

SUPPLEMENTARY INFORMATION

DFT Calculation of NMR $\delta(^{113}\text{Cd})$ in Cadmium Complexes.

Girolamo Casella,^{a,b} Francesco Ferrante,^c Giacomo Saielli^{d,e}

^a*Dipartimento di Scienze della Terra e del Mare (DiSTeM) dell'Università degli Studi di Palermo– Via Archirafi, 20 – 90123, Palermo, Italy*

^b*Consorzio Interuniversitario di Ricerca in Chimica dei Metalli nei Sistemi Biologici (C.I.R.C.M.S.B.) - Piazza Umberto I, 1-70121 Bari, Italy*

^c*Dipartimento di Fisica e Chimica dell'Università degli Studi di Palermo, Parco d' Orleans II, Viale delle Scienze, Ed. 17 - 90128, Palermo, Italy*

^d*Dipartimento di Scienze Chimiche dell'Università, Via Marzolo, 1 - 35131, Padova, Italy*

^e*Istituto per la Tecnologia delle Membrane del CNR, Unità di Padova, Via Marzolo, 1 -35131, Padova, Italy*

• Cartesian coordinates optimized with OP2 protocol [Gassuain09: B3LYP/cc-pvdz-PP(Cd);cc-pvdz].....	pag. S3
• Cartesian coordinates optimized with OP3 protocol [ADF: Relativistic ZORA scalar B3LYP/TZ2P].....	pag. S32
• Table S1 Calculated non-relativistic $\sigma(^{113}\text{Cd})$ at NR-1[F/B]level.....	pag. S57
• Table S2 Calculated $\sigma(^{113}\text{Cd})$, and ZORA spinorbit contributions, for the calculated $\delta(^{113}\text{Cd})$ of Table 2.....	pag. S58
• Table S3 Calculated $\sigma(^{113}\text{Cd})$, for different Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd at SO[B3LYP/TZ2P;DZP], SC[B3LYP/TZ2P;DZP], NR-2[B3LYP/TZ2P;DZP] levels	pag. S60
• Figure S1 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SO[B3LYP/TZ2P;DZP]....	pag. S61
• Figure S2 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SC[B3LYP/TZ2P;DZP]....	pag. S61
• Figure S3 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd NR-2[B3LYP/TZ2P;DZP].	pag. S61
• Tables S4 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3LYP/Sadleji (Cd);6-31G(d) (H,O,Cl).....	pag. S62
• Tables S5 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3LYP/Sadleji (Cd);6-31G(d,p) (H,O,Cl).....	pag. S62
• Tables S6 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3LYP/Sadleji (Cd);6-31+G(d,p) (H,O,Cl).....	pag. S63
• Tables S7 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3PW91/Sadleji (Cd);6-31G(d) (H,O,Cl).....	pag. S63
• Tables S8 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3PW91/Sadleji (Cd);6-31G(d,p) (H,O,Cl).....	pag. S64
• Tables S9 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} at B3PW91/Sadleji (Cd);6-31+G(d,p) (H,O,Cl).....	pag. S64
• Table S10 Correlations at NR-1 [F/B=DZVP(Cd), 6-31G(d,p)] [F=B3LYP,B3PW9] levels of calculated $\delta(^{113}\text{Cd})$ (ppm), wrt $\text{Cd}(\text{ClO}_4)_2$ and Me_2Cd , respectively, on OP2 geometries, and relevant statistical data.....	pag. S65
• Table S11 Calculated Cd-N, Cd-O and Cd-S bond lengths (pm) for the models of Scheme 1 with OP2 and OP3 protocols.....	pag. S66
• Table S12 Calculated plane and dihedral angles for the models of Scheme 1 with OP2 and OP3 protocols.....	pag. S67
• Table S13 Coordinates of the 20 snapshots obtained from MD simulation.....	pag. S68
• Tables S14-S44 Statistical data, experimental and calculated $\delta(^{113}\text{Cd})$ for all the models used.....	pag. S168

OP2 protocol

Model 1

93

C	0.758961	1.476816	-2.567189	H	-2.448342	4.125865	0.388673
N	0.103165	0.457519	-2.030670	H	6.699301	-0.774381	-1.507123
C	-0.465946	-0.231386	-3.081456	H	6.426352	-1.716616	-0.018601
C	-0.139946	0.388841	-4.262315	H	5.500987	-2.107227	-1.473866
N	0.641522	1.478212	-3.919346	H	4.999483	-2.048455	1.963336
Cd	-0.042202	0.003811	0.304094	H	6.038556	-4.228251	2.569248
O	-1.842073	-1.294593	-0.240883	H	5.178395	-6.342111	1.563818
C	-3.003383	-0.832814	-0.448363	H	3.248524	-6.269043	-0.015168
C	-3.619951	0.427006	-0.094654	H	2.175883	-4.083499	-0.567564
C	-4.956083	0.343662	-0.646078	C	-2.843229	-3.694237	-1.491805
N	-5.161001	-0.803825	-1.248219	C	-2.840555	-4.958456	-2.087853
N	-3.996744	-1.545297	-1.107505	C	-3.911129	-5.390086	-2.874312
C	-2.954111	1.488239	0.584844	C	-5.001739	-4.534475	-3.060770
C	-3.730789	2.608016	1.224274	C	-5.024223	-3.268311	-2.477364
C	-4.795376	2.351313	2.101779	H	-2.009713	-3.363708	-0.878335
C	-5.430288	3.401639	2.771349	H	-1.981711	-5.614881	-1.926035
C	-5.019392	4.720216	2.556547	H	-3.898276	-6.380694	-3.334219
C	-3.953421	4.983535	1.688347	H	-5.850986	-4.853612	-3.670220
C	-3.300365	3.932829	1.042769	H	-5.869300	-2.596902	-2.614355
C	-3.941794	-2.836277	-1.688545	C	2.982386	3.930319	-0.066250
C	-6.049893	1.368381	-0.708924	C	3.010643	5.308178	-0.301100
C	1.233596	2.443881	-4.831420	C	4.039438	5.894387	-1.042356
O	1.852588	1.311068	0.394928	C	5.056977	5.080010	-1.550828
C	2.991828	0.881846	0.047024	C	5.046066	3.702709	-1.332257
C	3.551175	-0.449926	-0.000652	H	2.184616	3.480406	0.518785
C	4.889039	-0.265597	-0.521261	H	2.212989	5.929284	0.114107
N	5.146117	0.999051	-0.761249	H	4.053066	6.972534	-1.216400
N	4.017958	1.714454	-0.386715	H	5.874925	5.520220	-2.126744
C	2.828884	-1.634076	0.330756	H	5.836276	3.061560	-1.717953
O	1.569595	-1.693447	0.426652				
C	4.004117	3.115228	-0.590144				
C	5.933463	-1.274419	-0.897827				
C	3.544751	-2.923915	0.627375				
C	3.039516	-4.123695	0.098376				
C	3.635376	-5.344089	0.419074				
C	4.718724	-5.385383	1.304704				
C	5.205170	-4.199792	1.863211				
C	4.626741	-2.974135	1.520084				
N	-0.177392	-0.403625	2.633423				
C	0.288335	-1.486280	3.237814				
N	0.017241	-1.458778	4.568280				
C	-0.664583	-0.280836	4.821502				
C	-0.777863	0.359599	3.612248				
C	0.369521	-2.480335	5.540392				
O	-1.700084	1.570640	0.728501				
H	1.322758	2.223504	-2.014047				
H	-0.386133	0.160929	-5.294859				
H	-1.067250	-1.120152	-2.914392				
H	1.826235	3.163935	-4.252443				
H	1.895733	1.937835	-5.550100				
H	0.451059	2.986507	-5.383594				
H	-1.246468	1.309534	3.372535				
H	-0.997944	-0.014566	5.819843				
H	0.820479	-2.294137	2.741843				
H	1.005298	-2.057081	6.332895				
H	-0.535183	-2.910220	5.996929				
H	0.923624	-3.280229	5.032259				
H	-6.803671	1.029603	-1.433362				
H	-6.544740	1.514686	0.263232				
H	-5.664993	2.351482	-1.021732				
H	-5.109311	1.320201	2.276540				
H	-6.248325	3.188438	3.463585				
H	-5.522970	5.542054	3.071107				
H	-3.623686	6.012146	1.523818				

Model 2

79

Cd	0.066494	0.142531	0.049576	H	-6.562307	2.083393	-1.593702
C	-4.539236	-0.976817	2.137305	H	-6.508391	0.326673	-1.299748
C	-4.387957	-0.918138	0.741656	H	-6.099806	1.437906	0.013009
C	-5.244999	-1.679107	-0.068194	H	-5.109345	-1.665498	-1.151536
C	-6.247591	-2.467829	0.504795	H	-6.901290	-3.065041	-0.135660
C	-6.414258	-2.491140	1.892416	H	-7.205204	-3.097979	2.339680
C	-5.557930	-1.741514	2.707596	H	-5.679685	-1.762225	3.793290
C	-3.225449	-0.155048	0.161138	H	-3.846879	-0.414414	2.766160
C	-3.396647	0.717212	-0.949677				
C	-2.305886	1.231051	-1.757908				
N	-2.918421	1.999121	-2.714165				
N	-4.285769	2.080494	-2.559408				
C	-4.583915	1.319454	-1.527482				
O	-1.043506	1.085169	-1.716462				
C	-2.268681	2.687837	-3.801939				
C	-6.014280	1.284430	-1.074270				
O	-2.115497	-0.388657	0.722617				
N	0.022751	-2.091460	-0.777513				
C	-0.836252	-3.018885	-0.384784				
N	-0.580394	-4.210371	-0.985753				
C	0.514455	-4.022743	-1.812099				
C	0.875374	-2.705254	-1.669674				
C	-1.311870	-5.449941	-0.785862				
O	2.218210	0.205179	-0.808929				
C	3.324647	-0.062213	-0.253927				
C	4.476477	-0.220065	-1.212126				
C	5.295543	-1.359218	-1.193847				
C	6.287002	-1.535725	-2.163929				
C	6.480389	-0.567595	-3.153239				
C	5.662092	0.567680	-3.183108				
C	4.654467	0.729959	-2.231463				
C	3.501053	-0.235904	1.146630				
C	2.411949	-0.393120	2.093959				
N	3.028996	-0.529866	3.309402				
N	4.400714	-0.412648	3.244265				
C	4.695224	-0.250405	1.971680				
O	1.146504	-0.430058	1.971745				
C	6.133105	-0.014987	1.612266				
C	2.378440	-0.739161	4.579178				
N	0.061550	2.364721	0.936264				
C	0.381844	2.780860	2.210390				
C	0.247960	4.145158	2.292573				
N	-0.161435	4.564752	1.038628				
C	-0.259206	3.455849	0.259311				
C	-0.439887	5.932135	0.632936				
H	-0.565414	3.474575	-0.783050				
H	0.402925	4.844698	3.108370				
H	0.685736	2.068101	2.970792				
H	-0.742103	5.936948	-0.422400				
H	-1.256935	6.356925	1.235958				
H	0.456053	6.561161	0.748221				
H	1.683924	-2.154081	-2.141324				
H	0.923883	-4.829092	-2.412919				
H	-1.645229	-2.857312	0.323323				
H	-1.706033	-5.824627	-1.742795				
H	-0.662014	-6.218800	-0.340060				
H	-2.154097	-5.261420	-0.107353				
H	1.297920	-0.794211	4.393026				
H	2.722375	-1.678664	5.041867				
H	2.596683	0.090225	5.272427				
H	6.697212	0.161397	2.539178				
H	6.586543	-0.872030	1.090739				
H	6.248863	0.857293	0.949751				
H	5.137108	-2.120011	-0.426896				
H	6.909271	-2.433818	-2.147044				
H	7.261583	-0.700561	-3.905563				
H	5.803985	1.323369	-3.959574				
H	3.990528	1.595410	-2.266702				
H	-2.661214	2.339247	-4.770979				
H	-2.432938	3.776571	-3.733728				
H	-1.194914	2.467286	-3.740023				

Model 3

113

Cd	0.269041	0.049400	-0.072127	H	-2.264948	-6.392220	1.059200
C	3.455303	0.331846	-1.257141	H	-0.568959	-6.373380	1.608553
N	2.623694	-0.155922	-0.268898	H	-1.733869	-5.269361	2.351081
C	3.399433	-0.769648	0.607095	H	1.618859	-5.275312	1.379471
N	4.710986	-0.704893	0.231838	H	2.635769	-6.506996	3.290329
C	4.753189	0.003735	-0.963715	H	2.397385	-5.624241	5.610829
O	0.579039	-1.641092	1.518609	H	1.174557	-3.486495	6.005304
C	0.293116	-2.871537	1.464058	H	0.211116	-2.230242	4.075250
C	0.817256	-3.691629	2.611231	H	0.236793	1.989552	3.503211
C	0.722425	-3.181217	3.917053	H	-0.196460	1.989762	5.948285
C	1.272131	-3.881617	4.991429	H	-1.122217	4.021110	7.070440
C	1.958131	-5.081642	4.770380	H	-1.602190	6.058578	5.700701
C	2.086902	-5.579527	3.470341	H	-1.165718	6.047469	3.247932
C	1.512166	-4.892524	2.396494	H	-0.740053	-1.977076	-3.503647
C	5.829953	-1.256698	0.950883	H	-1.680424	-1.878573	-5.798048
O	-0.241538	-1.769062	-1.386772	H	-3.381888	-3.548894	-6.543927
C	-0.636209	-2.868451	-0.897426	H	-4.119460	-5.332669	-4.952779
N	-1.404411	-3.785459	-1.606552	H	-3.172282	-5.422758	-2.648656
N	-1.752899	-4.882254	-0.830960	C	7.054817	-0.977893	0.226677
C	-1.175160	-4.719304	0.336484	H	5.883054	-0.806216	1.940917
C	-0.435030	-3.477409	0.397622	H	5.703153	-2.333873	1.048531
C	-1.913057	-3.698726	-2.925154	C	-6.618373	-0.056293	-0.297045
C	-2.865815	-4.646107	-3.346642	H	-5.464728	-0.018791	-2.031639
C	-3.384826	-4.586246	-4.640088	H	-5.455203	-1.561486	-1.147074
C	-2.972209	-3.591167	-5.532474	C	8.070942	-0.228909	0.832080
C	-2.022407	-2.657386	-5.111965	C	9.253571	0.040281	0.132846
C	-1.486162	-2.700433	-3.821800	C	9.420073	-0.439512	-1.171790
C	-1.446321	-5.742766	1.399404	C	8.403948	-1.188496	-1.777193
O	0.509333	1.698107	-1.678236	C	7.221319	-1.457686	-1.077959
C	0.529602	2.957243	-1.549910	H	7.941427	0.144301	1.846901
C	0.214833	3.649815	-0.345061	H	10.043971	0.622884	0.603763
C	0.129136	3.029607	0.958856	H	10.339989	-0.230121	-1.715694
N	-0.213064	4.059669	1.824353	H	8.533463	-1.561707	-2.792013
N	-0.410357	5.257680	1.152932	H	6.430919	-2.040289	-1.548876
C	-0.147825	5.032306	-0.112480	C	-7.546962	0.813035	-0.881845
O	0.319854	1.836824	1.342243	C	-8.675910	1.219610	-0.160614
C	-0.354402	6.160946	-1.078828	C	-8.876268	0.756859	1.145417
C	-0.446135	4.019696	3.221370	C	-7.947678	-0.112469	1.730217
C	-0.168958	2.872624	3.988892	C	-6.818731	-0.519044	1.008986
C	-0.417538	2.886770	5.364168	H	-7.391112	1.172989	-1.897751
C	-0.933453	4.021297	5.994657	H	-9.398220	1.895823	-0.615505
C	-1.201055	5.159214	5.226684	H	-9.754428	1.073117	1.706432
C	-0.962937	5.166199	3.852926	H	-8.103528	-0.472423	2.746123
N	-2.109494	0.210955	0.121080	H	-6.096422	-1.195256	1.463878
C	-2.973769	-0.290562	-0.744857				
N	-4.259183	-0.068476	-0.343695				
C	-4.191066	0.624957	0.858525				
C	-2.857202	0.786746	1.129460				
C	-5.449106	-0.477389	-1.044034				
C	0.950667	3.704070	-2.786784				
C	1.974441	4.663192	-2.747425				
C	2.427827	5.263224	-3.925870				
C	1.850615	4.923541	-5.152727				
C	0.833604	3.962912	-5.200626				
C	0.400797	3.342717	-4.027896				
H	-2.715349	-0.795269	-1.670995				
H	-5.082666	0.900322	1.411085				
H	-2.384183	1.271281	1.978542				
H	3.054529	0.878066	-2.105936				
H	5.683047	0.169119	-1.496802				
H	3.051245	-1.243353	1.520259				
H	-0.875610	6.975588	-0.556858				
H	0.593738	6.553840	-1.476015				
H	-0.956447	5.844929	-1.945063				
H	2.431310	4.920575	-1.789667				
H	3.235617	5.997798	-3.885025				
H	2.197694	5.400467	-6.072410				
H	0.384565	3.689208	-6.158334				
H	-0.369994	2.570771	-4.058942				

Model 4

99

Cd	0.142493	-0.426020	0.112555	H	0.025646	3.216936	3.960445
C	4.207441	-2.606401	1.994412	C	5.079870	2.188742	-1.533598
C	4.411181	-3.399450	0.849473	H	5.551813	1.310397	-1.067725
C	5.594067	-4.152747	0.731468	H	5.353250	2.177079	-2.599866
C	6.555051	-4.106911	1.740717	C	5.573215	3.468297	-0.885306
C	6.361960	-3.316449	2.878330	C	6.301581	4.402965	-1.631423
C	5.184874	-2.573272	2.992926	C	6.781953	5.573225	-1.033766
N	3.454949	-3.469001	-0.194533	C	6.532423	5.820141	0.317612
C	2.312401	-2.704252	-0.396200	C	5.802550	4.892101	1.069485
C	1.757874	-3.181283	-1.641448	C	5.327235	3.723759	0.472756
C	2.668409	-4.221912	-2.065683	H	6.497845	4.214610	-2.690594
N	3.656759	-4.382404	-1.217922	H	7.348777	6.293117	-1.628360
O	1.946506	-1.791898	0.405667	H	6.904099	6.734002	0.786336
O	-0.145182	-1.762963	-1.779061	H	5.604241	5.079648	2.127124
C	0.570015	-2.686232	-2.256621	H	4.755134	3.005260	1.065296
C	0.087672	-3.277790	-3.572155	C	-4.805651	-3.318051	0.353771
C	2.643621	-5.106343	-3.276393	C	-5.979417	-2.354390	0.361441
N	1.697109	1.065590	-0.878828	H	-4.561139	-3.623419	-0.675560
C	3.013774	0.954435	-0.793895	H	-5.060463	-4.232774	0.909448
N	3.633958	1.992437	-1.414633	C	-7.218606	-2.760859	0.872088
C	2.642555	2.813375	-1.925700	C	-8.315552	-1.893036	0.849824
C	1.450329	2.225118	-1.583675	C	-8.178693	-0.607532	0.321072
O	0.174623	0.718719	2.117592	C	-6.942472	-0.191840	-0.186774
C	-0.544840	1.661259	2.546307	C	-5.850348	-1.061086	-0.168057
C	-1.607217	2.263721	1.807007	H	-7.329742	-3.765335	1.290500
C	-1.973980	1.928172	0.451194	H	-9.276221	-2.222773	1.252099
N	-3.074262	2.731392	0.167226	H	-9.032965	0.073084	0.306792
N	-3.414747	3.544324	1.237906	H	-6.822528	0.812285	-0.599009
C	-2.558841	3.280127	2.196752	H	-4.890231	-0.720923	-0.563768
O	-1.476711	1.120790	-0.389386				
C	-2.704822	4.036480	3.483256				
C	-3.873901	2.780336	-0.999481				
C	-3.574251	2.015581	-2.143747				
C	-4.403770	2.097651	-3.265891				
C	-5.527529	2.927252	-3.277455				
C	-5.818055	3.686822	-2.138978				
C	-5.005303	3.618924	-1.007508				
N	-1.585242	-1.796982	1.016559				
C	-2.100571	-1.876768	2.293308				
C	-3.338618	-2.468490	2.252248				
N	-3.579645	-2.755290	0.919831				
C	-2.497534	-2.329615	0.217926				
C	-0.221289	2.144136	3.951745				
H	3.541412	0.144106	-0.297193				
H	2.876031	3.726706	-2.463414				
H	0.434345	2.549739	-1.788418				
H	-1.546456	-1.504048	3.149732				
H	-4.061302	-2.700706	3.027989				
H	-2.404293	-2.412899	-0.861849				
H	-3.556054	4.724739	3.389435				
H	-2.891423	3.366610	4.338234				
H	-1.804654	4.625860	3.720780				
H	3.511755	-5.778456	-3.235426				
H	1.729991	-5.720749	-3.321712				
H	2.694815	-4.528197	-4.213273				
H	-2.699684	1.371105	-2.140723				
H	-4.157316	1.499290	-4.146739				
H	-6.166655	2.984863	-4.161234				
H	-6.689534	4.346438	-2.127762				
H	-5.222509	4.207413	-0.118537				
H	3.291458	-2.030512	2.091227				
H	5.012242	-1.955182	3.877662				
H	7.117933	-3.284095	3.665994				
H	7.467208	-4.699204	1.632979				
H	5.733646	-4.768258	-0.154845				
H	-0.818041	-2.741376	-3.882423				
H	0.851326	-3.180187	-4.358670				
H	-0.139912	-4.350403	-3.469237				
H	-1.076298	2.000068	4.630389				
H	0.635959	1.569982	4.325285				

Model 5

99

Cd	-0.108541	0.266141	0.147138	H	0.053339	-7.546971	-0.234524
C	-3.494933	0.240738	0.699262	H	0.463076	-7.574658	-2.694516
N	-2.396789	-0.393344	0.154418	H	1.034700	-5.456103	-3.880462
C	-2.847328	-1.485076	-0.436487	H	1.175710	-3.314584	-2.602847
N	-4.202835	-1.593515	-0.301494	C	-6.412551	-2.403410	-0.472732
C	-4.624770	-0.485340	0.424862	H	-4.933228	-2.674864	-1.914619
O	0.181419	-1.975607	-0.555050	H	-4.709574	-3.602381	-0.413904
C	0.792382	-2.916647	0.027397	C	-7.376892	-2.244695	-1.475158
C	0.768379	-4.234958	-0.697673	C	-8.712980	-2.008514	-1.130068
C	0.956776	-4.252739	-2.090162	C	-9.084727	-1.931048	0.217450
C	0.865516	-5.449967	-2.801023	C	-8.120387	-2.089763	1.219876
C	0.545372	-6.639325	-2.135701	C	-6.784299	-2.325944	0.874785
C	0.321982	-6.624978	-0.755801	H	-7.087725	-2.304954	-2.523334
C	0.440965	-5.430540	-0.038759	H	-9.463098	-1.885056	-1.909812
C	-5.028747	-2.648027	-0.830149	H	-10.124013	-1.747332	0.485882
N	2.265126	0.689525	-0.031947	H	-8.409554	-2.029505	2.268052
C	3.167223	0.501314	0.914474	H	-6.034181	-2.449402	1.654529
N	4.435035	0.600507	0.420303	C	6.791293	0.607693	0.293435
C	4.315432	0.878109	-0.936466	H	5.691051	1.151984	1.976983
C	2.969629	0.924705	-1.195847	H	5.675431	-0.583342	1.588583
C	5.651374	0.421743	1.170079	C	7.725448	1.614763	0.563926
O	-0.837504	2.321565	0.873106	C	8.826060	1.794300	-0.282489
C	-1.142303	3.357685	0.209445	C	8.992518	0.966767	-1.399397
C	-0.869042	3.537267	-1.173744	C	8.058364	-0.040304	-1.669887
C	-0.441719	2.476594	-2.068713	C	6.957752	-0.219841	-0.823473
N	-0.304710	3.086719	-3.286507	H	7.595966	2.258465	1.432720
N	-0.538686	4.444716	-3.248854	H	9.552698	2.577656	-0.072086
C	-0.884302	4.723837	-2.010178	H	9.848638	1.106421	-2.057786
O	-0.222318	1.233223	-1.907437	H	8.187844	-0.684006	-2.538682
C	-1.126230	6.162497	-1.659007	H	6.231113	-1.003198	-1.033876
C	0.081014	2.452480	-4.522916				
O	0.406637	-0.679747	2.164416				
C	1.175968	-1.688937	2.211572				
C	1.434467	-2.780252	1.293635				
C	2.469529	-3.559134	1.940523				
N	2.806871	-3.041099	3.106685				
N	2.000115	-1.934851	3.281878				
C	3.248194	-4.742158	1.444844				
C	2.045079	-1.185696	4.514982				
C	-1.867526	4.409484	1.006881				
C	-3.096313	4.934777	0.579089				
C	-3.806573	5.826304	1.388904				
C	-3.287631	6.214555	2.627146				
C	-2.066126	5.688911	3.064091				
C	-1.371096	4.777282	2.268314				
H	2.955989	0.307965	1.960365				
H	5.185471	0.977278	-1.576595				
H	2.451152	1.101119	-2.133217				
H	-3.389478	1.168322	1.254591				
H	-5.664104	-0.347066	0.702292				
H	-2.230104	-2.195508	-0.979191				
H	0.172284	1.375625	-4.329978				
H	-0.681623	2.626551	-5.298896				
H	1.044062	2.849116	-4.886209				
H	-0.794711	6.785004	-2.502178				
H	-2.188097	6.379323	-1.465620				
H	-0.571905	6.458080	-0.754299				
H	-3.504616	4.624086	-0.384743				
H	-4.768985	6.218121	1.050894				
H	-3.837476	6.919310	3.255534				
H	-1.660288	5.983319	4.034945				
H	-0.434239	4.337985	2.615213				
H	1.759870	-1.821862	5.368734				
H	3.057960	-0.790619	4.699147				
H	1.333257	-0.354845	4.422456				
H	4.114419	-4.893360	2.104605				
H	2.652821	-5.667947	1.442215				
H	3.604102	-4.590625	0.413371				
H	0.255776	-5.415459	1.037131				

Model 6

71

Cd	0.000211	-0.000211	0.000516
C	-2.818382	2.734498	-2.478482
C	-1.508765	2.347349	-2.124415
N	-1.560997	1.351853	-1.220076
N	-2.875200	1.090039	-0.984276
C	-3.648798	1.910356	-1.731181
N	1.559781	-1.353108	1.221668
N	2.874076	-1.089964	0.986846
C	3.647768	-1.908964	1.735118
C	2.817591	-2.733548	2.482118
C	1.507926	-2.347889	2.126609
B	-3.356606	-0.002704	0.007273
N	-2.866972	0.309494	1.446224
N	-1.551345	0.381157	1.786287
C	-1.494009	0.667852	3.100020
C	-2.801626	0.784067	3.616700
C	-3.636237	0.548894	2.532652
B	3.356604	0.001297	-0.005315
N	2.871586	1.405202	0.444637
N	1.556688	1.736317	0.558978
C	1.502082	3.018456	0.964516
C	2.810732	3.523766	1.114367
C	3.643099	2.466107	0.774094
N	-1.556565	-1.736838	-0.557972
N	-2.871594	-1.405446	-0.445295
C	-3.642934	-2.463860	-0.782891
C	-2.810456	-3.520279	-1.126614
C	-1.501862	-3.016706	-0.970420
N	1.552438	-0.381280	-1.784337
N	2.868183	-0.311610	-1.444624
C	3.636928	-0.552013	-2.531098
C	2.801745	-0.785587	-3.615102
C	1.494362	-0.667737	-3.098238
H	-4.567638	-0.004016	0.011649
H	4.567650	0.001795	-0.008487
C	0.210654	-2.907725	2.630284
H	4.731137	-1.845552	1.681521
H	3.109664	-3.507193	3.186700
H	-4.726474	-2.388422	-0.753725
H	-3.100472	-4.517298	-1.446178
C	-0.203017	-3.728923	-1.206479
C	0.194458	-0.822507	-3.830380
H	3.089408	-1.009733	-4.638484
H	4.720651	-0.538829	-2.453924
C	0.203318	3.730697	1.201128
H	3.100851	4.522461	1.428569
H	4.726607	2.391084	0.742988
C	-0.194223	0.822105	3.832556
H	-3.089741	1.008212	4.639940
H	-4.719922	0.534499	2.455285
C	-0.211694	2.907936	-2.627686
H	-3.110321	3.508607	-3.182629
H	-4.732163	1.847718	-1.676694
H	-0.381262	1.062759	4.888974
H	0.408957	-0.097701	3.791780
H	0.424938	1.623574	3.401767
H	0.391229	4.769959	1.507050
H	-0.424398	3.745806	0.297256
H	-0.392014	3.244113	1.988842
H	-0.402503	3.698581	-3.367604
H	0.390382	3.338738	-1.813184
H	0.410880	2.134986	-3.103256
H	-0.390405	-4.772372	-1.498146
H	0.386194	-3.251312	-2.004385
H	0.430335	-3.730674	-0.306617
H	0.381453	-1.041213	-4.891573
H	-0.414420	-1.639377	-3.413815
H	-0.419151	0.089073	-3.770318
H	0.401105	-3.711197	3.356318
H	-0.402814	-2.138030	3.122973
H	-0.400388	-3.320664	1.813372

Model 7

91

Cd	-0.000092	-0.001481	-0.032886
C	2.938706	3.507415	-0.224016
C	1.621896	3.027851	-0.064465
N	1.633260	1.685106	-0.032015
N	2.929174	1.281480	-0.173869
C	3.729817	2.372809	-0.284030
N	-1.634757	-1.683967	-0.077485
N	-2.930876	-1.275919	-0.203837
C	-3.733551	-2.363938	-0.331304
C	-2.943483	-3.500402	-0.299070
C	-1.625184	-3.025569	-0.137479
B	3.400076	-0.212697	-0.065205
N	2.799485	-1.081666	-1.220382
N	1.535388	-0.895474	-1.699448
C	1.310596	-1.858524	-2.610521
C	2.442098	-2.696279	-2.710532
C	3.351293	-2.176670	-1.803286
B	-3.400099	0.215899	-0.059979
N	-2.797999	1.111947	-1.193567
N	-1.533020	0.938035	-1.674839
C	-1.307331	1.922545	-2.562453
C	-2.439359	2.761485	-2.644680
C	-3.349718	2.219952	-1.751563
N	1.572034	-1.019828	1.476528
N	2.913579	-0.819685	1.287960
C	3.597529	-1.269264	2.369670
C	2.685804	-1.772805	3.283605
C	1.422885	-1.593109	2.683138
N	-1.571619	0.975674	1.504633
N	-2.913898	0.788776	1.308070
C	-3.597942	1.220497	2.396961
C	-2.685461	1.697953	3.324067
C	-1.421931	1.521244	2.724010
N	4.930213	-0.217508	-0.221268
N	-4.930009	0.226196	-0.217059
C	-0.358578	-3.819432	-0.041858
H	-4.809886	-2.260678	-0.420222
H	-3.272029	-4.533248	-0.372783
H	4.676755	-1.170037	2.397991
H	2.901503	-2.209127	4.254962
C	0.078812	-1.969073	3.228500
C	-0.075508	1.861932	3.286280
H	-2.901186	2.115647	4.303576
H	-4.678003	1.129405	2.419818
C	-0.019456	2.018633	-3.322375
H	-2.574881	3.637279	-3.273276
H	-4.351135	2.541656	-1.483326
C	0.024156	-1.935484	-3.375114
H	2.578168	-3.557008	-3.359492
H	4.352029	-2.505415	-1.541080
C	0.355552	3.818514	0.057173
H	3.265724	4.541961	-0.278111
H	4.805708	2.272706	-0.381551
N	5.766001	-0.025212	0.841153
C	6.982128	0.186457	0.337402
C	6.947610	0.161230	-1.082271
C	5.626205	-0.088479	-1.394225
H	5.132039	-0.167617	-2.357934
H	7.772132	0.299245	-1.776885
C	8.158118	0.399019	1.241682
C	-5.624574	0.122494	-1.393382
C	-6.946765	-0.131554	-1.088454
C	-6.983262	-0.186139	0.330352
N	-5.767527	0.013274	0.840067
C	-8.160868	-0.415640	1.228377
H	-7.770525	-0.253991	-1.786883
H	-5.128885	0.220744	-2.354560
H	0.130730	1.278158	4.198344
H	0.726162	1.658975	2.564918
H	-0.028080	2.927154	3.565800
H	0.415351	3.027489	-3.239124

H	0.714837	1.293586	-2.948117
H	-0.184472	1.823089	-4.395460
H	-0.471885	-4.641947	0.682284
H	-0.097033	-4.272377	-1.012273
H	0.484439	-3.191457	0.273921
H	-0.414270	-2.944292	-3.312666
H	-0.708734	-1.215529	-2.988478
H	0.192513	-1.719602	-4.443754
H	-0.074180	-1.535232	4.229784
H	-0.733350	-1.623290	2.576654
H	-0.008821	-3.063415	3.333459
H	0.469177	4.616910	0.807870
H	0.094144	4.302939	-0.897918
H	-0.487422	3.181039	0.353205
H	-7.826280	-0.520726	2.270056
H	-8.875710	0.423342	1.179052
H	-8.710330	-1.328205	0.944672
H	8.705280	1.319340	0.979361
H	7.822109	0.479539	2.285093
H	8.875444	-0.436568	1.174200

Model 8

53

Cd	0.002026	-0.001099	0.000085
Br	-0.349291	-5.714407	2.851333
Br	4.910350	-2.332095	-3.370198
Br	4.897968	2.232166	3.451887
Br	-4.643591	2.788751	3.390989
Br	-4.639542	-2.693634	-3.470689
Br	-0.181964	5.720617	-2.853641
C	-0.114608	3.864766	-2.514669
C	-0.105728	3.222735	-1.264503
N	-0.054530	1.897028	-1.439571
N	-0.030389	1.667048	-2.777541
C	-0.064450	2.840774	-3.452347
N	-0.120667	-1.895606	1.438221
N	-0.113431	-1.665825	2.776482
C	-0.186169	-2.838103	3.450761
C	-0.239293	-3.861336	2.512594
C	-0.192113	-3.220404	1.262643
B	0.030323	0.235110	-3.377179
N	-1.218164	-0.580252	-2.941580
N	-1.499126	-0.846062	-1.640000
C	-2.629572	-1.561853	-1.615117
C	-3.093108	-1.759339	-2.927099
C	-2.166873	-1.121172	-3.742523
B	-0.032763	-0.235786	3.377533
N	-1.256331	0.606119	2.921381
N	-1.509084	0.877627	1.615197
C	-2.624569	1.615544	1.570902
C	-3.105152	1.825000	2.874937
C	-2.205193	1.169719	3.706162
N	1.604810	-0.720226	-1.607239
N	1.328049	-0.483548	-2.915283
C	2.329006	-0.955432	-3.695855
C	3.286636	-1.516425	-2.860106
C	2.786446	-1.346475	-1.557710
N	1.589477	0.687953	1.633792
N	1.287062	0.455613	2.936865
C	2.286146	0.903752	3.733734
C	3.266257	1.449941	2.914351
C	2.783812	1.290701	1.603941
H	0.039758	0.317245	-4.582470
H	-0.045039	-0.318560	4.582817
H	-0.209325	-3.652264	0.265013
H	-0.195794	-2.870808	4.535793
H	2.298599	-0.863350	-4.777065
H	3.222953	-1.643496	-0.607340
H	3.240893	1.579503	0.660679
H	2.238576	0.808312	4.814051
H	-3.031636	1.957980	0.622709
H	-2.182898	1.069010	4.786804
H	-3.057832	-1.898650	-0.674265
H	-2.124977	-1.019927	-4.822542
H	-0.135110	3.654720	-0.267168
H	-0.053315	2.874033	-4.537345

Model 9

71

Cd	-0.000171	0.000104	-0.005001
C	2.771987	3.699617	-0.337696
C	1.486171	3.119344	-0.294683
N	1.562674	1.788473	-0.170996
N	2.879885	1.472368	-0.131738
C	3.622429	2.602989	-0.230409
N	-1.562668	-1.792844	-0.109125
N	-2.879903	-1.475703	-0.080459
C	-3.622337	-2.609073	-0.140827
C	-2.771798	-3.708616	-0.211369
C	-1.486039	-3.127107	-0.188342
B	3.383879	0.009852	0.003458
N	2.891518	-0.840909	-1.198849
N	1.576758	-1.035884	-1.462919
C	1.510214	-1.806621	-2.555407
C	2.800329	-2.131803	-3.026404
C	3.642579	-1.489554	-2.123348
B	-3.383909	-0.009408	0.004239
N	-2.891672	0.799397	-1.226689
N	-1.576933	0.985403	-1.497385
C	-1.510594	1.718229	-2.615685
C	-2.800785	2.026871	-3.097452
C	-3.642873	1.415899	-2.172797
N	1.568251	-0.744652	1.627721
N	2.884684	-0.608008	1.337375
C	3.629596	-1.083970	2.366070
C	2.781175	-1.549558	3.366497
C	1.494204	-1.307569	2.840059
N	-1.568059	0.800782	1.601142
N	-2.884579	0.654007	1.316116
C	-3.629208	1.163578	2.328778
C	-2.780519	1.662851	3.312608
C	-1.493689	1.404058	2.793894
H	4.594815	0.015302	0.006096
H	-4.594847	-0.014778	0.007159
H	-0.510645	-3.610038	-0.225837
H	-4.708390	-2.558807	-0.130218
C	-3.139522	-5.161262	-0.292321
H	4.715601	-1.060003	2.318878
C	3.151462	-2.161071	4.685916
H	0.519429	-1.512982	3.280062
H	-0.518796	1.624597	3.226237
C	-3.150538	2.317716	4.611134
H	-4.715228	1.137535	2.282969
H	-0.538669	1.992257	-3.023473
C	-3.179174	2.819688	-4.314100
H	-4.728503	1.379908	-2.125551
H	0.538237	-2.094335	-2.953531
C	3.178398	-2.966057	-4.215125
H	4.728213	-1.452093	-2.077437
H	0.510842	3.600907	-0.348110
C	3.139725	5.148701	-0.467554
H	4.708474	2.552937	-0.218387
H	4.271789	-3.055086	-4.303779
H	2.768636	-3.987823	-4.146483
H	2.805523	-2.530507	-5.157586
H	4.244381	-2.222304	4.800221
H	2.763657	-1.572704	5.534647
H	2.750982	-3.183483	4.790858
H	4.232450	5.279561	-0.476658
H	2.746960	5.590041	-1.399079
H	2.742363	5.749395	0.367952
H	-4.272600	2.905323	-4.405630
H	-2.769699	3.843326	-4.280685
H	-2.806267	2.352096	-5.241067
H	-4.232247	-5.292316	-0.297375
H	-2.746444	-5.633788	-1.208283
H	-2.742459	-5.733412	0.563124
H	-4.243441	2.381685	4.724057
H	-2.761629	1.758281	5.478714
H	-2.750974	3.343431	4.681768

Model 10

91

Cd	0.000098	-0.064428	0.000141	H	-3.891675	4.713033	-2.774190
N	5.749541	0.491783	0.972483	H	-2.498806	5.459045	-1.962315
N	4.951392	-0.056060	0.017004	H	-3.908918	1.487345	5.093871
C	5.679552	-0.908406	-0.774600	H	-2.914439	0.149889	5.708301
C	6.995264	-0.895615	-0.344486	H	-2.168113	1.721496	5.361900
C	6.968251	0.005304	0.752264	H	4.226322	-4.315156	3.067468
B	3.419474	0.050146	0.057918	H	2.702540	-4.170616	3.968646
N	2.895541	1.343902	0.759882	H	2.774993	-5.171724	2.505549
N	1.555405	1.585606	0.738847	H	2.164191	1.715772	-5.363426
C	1.363189	2.750882	1.367027	H	3.905682	1.488375	-5.093986
C	2.585390	3.298188	1.807451	H	2.916643	0.146651	-5.707855
C	3.530463	2.363795	1.397225	H	2.500079	5.460113	1.959389
N	-1.555245	1.584572	-0.740947	H	2.275040	4.613673	3.502527
N	-2.895476	1.343342	-0.761067	H	3.891661	4.713608	2.773008
C	-3.530428	2.363340	-1.398234	H	8.665675	-2.258939	-0.142215
C	-2.585267	3.297246	-1.809347	H	7.851755	-2.321051	-1.720605
C	-1.362989	2.749603	-1.369549	H	8.927388	-0.963811	-1.324312
B	-3.419416	0.050174	-0.058029	H	-7.851806	-2.320386	1.721038
N	-4.951321	-0.056135	-0.017267	H	-8.927749	-0.963827	1.323242
N	-5.749432	0.491541	-0.972870	H	-8.665037	-2.259747	0.142240
C	-6.968146	0.005075	-0.752640				
C	-6.995199	-0.895667	0.344256				
C	-5.679513	-0.908361	0.774441				
N	-1.619602	-0.240249	1.747842				
C	-1.468344	0.048063	3.045913				
C	-2.657946	0.569042	3.596351				
C	-3.533535	0.578410	2.516926				
N	-2.900144	0.073701	1.422183				
N	1.619744	-0.242979	-1.747576				
N	2.900014	0.072391	-1.422199				
C	3.532760	0.577436	-2.517152				
C	2.657045	0.566845	-3.596470				
C	1.468043	0.044831	-3.045721				
N	-1.566583	-1.461028	-1.029318				
N	-2.884546	-1.210359	-0.828636				
C	-3.623970	-2.145869	-1.485538				
C	-2.769481	-3.039248	-2.120510				
C	-1.485707	-2.554232	-1.794218				
N	1.566807	-1.459767	1.031333				
N	2.884741	-1.209709	0.829663				
C	3.624242	-2.145086	1.486649				
C	2.769834	-3.037763	2.122718				
C	1.486027	-2.552487	1.796937				
H	0.505655	-0.130137	-3.524720				
H	4.565625	0.908153	-2.463972				
C	2.923395	0.999772	-5.008159				
H	-4.607026	2.326921	-1.525145				
C	-2.822858	4.581934	-2.547899				
H	-0.351824	3.139648	-1.476837				
H	0.352109	3.141349	1.473573				
C	2.822997	4.583056	2.545684				
H	4.606975	2.326943	1.524768				
H	0.507591	-2.939153	2.078590				
C	3.134846	-4.231112	2.955894				
H	4.709295	-2.114382	1.471425				
H	-0.507226	-2.941393	-2.075033				
C	-3.134393	-4.233039	-2.953097				
H	-4.709020	-2.114774	-1.471015				
H	-0.505831	-0.125790	3.525067				
C	-2.924882	1.002319	5.007822				
H	-4.566719	0.908085	2.463555				
H	-5.211969	-1.471891	1.577312				
C	-8.164926	-1.645615	0.909873				
H	-7.794222	0.320427	-1.390116				
H	7.794357	0.320777	1.389643				
C	8.164998	-1.645566	-0.910082				
H	5.211964	-1.472048	-1.577366				
H	-4.225784	-4.316178	-3.066179				
H	-2.700547	-4.173888	-3.965265				
H	-2.776075	-5.173570	-2.501353				
H	-2.275866	4.611806	-3.505320				

Model 11

89

Cd	-0.000031	0.000315	-0.000305	H	-5.503270	2.513145	-2.655994
C	2.779863	-2.535009	2.692698	H	-5.564386	0.809917	-2.143224
C	1.480839	-2.155989	2.301357	H	-5.557746	2.099092	-0.926054
N	1.558770	-1.235285	1.327727	H	-5.506826	1.043236	3.499423
N	2.883340	-1.010601	1.082209	H	-5.567329	1.441375	1.765754
C	3.645979	-1.789243	1.898909	H	-5.557052	-0.254525	2.282465
N	-1.558546	1.237284	-1.326298	H	5.503564	-2.513376	2.655434
N	-2.883072	1.011776	-1.081312	H	5.557773	-2.100459	0.925200
C	-3.645850	1.788746	-1.899488	H	5.564384	-0.810412	2.141521
C	-2.779842	2.533959	-2.693972	H	5.506767	-1.046011	-3.497940
C	-1.480781	2.156325	-2.301460	H	5.558089	0.250950	-2.280131
B	3.361059	0.003904	0.002180	H	5.565602	-1.445252	-1.764463
N	2.880105	1.445674	0.338728	H	-5.497497	-3.563425	-0.850019
N	1.555029	1.769049	0.408806	H	-5.561351	-2.265803	0.366465
C	1.475146	3.073468	0.714756	H	-5.551731	-1.858838	-1.359063
C	2.773292	3.604523	0.845204	H	5.497192	3.564631	0.848223
C	3.641008	2.544545	0.600108	H	5.552691	1.860579	1.358869
B	-3.361088	-0.003349	-0.002162	H	5.560740	2.265799	-0.367094
N	-2.884161	0.425404	1.416455				
N	-1.559893	0.528768	1.733876				
C	-1.483102	0.916991	3.016463				
C	-2.782565	1.068594	3.538756				
C	-3.647772	0.748594	2.496829				
N	1.559533	-0.529464	-1.733583				
N	2.883833	-0.426294	-1.415968				
C	3.647513	-0.749753	-2.496137				
C	2.782429	-1.069610	-3.538207				
C	1.482898	-0.917786	-3.016167				
N	-1.554996	-1.768287	-0.409416				
N	-2.880166	-1.444993	-0.339991				
C	-3.640929	-2.544286	-0.599694				
C	-2.773070	-3.604414	-0.843710				
C	-1.474960	-3.073038	-0.714097				
H	4.563444	0.005652	0.002786				
H	-4.563449	-0.005295	-0.003215				
C	-0.172086	2.655000	-2.839718				
C	-5.143629	1.798797	-1.901570				
H	-3.055354	3.256053	-3.458335				
C	5.145373	-0.745446	-2.504036				
H	3.058825	-1.373184	-4.544688				
C	0.174941	-1.136149	-3.718012				
C	-0.164966	-3.786333	-0.875482				
H	-3.046762	-4.628532	-1.084156				
C	-5.138769	-2.552352	-0.609565				
C	-0.175016	1.136558	3.717714				
H	-3.058834	1.372232	4.545246				
C	-5.145617	0.742612	2.505462				
C	0.165245	3.787041	0.875686				
H	3.047090	4.628390	1.086680				
C	5.138819	2.553149	0.608963				
C	0.172188	-2.655126	2.839341				
H	3.055271	-3.258517	3.455730				
C	5.143822	-1.799517	1.900596				
H	0.338646	4.843060	1.128710				
H	-0.437200	3.748865	-0.044511				
H	-0.449717	3.339511	1.671046				
H	-0.351293	1.442440	4.759158				
H	0.442289	0.225587	3.726658				
H	0.426273	1.917399	3.227897				
H	0.347351	-3.410252	3.619309				
H	-0.426810	-1.842465	3.277463				
H	-0.447075	-3.111109	2.052220				
H	0.351485	-1.458797	-4.754338				
H	-0.434498	-1.903998	-3.217989				
H	-0.434395	-0.220020	-3.742951				
H	-0.338331	-4.842104	-1.129521				
H	0.449720	-3.337777	-1.670502				
H	0.437634	-3.749156	0.044649				
H	-0.347202	3.408298	-3.621449				
H	0.446110	3.113046	-2.052950				
H	0.427968	1.841863	-3.275540				

Model 12

53

Cd	0.000061	0.000513	-0.004981
N	-1.566412	0.773044	1.615461
N	-1.562727	-1.788764	-0.140788
N	1.574240	-0.997745	-1.489919
N	-1.574566	1.015110	-1.478425
N	1.566392	-0.790328	1.606779
N	1.563029	1.790686	-0.120699
N	-2.882273	-1.471494	-0.109533
N	-2.885474	0.631083	1.328695
N	-2.891982	0.826385	-1.211060
B	-3.385008	-0.006378	0.003816
H	-4.595450	-0.010936	0.006323
N	2.885457	-0.646488	1.320951
N	2.891739	-0.812009	-1.220912
N	2.882511	1.472831	-0.092438
B	3.385003	0.006467	0.003614
H	4.595447	0.010611	0.006045
C	1.485598	3.124348	-0.209703
C	3.628377	2.601646	-0.163110
C	2.771697	3.693173	-0.239975
H	0.511398	3.607942	-0.248269
H	4.713567	2.546303	-0.154066
H	3.039546	4.743307	-0.307962
C	-1.489860	1.352728	2.819780
C	-3.632353	1.119049	2.348439
C	-2.776403	1.595744	3.334024
H	-4.717548	1.091531	2.299117
H	-3.045029	2.051229	4.282459
H	-0.515617	1.565446	3.255656
C	1.489858	-1.385275	2.803648
C	3.632345	-1.148237	2.333968
C	2.776411	-1.636333	3.313975
H	0.515624	-1.602226	3.237448
H	3.045074	-2.104075	4.256415
H	4.717549	-1.121474	2.284366
C	1.504754	-1.741170	-2.601101
C	3.644388	-1.436940	-2.158230
C	2.794246	-2.050684	-3.070287
H	0.533133	-2.016729	-3.006606
H	3.068327	-2.634458	-3.943940
H	4.729224	-1.400043	-2.107935
C	-1.505478	1.770569	-2.581496
C	-3.644949	1.461469	-2.141285
C	-2.795119	2.085094	-3.046896
H	-0.534015	2.050702	-2.984239
H	-3.069500	2.678424	-3.913991
H	-4.729768	1.424055	-2.091021
C	-1.484992	-3.121252	-0.245567
C	-3.627893	-2.599508	-0.193990
C	-2.770973	-3.689910	-0.283330
H	-0.510666	-3.604162	-0.289186
H	-3.038576	-4.739227	-0.363791
H	-4.713104	-2.544518	-0.184883

Model 13

67

Cd	-0.000889	0.010044	-0.078723
C	2.585808	3.706648	0.123644
C	1.402725	3.087467	-0.315582
N	1.579192	1.767379	-0.448260
N	2.870131	1.505538	-0.107939
C	3.488512	2.661310	0.255853
N	-1.558737	-1.806740	-0.052345
N	-2.848454	-1.489434	0.241085
C	-3.442523	-2.535782	0.875526
C	-2.524931	-3.572069	0.973263
C	-1.358734	-3.057389	0.380443
B	3.420027	0.041701	0.028608
N	2.903115	-0.873407	-1.139591
N	1.586881	-1.119793	-1.370220
C	1.519943	-2.004338	-2.370176
C	2.810245	-2.356136	-2.803505
C	3.658687	-1.617847	-1.991193
B	-3.420739	-0.042303	0.041249
N	-2.912186	0.592257	-1.303690
N	-1.599626	0.816928	-1.574926
C	-1.541846	1.447038	-2.752477
C	-2.834542	1.651548	-3.265397
C	-3.674652	1.097313	-2.310414
N	1.567230	-0.516881	1.629239
N	2.911068	-0.524694	1.393333
C	3.563149	-1.010782	2.481875
C	2.620505	-1.330246	3.450101
C	1.387054	-1.004217	2.861827
N	-1.582197	0.886741	1.475734
N	-2.924712	0.828294	1.239923
C	-3.586635	1.552846	2.179467
C	-2.651780	2.099143	3.048867
C	-1.412782	1.652681	2.559353
N	4.951338	0.100308	-0.085247
N	-4.950182	-0.150663	-0.056384
H	-0.383054	-3.521508	0.249076
H	-4.473484	-2.475479	1.209134
H	-2.682551	-4.554355	1.408478
H	4.642760	-1.106415	2.458731
H	2.805590	-1.743087	4.437239
H	0.378654	-1.094256	3.261294
H	-0.407621	1.843018	2.930730
H	-2.845237	2.731861	3.909898
H	-4.666789	1.630982	2.129228
H	-0.574179	1.719669	-3.169445
H	-3.120816	2.135273	-4.194341
H	-4.757677	1.039220	-2.277495
H	0.548057	-2.340931	-2.726150
H	3.089453	-3.048642	-3.591789
H	4.742545	-1.580835	-1.958010
H	0.431397	3.525323	-0.538308
H	2.763484	4.760448	0.316112
H	4.524441	2.664239	0.579097
N	5.765411	-0.772688	0.570881
C	6.983125	-0.587724	0.066470
C	6.983150	0.397767	-0.948594
C	5.664380	0.805181	-1.020152
H	5.183378	1.529506	-1.670918
H	7.819099	0.762641	-1.538655
H	7.818242	-1.169261	0.454567
C	-5.647900	-1.068317	-0.798211
C	-6.972865	-0.675946	-0.827221
C	-6.992394	0.522300	-0.075188
N	-5.780097	0.840673	0.372502
H	-7.838060	1.166145	0.162675
H	-7.800529	-1.183456	-1.314606
H	-5.152282	-1.918608	-1.257276

Model 14

39

Cd	-0.007735	-0.917485	0.040310
C	-2.888044	-0.912998	0.912895
S	-2.348960	-1.997699	-0.355439
S	2.322672	-2.012235	0.459539
C	2.871984	-0.961675	-0.832948
N	4.162881	-0.988533	-1.232913
N	-4.179533	-0.917523	1.311919
S	-1.732741	0.173767	1.662206
S	1.727724	0.120899	-1.604920
C	4.690986	-0.160041	-2.346854
C	5.924854	0.651746	-1.902338
H	4.964142	-0.843209	-3.167096
H	3.893184	0.493412	-2.700501
C	7.014415	-0.258005	-1.296816
H	6.312717	1.196893	-2.773702
H	5.608789	1.402170	-1.163813
C	6.422434	-1.138740	-0.176443
H	7.431740	-0.903091	-2.086120
H	7.845006	0.346286	-0.909348
C	5.177325	-1.909959	-0.659820
H	7.164058	-1.867048	0.179169
H	6.141693	-0.514465	0.683737
H	5.459168	-2.624666	-1.449685
H	4.716296	-2.468632	0.154945
C	-4.700064	-0.059466	2.406957
C	-5.925810	0.754253	1.943836
H	-4.980134	-0.721604	3.241997
H	-3.896081	0.593871	2.746517
C	-7.023851	-0.158211	1.358006
H	-6.308735	1.322657	2.802495
H	-5.602192	1.484921	1.188954
C	-6.439984	-1.068911	0.257527
H	-7.447486	-0.781805	2.161106
H	-7.848557	0.445254	0.956947
C	-5.202570	-1.841366	0.758345
H	-7.188415	-1.797684	-0.082531
H	-6.152909	-0.466315	-0.615924
H	-5.491589	-2.536109	1.563290
H	-4.746622	-2.421951	-0.043866

(For models 15 and 16 contributions of several configurational isomers has been taken into account. The corresponding averaged weights are also given together the relevant coordinates.)

Model 15A avgd weight 37%				Model 15B avgd weight 31%				Model 15C avgd weight 32%			
45				45				45			
Cd	-0.0076	-0.8342	0.0376	Cd	0.0269	-0.7813	-0.0004	Cd	0.0361	-0.6247	-0.0733
C	5.1839	-1.6956	-0.3682	C	-4.7363	0.4192	1.9295	C	-4.6807	0.2509	2.1319
C	4.7441	0.0547	-2.0989	C	-5.1698	-1.5952	0.5108	C	-5.1338	-1.5624	0.4688
C	5.9583	0.8416	-1.5694	C	-6.3925	-0.8719	-0.0865	C	-6.3793	-0.7840	0.0037
C	7.0171	-0.0434	-0.9035	C	-7.0050	0.1706	0.8542	C	-6.9807	0.1070	1.0951
C	6.3666	-0.8989	0.1874	C	-5.9252	1.1560	1.3084	C	-5.9019	1.0399	1.6527
C	2.8888	-0.8311	-0.7020	C	-2.8762	-0.6569	0.7032	C	-2.8465	-0.6264	0.7195
C	-2.9036	-0.7854	0.7766	C	2.9304	-0.8654	-0.7061	C	2.9182	-0.6793	-0.8659
C	-5.2073	-1.6342	0.4621	C	5.2298	-1.6432	-0.2224	C	5.1927	-1.6411	-0.5983
C	-6.3821	-0.8383	-0.1112	C	6.4112	-0.7635	0.1934	C	6.4484	-0.8710	-0.1469
C	-7.0238	0.0480	0.9602	C	7.0585	-0.0978	-1.0240	C	7.0615	-0.0077	-1.2539
C	-5.9561	0.9370	1.6061	C	5.9969	0.6634	-1.8249	C	5.9951	0.9292	-1.8284
C	-4.7497	0.1501	2.1532	C	4.7862	-0.2044	-2.2193	C	4.7637	0.1478	-2.2937
C	5.0226	-0.7605	-3.3685	C	5.0709	-1.2149	-3.3378	C	5.4813	-2.8198	-1.5373
C	-5.0362	-0.6336	3.4407	C	-5.5123	-2.6170	1.6029	C	-5.4376	-2.7201	1.4288
N	4.1974	-0.8111	-1.0179	N	-4.1863	-0.5932	1.0074	N	-4.1475	-0.6203	1.0668
N	-4.2120	-0.7452	1.0919	N	4.2414	-0.8831	-1.0114	N	4.2190	-0.6969	-1.2133
S	2.2939	-1.8875	0.5617	S	-1.7567	0.5318	1.3346	S	-1.7138	0.4667	1.4869
S	-2.3195	-1.8758	-0.4631	S	1.7952	-0.0048	-1.7248	S	1.8001	0.4149	-1.6529
S	-1.7600	0.2517	1.6036	S	2.3347	-1.6994	0.7138	S	2.3193	-1.7553	0.3793
S	1.7556	0.1986	-1.5522	S	-2.2658	-1.9349	-0.3275	S	-2.2622	-1.7325	-0.5061
H	4.6733	-2.2533	0.4231	H	-3.9314	1.1126	2.1931	H	-3.8784	0.9210	2.4570
H	-4.7025	-2.2145	-0.3165	H	4.7199	-2.0620	0.6511	H	4.7005	-2.0380	0.2971
H	3.9524	0.7759	-2.3334	H	-4.6663	-2.1318	-0.3016	H	-4.6470	-1.9817	-0.4193
H	6.3916	1.4146	-2.4057	H	3.9919	0.4648	-2.5696	H	5.0270	-0.5056	-3.1449
H	5.5924	1.5790	-0.8338	H	6.4287	1.0944	-2.7432	H	3.9703	0.8225	-2.6311
H	7.4968	-0.6989	-1.6525	H	5.6280	1.5101	-1.2200	H	6.3886	1.5036	-2.6834
H	7.8192	0.5823	-0.4793	H	7.5376	-0.8677	-1.6554	H	5.6853	1.6612	-1.0617
H	7.0917	-1.6052	0.6242	H	7.8601	0.5904	-0.7102	H	7.4662	-0.6470	-2.0591
H	6.0080	-0.2532	1.0085	H	7.1385	-1.3873	0.7391	H	7.9123	0.5696	-0.8569
H	5.5372	-2.4277	-1.1164	H	6.0527	0.0072	0.8987	H	7.1817	-1.5984	0.2388
H	-3.9508	0.8684	2.3714	H	5.5844	-2.4904	-0.8368	H	6.1667	-0.2227	0.7011
H	-6.3834	1.5330	2.4292	H	-5.0503	-0.0935	2.8566	H	-4.9523	-0.3836	2.9947
H	-5.5829	1.6541	0.8541	H	-6.3230	1.8684	2.0500	H	-6.2875	1.6346	2.4972
H	-7.5099	-0.5857	1.7237	H	-5.5692	1.7491	0.4475	H	-5.5826	1.7539	0.8730
H	-7.8197	0.6720	0.5219	H	-7.4509	-0.3226	1.7367	H	-7.3935	-0.5124	1.9116
H	-7.1144	-1.5469	-0.5321	H	-7.8265	0.7015	0.3461	H	-7.8239	0.6883	0.6879
H	-6.0172	-0.2147	-0.9466	H	-7.1382	-1.6313	-0.3741	H	-7.1222	-1.5083	-0.3689
H	-5.5678	-2.3457	1.2265	H	-6.0734	-0.3715	-1.0175	H	-6.0893	-0.1547	-0.8557
H	-5.3584	0.0628	4.2313	H	5.3999	-0.6797	-4.2428	H	6.1397	-3.5426	-1.0297
H	-5.8282	-1.3890	3.3195	H	5.8579	-1.9382	-3.0737	H	4.5460	-3.3376	-1.7984
H	-4.1240	-1.1423	3.7877	H	4.1564	-1.7740	-3.5872	H	5.9795	-2.5130	-2.4701
H	5.3517	-0.0853	-4.1745	H	-6.1843	-3.3864	1.1902	H	-6.1056	-3.4432	0.9342
H	5.8071	-1.5209	-3.2303	H	-4.5984	-3.1182	1.9558	H	-4.5092	-3.2454	1.6992
H	4.1054	-1.2677	-3.7041	H	-6.0167	-2.1651	2.4711	H	-5.9317	-2.3901	2.3558

Model 16A avgd weight 29%

45

Cd	3.6038	-4.2110	1.9450
C	5.9578	-8.6696	3.5395
C	6.4588	-7.0857	5.3411
C	5.8765	-8.0260	6.4108
C	5.9693	-9.4848	5.9357
C	5.3595	-9.6632	4.5404
C	5.1202	-6.3364	3.3900
C	2.0917	-2.0867	0.4940
C	2.0257	-0.2067	-1.1260
C	1.8743	1.2534	-0.6660
C	0.3922	1.5735	-0.4155
C	-0.2541	0.5497	0.5248
C	-0.0292	-0.8822	0.0276
C	2.5103	2.2048	-1.6825
C	6.5744	-7.8072	7.7553
N	5.8122	-7.2920	4.0366
N	1.4071	-1.1369	-0.1689
S	4.3640	-6.6824	1.8506
S	3.8080	-2.2912	0.2219
S	1.2729	-3.1314	1.6343
S	4.9702	-4.7350	4.0794
H	4.2671	-9.5094	4.5807
H	0.1724	0.6431	1.5387
H	2.4169	1.3472	0.2932
H	-1.3383	0.7294	0.6128
H	5.4767	-8.7445	2.5592
H	3.0799	-0.4766	-1.2487
H	7.5397	-7.2875	5.2159
H	6.3420	-6.0358	5.6301
H	4.8076	-7.7642	6.5215
H	7.0347	-9.7856	5.9119
H	5.4725	-10.1512	6.6607
H	5.5276	-10.6875	4.1684
H	7.0384	-8.8641	3.4082
H	-0.5301	-1.0300	-0.9471
H	-0.4262	-1.6218	0.7301
H	-0.1423	1.5702	-1.3851
H	0.2887	2.5917	-0.0044
H	1.5214	-0.3438	-2.1013
H	6.1488	-8.4648	8.5300
H	7.6534	-8.0298	7.6856
H	6.4672	-6.7664	8.1010
H	2.4220	3.2515	-1.3502
H	3.5809	1.9864	-1.8252
H	2.0160	2.1249	-2.6663

Model 16B avgd weight 35%

45

Cd	3.6846	-4.1403	2.0252
C	6.4306	-7.1017	5.4407
C	5.9728	-8.6465	3.5919
C	5.3623	-9.7003	4.5359
C	5.9623	-9.5366	5.9475
C	5.8488	-8.0925	6.4543
C	5.1526	-6.3032	3.4657
C	2.1512	-2.0268	0.5794
C	0.0104	-0.8699	0.0878
C	-0.2734	0.5771	0.5035
C	0.3490	1.5708	-0.4867
C	1.8493	1.2944	-0.7167
C	2.0495	-0.1872	-1.0908
C	3.8275	-9.6613	4.5277
C	2.7269	1.7118	0.4715
N	5.8023	-7.2824	4.1207
N	1.4569	-1.0850	-0.0850
S	4.4375	-6.6116	1.8984
S	3.8672	-2.2254	0.2967
S	1.3469	-3.0671	1.7334
S	5.0152	-4.7076	4.1715
H	5.6782	-10.6829	4.1420
H	2.1724	1.8778	-1.5975
H	-1.3653	0.7210	0.5589
H	0.1202	0.7405	1.5209
H	5.5233	-8.6956	2.5946
H	3.1114	-0.4318	-1.1987
H	7.5159	-7.2766	5.3182
H	6.2874	-6.0649	5.7611
H	6.3853	-7.9756	7.4106
H	4.7953	-7.8284	6.6464
H	7.0301	-9.8210	5.9168
H	5.4736	-10.2309	6.6511
H	7.0588	-8.8248	3.4875
H	-0.4760	-1.0885	-0.8814
H	-0.3673	-1.5843	0.8261
H	-0.1809	1.4893	-1.4534
H	0.2039	2.6061	-0.1360
H	1.5501	-0.3985	-2.0541
H	3.4159	-10.4393	5.1911
H	3.4350	-8.6893	4.8656
H	3.4337	-9.8351	3.5141
H	2.5791	2.7781	0.7082
H	2.5004	1.1313	1.3797
H	3.7941	1.5586	0.2468

Model 16C avgd weight 28%

45

Cd	3.6452	-4.1408	1.9779
C	2.0086	-0.2201	-1.1657
C	-0.0359	-0.8968	0.0036
C	-0.2545	0.5329	0.5096
C	0.3895	1.5611	-0.4279
C	1.8683	1.2368	-0.6925
C	2.0950	-2.0875	0.4663
C	5.2674	-6.1165	3.5170
C	2.5013	2.1955	-1.7038
C	6.2010	-8.4016	3.7906
C	5.6635	-9.3713	4.8584
C	6.3069	-9.0659	6.2209
C	6.1732	-7.5839	6.5893
C	6.6959	-6.6838	5.4659
C	5.8848	-10.8222	4.4238
N	1.3987	-1.1525	-0.2053
N	6.0177	-7.0009	4.1989
S	3.8099	-2.2849	0.1818
S	4.4769	-6.5896	2.0290
S	5.0756	-4.4813	4.1086
S	1.2937	-3.1185	1.6317
H	4.5757	-9.1890	4.9402
H	2.4182	1.3184	0.2635
H	6.7298	-7.3597	7.5143
H	3.0601	-0.4933	-1.3033
H	5.7026	-8.5568	2.8277
H	-0.5432	-1.0389	-0.9685
H	-0.4291	-1.6390	0.7055
H	-1.3379	0.7149	0.6043
H	0.1771	0.6192	1.5219
H	-0.1516	1.5683	-1.3938
H	0.2934	2.5765	-0.0081
H	1.4912	-0.3496	-2.1352
H	7.7783	-6.8523	5.3152
H	6.5442	-5.6238	5.6926
H	7.3794	-9.3381	6.1782
H	5.8546	-9.6993	7.0023
H	7.2849	-8.5705	3.6456
H	2.4205	3.2390	-1.3597
H	3.5700	1.9738	-1.8562
H	1.9999	2.1290	-2.6850
H	5.1152	-7.3328	6.7800
H	5.4878	-11.5224	5.1761
H	5.3843	-11.0375	3.4660
H	6.9594	-11.0415	4.2990

Model 16D avgd weight 1.6 %

45

Cd	3.601459	-4.212041	1.955259
C	2.044965	-0.139253	-1.045586
N	1.423457	-1.089204	-0.107237
C	-0.023461	-0.865451	0.051704
C	-0.298132	0.556335	0.551297
C	0.357648	1.601951	-0.361128
C	1.858317	1.317867	-0.578862
C	2.099190	-2.062837	0.529593
S	1.268816	-3.137743	1.632968
S	4.951196	-4.738239	4.101414
C	5.108425	-6.337580	3.409717
S	4.368070	-6.679756	1.861292
C	2.715697	1.641281	0.652674
S	3.816493	-2.268275	0.262083
N	5.793593	-7.295281	4.060478
C	6.428638	-7.092606	5.371501
C	5.829446	-8.028831	6.435015
C	5.919934	-9.488030	5.960513
C	5.323708	-9.663874	4.559078
C	5.937630	-8.673249	3.564155
H	4.231847	-9.503792	4.587936
H	-1.389045	0.711400	0.593509
H	2.208480	1.952964	-1.412271
H	5.466462	-8.745404	2.578854
H	3.105154	-0.391944	-1.151488
H	7.509131	-7.302350	5.256978
H	6.316080	-6.042027	5.659361
C	6.514470	-7.813896	7.786710
H	4.760860	-7.761323	6.533933
H	6.983940	-9.794232	5.948081
H	5.412349	-10.152077	6.680169
H	5.489996	-10.689329	4.189576
H	7.018519	-8.873370	3.444578
H	-0.492666	-1.017786	-0.938384
H	-0.424335	-1.618841	0.737117
H	0.075929	0.649617	1.584689
H	-0.153411	1.590002	-1.341350
H	0.219346	2.614760	0.052335
H	1.558674	-0.281503	-2.027938
H	2.580092	2.692424	0.955261
H	2.457956	1.006999	1.515426
H	3.784924	1.482962	0.441933
H	6.077193	-8.468723	8.557269
H	7.592803	-8.042737	7.728073
H	6.409933	-6.772439	8.131340

Model 16E avgd weight 1.5 %

45

Cd	3.508549	-4.166998	2.042821
C	-0.055707	-0.806887	0.048958
N	1.372038	-1.104197	-0.147140
C	2.005383	-0.221945	-1.138103
C	1.898666	1.256033	-0.724074
C	0.428623	1.624685	-0.466415
C	-0.237813	0.644254	0.506162
C	2.038947	-2.047314	0.542616
S	1.200126	-3.048107	1.707835
S	4.837447	-4.705999	4.197045
C	5.024165	-6.294595	3.486901
S	4.294955	-6.629266	1.931738
H	-1.316018	0.856394	0.596728
N	5.722942	-7.248137	4.129532
C	5.959498	-8.595648	3.583332
C	5.437288	-9.692646	4.530795
C	6.064169	-9.505871	5.927587
C	5.875742	-8.076770	6.453110
C	6.369403	-7.041524	5.436969
H	5.800782	-10.650699	4.118254
S	3.752045	-2.286782	0.280891
C	3.903458	-9.744463	4.562656
H	0.198552	0.753787	1.514219
H	2.455551	1.365497	0.225180
C	2.547520	2.156274	-1.778247
H	5.489280	-8.661708	2.596612
H	3.050443	-0.524445	-1.262816
H	7.460832	-7.144977	5.288475
H	6.168625	-6.018982	5.772050
H	6.429324	-7.936311	7.396313
H	4.813654	-7.879662	6.675932
H	7.146377	-9.722777	5.864959
H	5.638338	-10.235706	6.636027
H	7.051203	-8.708403	3.450037
H	-0.566466	-0.969071	-0.918242
H	-0.468240	-1.514626	0.774988
H	-0.116395	1.614191	-1.430253
H	0.359433	2.655517	-0.080271
H	1.487194	-0.376279	-2.103678
H	3.555426	-10.547113	5.233046
H	3.464310	-8.797862	4.914924
H	3.494047	-9.938326	3.558912
H	2.491382	3.215083	-1.479237
H	3.609992	1.903640	-1.925309
H	2.039795	2.057980	-2.753496

Model 16F avgd weight 1.6 %

45

Cd	3.599746	-4.190022	2.017766
C	2.070327	-0.226842	-1.128341
N	1.435066	-1.142065	-0.165823
C	-0.003226	-0.883488	0.004336
C	-0.261014	0.553565	0.489031
C	0.406168	1.557912	-0.463922
C	1.886154	1.227167	-0.683514
C	2.109901	-2.080672	0.522584
S	1.275810	-3.106702	1.669179
S	4.936418	-4.738193	4.164399
C	5.122654	-6.322767	3.444904
S	4.389468	-6.651064	1.890717
H	2.453460	1.385436	0.250167
S	3.829641	-2.288821	0.277466
N	5.825046	-7.278944	4.079470
C	6.445837	-7.092895	5.402588
C	5.869488	-8.075418	6.434239
C	6.003218	-9.517971	5.921379
C	5.414332	-9.671882	4.515144
C	6.005896	-6.640606	3.549585
H	4.318738	-9.539828	4.545358
H	5.607221	-10.682441	4.118644
H	2.326513	1.891075	-1.445724
C	-1.762638	0.807634	0.641396
H	0.215121	0.648652	1.482840
H	5.540872	-8.699184	2.560499
H	3.128567	-0.490619	-1.220754
H	7.533281	-7.265332	5.288045
H	6.298779	-6.054416	5.715419
C	6.542184	-7.878528	7.794913
H	4.793259	-7.841356	6.535994
H	7.075848	-9.792249	5.902055
H	5.514373	-10.215558	6.621922
H	7.092112	-8.809604	3.429142
H	-0.491216	-1.039005	-0.976748
H	-0.412534	-1.617930	0.706069
H	-0.123410	1.533843	-1.436071
H	0.294843	2.582850	-0.072165
H	1.588667	-0.389600	-2.110401
H	6.118408	-8.564965	8.545324
H	7.626431	-8.077639	7.736808
H	6.408476	-6.849851	8.166663
H	-1.952658	1.828745	1.008997
H	-2.285978	0.699169	-0.324516
H	-2.221415	0.103030	1.353648

Model 16G avgd weight 1.8 %

45

Cd	3.708815	-4.148309	2.008063
C	2.098016	-0.174357	-1.085269
N	1.489845	-1.084435	-0.099161
C	0.040305	-0.872109	0.055377
C	-0.276928	0.569056	0.500684
C	0.359694	1.565434	-0.489006
C	1.853818	1.287531	-0.698299
C	2.180106	-2.032265	0.560941
S	1.367813	-3.091756	1.692440
S	5.055867	-4.692907	4.148904
C	5.211944	-6.287724	3.445622
S	4.478874	-6.616055	1.891296
H	2.425443	1.515429	0.217029
N	5.890513	-7.251861	4.093641
C	6.498716	-7.068489	5.421246
C	5.867990	-8.031410	6.432818
C	5.957778	-9.484127	5.950651
C	5.387824	-9.645178	4.532089
C	6.040130	-8.623585	3.584794
H	4.307371	-9.411079	4.562893
S	3.899540	-2.219523	0.294371
C	5.565025	-11.066617	3.992784
H	2.259002	1.934461	-1.494018
H	-1.374537	0.674326	0.433408
C	0.132870	0.823797	1.957899
H	5.603443	-8.677850	2.581991
H	3.166721	-0.398961	-1.159811
H	7.580735	-7.273452	5.322558
H	6.375909	-6.024267	5.725657
H	6.375442	-7.910038	7.404171
H	4.812387	-7.744885	6.581672
H	7.017397	-9.805222	5.947323
H	5.429810	-10.154368	6.649548
H	7.123160	-8.833249	3.498654
H	-0.427934	-1.070345	-0.926244
H	-0.347764	-1.605015	0.770372
H	-0.158582	1.482036	-1.461837
H	0.205676	2.599595	-0.138809
H	1.633701	-0.389840	-2.066065
H	5.082131	-11.802133	4.655811
H	5.121788	-11.175593	2.989783
H	6.633327	-11.335005	3.919976
H	-0.120206	1.853414	2.259040
H	-0.386072	0.132557	2.640318
H	1.214017	0.683749	2.114726

Model 16H avgd weight 1.6 %

45

Cd	3.645202	-4.140765	1.977900
C	2.008574	-0.220142	-1.165740
N	1.398685	-1.152548	-0.205326
C	-0.035863	-0.896824	0.003589
C	-0.254525	0.532909	0.509624
C	0.389501	1.561128	-0.427888
C	1.868262	1.236768	-0.692526
C	2.094996	-2.087451	0.466330
S	3.809870	-2.284883	0.181762
S	4.476855	-6.589574	2.028981
C	5.267374	-6.116511	3.517014
S	5.075567	-4.481278	4.108565
C	2.501303	2.195454	-1.703771
N	6.017708	-7.000907	4.198869
C	6.200967	-8.401617	3.790596
C	5.663532	-9.371282	4.858408
C	6.306945	-9.065929	6.220900
C	6.173159	-7.583920	6.589316
C	6.695874	-6.683789	5.465935
S	1.293728	-3.118450	1.631678
H	4.575744	-9.188998	4.940179
H	2.418245	1.318392	0.263459
C	5.884754	-10.822191	4.423807
H	6.729828	-7.359661	7.514293
H	3.060088	-0.493306	-1.303262
H	5.702619	-8.556819	2.827730
H	-0.543242	-1.038897	-0.968486
H	-0.429096	-1.639041	0.705488
H	-1.337916	0.714895	0.604281
H	0.177137	0.619170	1.521926
H	-0.151628	1.568265	-1.393848
H	0.293381	2.576542	-0.008113
H	1.491178	-0.349575	-2.135182
H	7.778330	-6.852293	5.315245
H	6.544214	-5.623795	5.692573
H	7.379400	-9.338133	6.178244
H	5.854639	-9.699297	7.002332
H	7.284910	-8.570493	3.645569
H	2.420473	3.238997	-1.359660
H	3.569973	1.973839	-1.856174
H	1.999942	2.128969	-2.684996
H	5.115233	-7.332801	6.780038
H	5.487804	-11.522395	5.176066
H	5.384265	-11.037519	3.465969
H	6.959359	-11.041508	4.299021

Model 17

63

Cd	-0.000206	-0.000107	-0.204540
C	1.675939	1.630249	2.241666
N	1.568359	1.123039	1.000607
N	2.806639	1.148075	0.425024
C	3.699405	1.672704	1.299482
C	3.014091	1.992088	2.472924
N	1.537568	-1.358621	-1.086953
N	2.781801	-0.816234	-1.240474
C	3.656978	-1.790606	-1.583947
C	2.953324	-2.995741	-1.646950
C	1.623605	-2.680210	-1.324691
C	5.110151	-1.541245	-1.842171
B	2.970378	0.725871	-1.075167
C	0.425697	-3.577144	-1.267110
C	5.150983	1.859525	0.985287
C	0.489576	1.776157	3.144249
H	2.069111	1.267209	-1.702566
H	4.070653	1.045219	-1.464998
H	3.433119	2.439045	3.370699
H	-0.418389	1.367411	2.677825
H	0.647469	1.253419	4.101400
H	0.301100	2.836616	3.379866
H	5.297896	2.546124	0.137108
H	5.670189	2.275149	1.860590
H	5.636983	0.907837	0.719071
H	3.355111	-3.972629	-1.902737
H	-0.268769	-3.269828	-0.471303
H	-0.135701	-3.554365	-2.216285
H	0.730967	-4.617582	-1.082475
H	5.258693	-0.821575	-2.661948
H	5.619793	-1.132570	-0.955156
H	5.605946	-2.483670	-2.115121
N	-1.535974	1.355896	-1.089451
C	-1.619929	2.677007	-1.332334
C	-2.947976	2.992791	-1.658569
C	-3.654588	1.789215	-1.588635
N	-2.781627	0.815607	-1.238981
C	-5.106667	1.540360	-1.853494
H	-3.346162	3.968446	-1.924412
C	-0.428190	3.579613	-1.240968
H	-0.662991	4.566287	-1.665079
H	-0.111261	3.727114	-0.195172
H	0.433347	3.163322	-1.785465
H	-5.621040	1.134316	-0.968031
H	-5.600291	2.482592	-2.131028
H	-5.251922	0.818841	-2.672251
N	-1.567141	-1.133046	0.998516
N	-2.807812	-1.147509	0.426545
C	-3.702652	-1.661671	1.304673
C	-3.016946	-1.985286	2.476976
C	-1.676205	-1.637054	2.241264
C	-0.487825	-1.794690	3.139100
H	-3.437576	-2.427229	3.376492
C	-5.156805	-1.835331	0.994903
B	-2.970728	-0.726971	-1.074624
H	-2.069549	-1.269526	-1.700088
H	-4.071694	-1.045343	-1.463629
H	-0.637350	-1.271954	4.097533
H	-0.308109	-2.857247	3.372038
H	0.421909	-1.393805	2.669355
H	-5.677385	-2.245662	1.871881
H	-5.634612	-0.879260	0.729583
H	-5.312336	-2.520889	0.147435

Model 18

63

Cd	0.317371	0.102460	-0.049544
S	2.528054	-1.405644	0.589289
S	2.509784	1.370998	-0.584523
B	-2.971215	-0.131587	0.059704
N	-1.081380	-1.370819	-1.143126
N	-2.413986	-1.261578	-0.857672
N	-1.345534	1.674693	-0.706999
N	-2.637628	1.264099	-0.538326
N	-1.074489	-0.130551	1.777835
N	-2.409468	-0.249363	1.508028
N	4.744176	-0.000423	0.000388
C	-0.924455	-2.405325	-1.980824
C	-2.181090	-2.983992	-2.242508
C	-3.101661	-2.234740	-1.516120
C	0.416948	-2.787759	-2.525731
C	-4.585404	-2.418761	-1.430992
C	-1.379866	2.906668	-1.233267
C	-2.719284	3.303824	-1.409534
C	-3.491647	2.237409	-0.958217
C	-0.131719	3.671377	-1.556475
C	-4.984161	2.122199	-0.915624
C	-0.912562	-0.240029	3.103900
C	-2.168345	-0.438594	3.708954
C	-3.093824	-0.438279	2.669663
C	0.432926	-0.121550	3.750815
C	-4.578977	-0.612207	2.750902
C	5.516706	1.142699	-0.516678
C	5.843788	2.179212	0.558920
C	5.545302	-1.124102	0.517154
C	5.892890	-2.153459	-0.558500
C	3.395789	-0.020617	0.005702
H	-4.166722	-0.249231	0.111543
H	-2.395572	-3.839690	-2.877265
H	1.225535	-2.476105	-1.848313
H	0.482468	-3.877491	-2.666355
H	0.594671	-2.317104	-3.508128
H	-4.920009	-2.600580	-0.397530
H	-5.132897	-1.537357	-1.800669
H	-4.882948	-3.283405	-2.041180
H	-3.081625	4.246022	-1.812423
H	0.462782	3.166547	-2.335160
H	-0.384009	4.677487	-1.921243
H	0.516367	3.780610	-0.672457
H	-5.434697	3.045366	-1.307229
H	-5.351260	1.280897	-1.524739
H	-5.358137	1.970270	0.109322
H	-2.378990	-0.567908	4.767283
H	1.234257	-0.431657	3.063936
H	0.633960	0.918756	4.060058
H	0.485710	-0.749220	4.653385
H	-5.119245	0.266927	2.365643
H	-4.924770	-1.485487	2.175619
H	-4.873671	-0.758631	3.799810
H	4.943141	1.604506	-1.331042
H	6.441793	0.733412	-0.953036
H	6.449861	2.990921	0.124568
H	4.920640	2.618204	0.965661
H	6.417389	1.736340	1.389511
H	4.980979	-1.598617	1.330483
H	6.461615	-0.692235	0.950460
H	6.519772	-2.949915	-0.125427
H	4.978158	-2.614781	-0.959355
H	6.452341	-1.698886	-1.392531

Model 19

75

Cd	0.3610	0.0371	-0.1760	H	0.5420	0.3110	5.1825
C	1.7163	-0.4052	3.5233	H	1.6138	0.5214	2.9575
C	2.4648	-1.4646	2.9830	H	-4.7844	-1.2266	3.8818
C	2.6141	-2.6392	3.7431	H	-5.4568	-1.3170	2.2337
C	2.0267	-2.7524	5.0041	H	-3.7494	-1.7602	2.5324
C	1.2774	-1.6942	5.5283				
C	1.1237	-0.5222	4.7824				
C	3.1274	-1.3499	1.6698				
C	4.5978	-1.4305	0.0121				
C	4.4179	-1.8175	1.3289				
C	-2.5089	0.4938	0.7265				
C	-4.1187	0.3831	2.5974				
C	-4.5558	-1.0673	2.8150				
C	0.2448	-2.1843	-2.7920				
C	1.0455	-2.4490	-3.9261				
C	2.2229	-1.7529	-3.7023				
C	-1.0939	-2.7232	-2.4895				
C	-2.0092	-2.9570	-3.5313				
C	-3.2693	-3.4948	-3.2658				
C	-3.6374	-3.8090	-1.9536				
C	-2.7344	-3.5814	-0.9106				
C	-1.4724	-3.0468	-1.1750				
C	3.4063	2.2842	-2.3964				
C	2.7272	3.4513	-2.0873				
C	1.6770	3.0463	-1.2320				
C	0.6748	3.9063	-0.5755				
C	0.1962	3.6274	0.7161				
C	-0.7326	4.4704	1.3284				
C	-1.1952	5.6108	0.6655				
C	-0.7229	5.9010	-0.6183				
C	0.2029	5.0568	-1.2329				
C	-4.8109	1.2802	0.3497				
C	-5.5892	0.2480	-0.4688				
N	2.5697	-0.7298	0.6099				
N	3.4820	-0.7822	-0.3990				
N	-3.7548	0.7058	1.2054				
N	2.1229	-1.1099	-2.5163				
N	0.9137	-1.3668	-1.9527				
N	1.7319	1.7100	-1.0569				
N	2.7944	1.2521	-1.7704				
S	-1.2763	-0.1627	1.7977				
S	-2.1067	0.8668	-0.9124				
B	3.2097	-0.2420	-1.8221				
H	5.4408	-1.5590	-0.6611				
H	3.1314	-1.6799	-4.2937				
H	4.2879	2.1128	-3.0076				
H	-3.2507	0.6081	3.2330				
H	4.2248	-0.3255	-2.4754				
H	0.8087	-3.0967	-4.7645				
H	5.1281	-2.3240	1.9752				
H	2.9741	4.4622	-2.3962				
H	-4.9286	1.0723	2.8821				
H	-4.3316	2.0042	-0.3237				
H	-5.4913	1.8348	1.0146				
H	-6.3270	0.7652	-1.1042				
H	-4.9109	-0.3184	-1.1237				
H	-6.1343	-0.4606	0.1739				
H	-1.7351	-2.6949	-4.5555				
H	-3.9695	-3.6641	-4.0871				
H	-4.6232	-4.2315	-1.7456				
H	-3.0089	-3.8282	0.1174				
H	-0.7691	-2.8938	-0.3550				
H	0.5643	2.7530	1.2545				
H	-1.0911	4.2351	2.3329				
H	-1.9198	6.2715	1.1470				
H	-1.0821	6.7866	-1.1476				
H	0.5523	5.2783	-2.2435				
H	3.1832	-3.4752	3.3304				
H	2.1492	-3.6743	5.5775				
H	0.8157	-1.7831	6.5144				

Model 20

98

Cd	-0.7200	0.2803	0.0628	H	-2.5579	-3.9067	0.1990
N	2.2184	1.1698	-0.4203	H	-2.6504	-3.4823	1.9140
N	1.0930	1.7943	0.0114	H	-3.1391	-2.7771	-3.7967
N	2.0352	-0.9289	0.9665	H	-2.1536	-2.3021	-5.1803
N	0.8544	-0.5957	1.5505	H	-1.5433	-3.5256	-4.0346
N	0.2887	-0.6514	-1.8191	H	-2.5884	0.0912	-4.2811
N	1.5445	-1.0881	-1.4999	H	-3.2024	-0.2931	-2.6682
N	3.8887	-0.6656	-0.7731	H	-1.6938	0.6418	-2.8396
N	4.8224	-0.3848	0.1564	H	-1.8178	0.1860	4.4191
C	1.3362	3.1556	-0.0380	H	-0.8093	0.9418	3.1523
C	2.6559	3.3508	-0.5836	H	-1.9992	-0.3018	2.7189
C	3.1638	2.0981	-0.7827	H	-1.2728	-2.3422	5.0788
C	-3.5154	-1.2962	0.4175	H	0.4798	-2.6431	5.0299
C	-4.2801	-0.1479	0.0916	H	-0.1720	-1.1995	5.8508
C	-3.7956	1.1423	-0.1981	H	-1.2509	4.6000	1.6922
C	-4.8287	2.2644	-0.5086	H	-1.4831	3.1674	0.6591
C	-5.5838	2.6062	0.7967	H	-0.4791	3.0454	2.1089
C	0.4660	4.1159	0.4883	H	-0.0995	6.1301	-0.0201
C	-0.7457	3.7189	1.2678	H	0.9704	6.0210	1.3783
C	2.7131	-1.8319	1.7495	H	1.6324	5.7991	-0.2630
C	1.9731	-2.0920	2.8682	H	3.8575	-1.0184	-2.8995
C	0.7885	-1.2750	2.7561	H	6.5548	-0.7644	-2.6824
C	-0.2221	-1.0684	3.6944	H	7.7488	1.0775	1.8838
C	-1.2618	-0.0114	3.4896	H	6.2141	0.1721	2.0730
C	1.7451	-2.3502	-2.0068	H	7.7965	-0.6521	2.2288
C	0.6440	-2.7304	-2.7191	H	9.1083	0.7426	-0.3517
C	-0.2859	-1.6287	-2.6273	H	9.2172	-0.9870	-0.0299
C	-1.5009	-1.4731	-3.2908	H	8.4936	-0.4201	-1.5569
C	-2.2710	-0.1917	-3.2593				
C	-4.1144	3.5269	-1.0199				
C	-5.8368	1.8041	-1.5841				
C	-2.0949	-2.5788	-4.1084				
C	-0.2841	-1.8568	4.9658				
C	0.7712	5.5776	0.3815				
C	-4.2664	-2.6278	0.7015				
C	-5.0797	-3.0430	-0.5443				
C	-3.2554	-3.7381	1.0321				
C	-5.2170	-2.4372	1.9044				
C	6.0368	-0.3998	-0.4879				
C	5.8181	-0.6845	-1.8892				
C	4.4637	-0.8305	-2.0194				
C	7.2355	-0.1688	0.2032				
C	8.5632	-0.2135	-0.4804				
C	7.2325	0.1211	1.6693				
O	-2.2512	-1.3331	0.5079				
O	-2.5660	1.4944	-0.2161				
B	2.4158	-0.3791	-0.4335				
H	3.6976	-2.1767	1.4545				
H	4.1389	1.7901	-1.1424				
H	2.6759	-2.8793	-1.8259				
H	2.2576	-2.7353	3.6943				
H	3.1735	4.2902	-0.7462				
H	0.5264	-3.6505	-3.2819				
H	-5.3596	-0.2772	0.0646				
H	-6.2981	3.4279	0.6185				
H	-6.1478	1.7424	1.1809				
H	-4.8844	2.9312	1.5839				
H	-4.8613	4.2990	-1.2668				
H	-3.4310	3.9415	-0.2663				
H	-3.5226	3.3175	-1.9236				
H	-6.5271	2.6297	-1.8253				
H	-5.3227	1.5130	-2.5143				
H	-6.4472	0.9505	-1.2543				
H	-5.7160	-3.3910	2.1454				
H	-4.6634	-2.1110	2.8000				
H	-6.0005	-1.6908	1.7028				
H	-5.5896	-4.0035	-0.3591				
H	-5.8480	-2.3001	-0.8068				
H	-4.4220	-3.1744	-1.4190				
H	-3.7906	-4.6801	1.2361				

Model 21

89				H	2.7950	2.6150	-1.5060
				H	5.6751	-0.2297	0.6715
Cd	-0.2821	-0.3725	0.2053	H	4.4740	0.8989	1.3581
C	0.2377	-1.8113	-3.0999	H	4.0336	-0.8053	1.0893
C	0.5811	-3.0310	-2.4908	H	5.4038	-1.1314	-1.6877
C	1.5473	-3.8422	-3.1128	H	3.7573	-1.7104	-1.2936
C	2.1547	-3.4427	-4.3043	H	4.0134	-0.6421	-2.6939
C	1.8107	-2.2233	-4.8960	H	6.0312	1.2705	-1.2982
C	0.8506	-1.4089	-4.2875	H	4.6872	1.8130	-2.3236
C	-0.0682	-3.4803	-1.2457	H	4.8646	2.4513	-0.6656
C	-1.0161	-4.6755	0.3671	H	1.1349	5.5927	-2.3178
C	-0.3726	-4.8040	-0.8533	H	2.0314	4.8014	-0.9997
C	0.7253	2.2697	-1.1900	H	2.2484	4.2632	-2.6863
C	2.0787	1.8894	-1.1420	H	-0.6452	4.3131	-3.6298
C	2.6049	0.6543	-0.6858	H	0.4446	2.9179	-3.8535
C	4.1314	0.3771	-0.7494	H	-1.1502	2.6904	-3.0802
C	-0.2837	-2.3759	4.0795	H	-1.0823	5.2442	-1.3082
C	0.6126	-1.4262	4.5429	H	-1.5849	3.6327	-0.7187
C	0.7100	-0.4772	3.4996	H	-0.2963	4.5321	0.1228
C	1.4928	0.7714	3.4875				
C	1.0530	1.9083	2.7866				
C	1.7967	3.0894	2.8093				
C	2.9857	3.1620	3.5412				
C	3.4294	2.0394	4.2476				
C	2.6914	0.8552	4.2193				
C	0.3298	3.6490	-1.7853				
C	-3.8154	-0.0264	0.5999				
C	-4.7711	-0.6321	1.4472				
C	-4.1100	-1.7085	2.0138				
C	-4.0514	1.1110	-0.3105				
C	-3.6016	1.0827	-1.6411				
C	-3.9175	2.1218	-2.5184				
C	-4.6760	3.2114	-2.0795				
C	-5.1192	3.2549	-0.7541				
C	-4.8134	2.2113	0.1216				
C	4.3370	-0.8525	-1.6614				
C	4.9649	1.5501	-1.2907				
C	4.6056	0.0394	0.6810				
C	-0.7255	4.2992	-0.8666				
C	1.5096	4.6222	-1.9531				
C	-0.2939	3.3727	-3.1725				
N	-0.5020	-2.6237	-0.3005				
N	-1.0832	-3.3604	0.6814				
N	-0.6853	-2.0171	2.8384				
N	-0.0812	-0.8561	2.4754				
N	-2.6471	-0.6959	0.6738				
N	-2.8427	-1.7308	1.5388				
O	-0.2788	1.5629	-0.8166				
O	1.9206	-0.3034	-0.2110				
B	-1.7342	-2.7331	1.9431				
H	-0.6768	-3.2735	4.5487				
H	-1.4419	-5.4231	1.0302				
H	-4.4511	-2.4696	2.7101				
H	-2.2294	-3.6258	2.5923				
H	1.0962	-1.3934	5.5142				
H	-0.1836	-5.7182	-1.4072				
H	-5.8105	-0.3468	1.5766				
H	0.1112	1.8764	2.2362				
H	1.4371	3.9617	2.2595				
H	3.5631	4.0890	3.5624				
H	4.3593	2.0835	4.8192				
H	3.0558	-0.0230	4.7560				
H	1.8374	-4.7857	-2.6458				
H	2.9065	-4.0844	-4.7695				
H	2.2871	-1.9102	-5.8277				
H	0.5691	-0.4572	-4.7434				
H	-0.5326	-1.1803	-2.6532				
H	-5.1595	2.2486	1.1569				
H	-5.7076	4.1046	-0.4002				
H	-4.9224	4.0223	-2.7686				
H	-3.5776	2.0757	-3.5553				
H	-3.0272	0.2244	-1.9926				

Model 22

85				H	-5.3637	-2.0123	-1.2555
				H	-6.3567	-0.4322	-2.8909
Cd	-0.0077	-0.7681	0.1834	H	-4.8839	0.8552	-4.4422
C	-3.6850	2.4049	-0.6002	H	-2.4119	0.5323	-4.3474
C	-2.4427	3.0104	-0.3401	H	-1.4267	-1.0797	-2.7402
C	-2.4081	4.3970	-0.1025	H	0.0720	3.8004	-0.6235
C	-3.5799	5.1559	-0.1357	H	-1.4645	4.8897	0.1365
C	-4.8065	4.5443	-0.4125	H	-3.5348	6.2296	0.0614
C	-4.8535	3.1659	-0.6446	H	-5.7223	5.1397	-0.4412
C	-1.2168	2.1361	-0.2960	H	-5.8075	2.6788	-0.8600
C	0.0539	2.7305	-0.4423	H	-3.7123	1.3295	-0.7721
C	1.3073	2.0831	-0.3361	H	1.6858	4.5711	-1.5649
C	-2.7545	-2.6459	-0.9496	H	3.8012	5.8208	-1.7748
C	-3.3044	-3.9015	-0.6032	H	5.9178	4.8789	-0.8485
C	-2.3576	-4.4900	0.2185	H	5.8880	2.6518	0.2794
C	-3.3237	-1.6519	-1.8783	H	3.7434	1.3860	0.4731
C	-2.5060	-0.9212	-2.7576				
C	-3.0632	-0.0245	-3.6702				
C	-4.4489	0.1550	-3.7258				
C	-5.2731	-0.5673	-2.8573				
C	-4.7158	-1.4616	-1.9408				
C	0.1895	-3.3422	3.7040				
C	0.2292	-2.2098	4.5014				
C	0.0821	-1.1270	3.6057				
C	0.0277	0.3085	3.9395				
C	-0.8121	1.1953	3.2435				
C	-0.8621	2.5461	3.5952				
C	-0.0846	3.0309	4.6508				
C	0.7493	2.1554	5.3535				
C	0.8059	0.8065	5.0008				
C	2.2102	-4.5633	0.0272				
C	3.1342	-3.9801	-0.8239				
C	2.6288	-2.6841	-1.0772				
C	3.2010	-1.6632	-1.9743				
C	4.5963	-1.5259	-2.0828				
C	5.1550	-0.5900	-2.9549				
C	4.3294	0.2247	-3.7354				
C	2.9410	0.0937	-3.6387				
C	2.3822	-0.8432	-2.7688				
C	2.5647	2.8961	-0.4985				
C	2.5963	4.1484	-1.1380				
C	3.7945	4.8536	-1.2667				
C	4.9817	4.3235	-0.7522				
C	4.9638	3.0757	-0.1207				
C	3.7690	2.3656	-0.0035				
O	1.4905	0.8468	-0.0820				
O	-1.4503	0.8887	-0.1299				
N	-1.5553	-2.4964	-0.3516				
N	-1.3182	-3.6339	0.3568				
N	0.0348	-2.9564	2.4171				
N	-0.0304	-1.6001	2.3466				
N	1.4758	-2.5101	-0.4003				
N	1.2242	-3.6677	0.2687				
B	-0.0212	-3.8790	1.1688				
H	0.2505	-4.3964	3.9592				
H	2.1749	-5.5549	0.4696				
H	-2.3399	-5.4620	0.7034				
H	-0.0200	-5.0245	1.5576				
H	0.3097	-2.1638	5.5829				
H	4.0257	-4.4342	-1.2451				
H	-4.2389	-4.3315	-0.9499				
H	-1.4422	0.8275	2.4327				
H	-1.5211	3.2192	3.0429				
H	-0.1278	4.0873	4.9254				
H	1.3649	2.5259	6.1765				
H	1.4743	0.1315	5.5397				
H	5.2461	-2.1474	-1.4629				
H	6.2411	-0.4921	-3.0204				
H	4.7661	0.9596	-4.4151				
H	2.2881	0.7220	-4.2486				
H	1.2983	-0.9587	-2.7192				

Model 23

71

Cd	-0.4194	-0.2006	0.2907
C	2.2374	1.7783	2.0765
C	2.3840	0.6003	2.8303
C	3.6796	0.1642	3.1578
C	4.7983	0.8865	2.7383
C	4.6418	2.0541	1.9844
C	3.3575	2.4966	1.6531
C	1.2025	-0.1531	3.2899
C	-0.3044	-1.2809	4.4680
C	0.9861	-0.7772	4.5381
C	1.5232	1.5865	-1.5094
C	-1.8630	-3.2468	-0.4041
C	-2.7476	-4.1050	0.2843
C	-2.9169	-3.5228	1.5301
C	-1.3573	-3.4105	-1.7823
C	0.0023	-3.2397	-2.0930
C	0.4564	-3.4217	-3.4019
C	-0.4356	-3.7847	-4.4148
C	-1.7891	-3.9674	-4.1122
C	-2.2471	-3.7829	-2.8066
C	2.5437	-0.5953	-1.0089
C	-4.1218	0.4405	2.5871
C	-4.4885	1.4906	1.7651
C	-3.4378	1.6069	0.8265
C	-3.3694	2.5847	-0.2782
C	-4.5538	2.9293	-0.9581
C	-4.5382	3.8732	-1.9853
C	-3.3377	4.4883	-2.3552
C	-2.1566	4.1523	-1.6888
C	-2.1717	3.2134	-0.6546
C	2.5840	0.6818	-1.6013
C	3.7801	-1.5076	-1.1714
C	1.7177	2.9912	-2.1166
N	0.1014	-0.2934	2.5254
N	-0.8168	-0.9822	3.2519
N	-2.1822	-2.3883	1.5803
N	-1.5315	-2.2109	0.3961
N	-2.4965	0.6718	1.0824
N	-2.9285	-0.0393	2.1661
O	0.3873	1.4443	-0.9701
O	1.6170	-1.1184	-0.3458
B	-2.2281	-1.3145	2.7070
H	-3.5057	-3.8345	2.3881
H	-4.6213	-0.0020	3.4443
H	-0.9001	-1.8173	5.2012
H	-2.8891	-1.7612	3.6154
H	-3.1681	-5.0382	-0.0769
H	-5.3720	2.1163	1.8417
H	1.6646	-0.8108	5.3848
H	0.7103	-2.9798	-1.3070
H	1.5179	-3.2874	-3.6199
H	-0.0779	-3.9285	-5.4369
H	-2.4935	-4.2496	-4.8981
H	-3.3073	-3.9109	-2.5770
H	-5.4903	2.4368	-0.6882
H	-5.4664	4.1235	-2.5043
H	-3.3234	5.2249	-3.1618
H	-1.2120	4.6190	-1.9724
H	-1.2428	2.9731	-0.1416
H	3.8082	-0.7592	3.7263
H	5.7986	0.5301	2.9942
H	5.5183	2.6164	1.6551
H	3.2206	3.4047	1.0621
H	1.2375	2.1459	1.8404
H	3.4850	0.9874	-2.1233
F	4.2828	-1.8432	0.0282
F	3.4293	-2.6525	-1.8023
F	4.7707	-0.9408	-1.8899
F	2.9285	3.1717	-2.6780
F	0.7886	3.2414	-3.0580
F	1.5751	3.9294	-1.1494

Model 24

70

Cd	-0.0724	-0.0001	0.5013
C	1.5864	-2.2153	-2.8478
C	1.7558	-2.7249	-0.6884
C	2.1152	-3.1605	-1.9826
C	1.7552	2.7254	-0.6877
C	2.1139	3.1619	-1.9818
C	1.5855	2.2168	-2.8473
C	-0.6261	-0.0005	3.1144
C	-0.9860	-0.0007	4.5830
C	2.0720	3.4002	0.6424
C	0.7783	3.9861	1.2541
C	2.0724	-3.4002	0.6415
C	3.0726	-4.5492	0.4048
C	-2.2801	0.0009	-3.2158
C	-3.4755	0.0007	-2.5118
C	-3.1060	0.0002	-1.1499
C	-4.0163	-0.0005	0.0724
C	-3.7637	-1.2673	0.9202
C	2.7079	-2.3923	1.6230
C	0.7786	-3.9859	1.2531
C	2.7071	2.3918	1.6237
C	3.0726	4.5488	0.4062
C	-3.7641	1.2656	0.9215
C	-5.4882	-0.0005	-0.3842
N	0.9511	-1.2745	-2.1173
N	1.0492	-1.5794	-0.7903
N	0.9508	1.2753	-2.1171
N	1.0492	1.5795	-0.7900
N	-1.7596	-0.0001	-1.0612
N	-1.2614	0.0003	-2.3305
B	0.2560	0.0004	-2.6641
O	-0.4921	1.1060	2.5031
O	-0.4915	-1.1067	2.5027
H	1.6211	-2.1420	-3.9311
H	1.6200	2.1441	-3.9307
H	-2.0823	0.0012	-4.2840
H	0.3674	0.0005	-3.8683
H	2.6860	-4.0417	-2.2531
H	2.6841	4.0436	-2.2520
H	-4.4762	0.0011	-2.9292
H	-4.4613	-1.2944	1.7742
H	-3.9245	-2.1791	0.3226
H	-2.7420	-1.3035	1.3262
H	-4.4609	1.2909	1.7762
H	-2.7421	1.3021	1.3267
H	-3.9263	2.1779	0.3252
H	-6.1512	-0.0005	0.4951
H	-5.7278	0.8920	-0.9838
H	-5.7278	-0.8930	-0.9838
H	3.3252	5.0249	1.3666
H	4.0087	4.1867	-0.0482
H	2.6512	5.3279	-0.2486
H	1.0179	4.5439	2.1751
H	0.2945	4.6833	0.5510
H	0.0631	3.1970	1.5225
H	2.9898	2.9053	2.5574
H	2.0051	1.5914	1.8969
H	3.6140	1.9359	1.1950
H	1.0181	-4.5440	2.1740
H	0.0636	-3.1967	1.5217
H	0.2945	-4.6828	0.5499
H	2.9903	-2.9061	2.5566
H	3.6151	-1.9367	1.1945
H	2.0062	-1.5917	1.8963
H	3.3248	-5.0258	1.3650
H	2.6510	-5.3277	-0.2505
H	4.0090	-4.1872	-0.0492
H	-0.6056	-0.9056	5.0748
H	-0.6063	0.9043	5.0749
H	-2.0852	-0.0011	4.6712

Model 25

97

Cd	0.0000	0.0001	0.0006	C	-1.1341	6.4128	-0.1276
O	-2.1817	-0.4271	-0.3549	C	-5.0827	-0.9827	0.1018
O	-0.6090	2.0056	-0.8253	C	-4.3940	-2.2027	0.2186
O	-0.1424	-0.9887	-2.2360	C	-5.1140	-3.3831	0.4214
O	2.1820	0.4272	0.3552	C	-6.5076	-3.3727	0.5108
O	0.6092	-2.0051	0.8268	C	-7.1853	-2.1551	0.3957
O	0.1434	0.9893	2.2371	C	-6.4859	-0.9660	0.1925
H	-1.1118	-1.0280	-2.1233	C	0.1602	-0.2328	-3.4265
H	-4.7549	4.2587	-1.3632	C	-0.4372	-0.8742	-4.6678
H	-4.4578	4.4560	0.3784	C	3.0640	-0.4993	0.3105
H	-5.9777	3.7104	-0.1872	C	2.9497	-1.9313	0.4629
H	-2.6748	4.5331	-0.9747	C	4.3125	-2.4072	0.3218
H	-1.2137	4.2679	-1.9333	C	4.8980	-3.7875	0.3760
H	-0.9510	3.4941	1.7743	C	1.7211	-2.6091	0.7261
H	-2.3058	4.6555	1.7114	C	0.8247	-4.9208	-0.1035
H	-0.7021	5.1846	2.2684	C	1.6649	-4.1122	0.9392
H	1.0000	4.9874	-1.1055	C	1.2201	-4.5365	-1.5417
H	0.9529	3.6360	0.0474	C	-0.6850	-4.6911	0.0940
H	1.2576	5.2987	0.6302	C	1.1328	-6.4126	0.1298
H	-0.8997	6.7132	-1.1627	C	5.0827	0.9822	-0.1039
H	-0.5341	7.0447	0.5478	C	4.3941	2.2024	-0.2203
H	-2.1975	6.6400	0.0562	C	5.1141	3.3826	-0.4239
H	-3.3104	-2.2202	0.1519	C	6.5076	3.3720	-0.5145
H	-4.5661	-4.3242	0.5114	C	7.1852	2.1543	-0.3998
H	-7.0598	-4.3014	0.6694	C	6.4858	0.9653	-0.1958
H	-8.2754	-2.1250	0.4639	C	-0.1585	0.2334	3.4276
H	-7.0049	-0.0141	0.1042	C	0.4396	0.8747	4.6687
H	1.2589	-0.2156	-3.4819				
H	-0.1866	0.8082	-3.3044				
H	-0.1555	-0.3011	-5.5664				
H	-1.5394	-0.8923	-4.6161				
H	-0.0799	-1.9089	-4.7885				
H	1.1128	1.0285	2.1238				
H	4.7553	-4.2589	1.3619				
H	4.4565	-4.4563	-0.3795				
H	5.9771	-3.7110	0.1847				
H	2.6747	-4.5330	0.9753				
H	1.2144	-4.2673	1.9350				
H	0.9492	-3.4942	-1.7726				
H	2.3035	-4.6562	-1.7105				
H	0.6992	-5.1847	-2.2662				
H	-1.0002	-4.9865	1.1090				
H	-0.9537	-3.6354	-0.0442				
H	-1.2592	-5.2982	-0.6264				
H	0.8992	-6.7127	1.1651				
H	0.5322	-7.0445	-0.5450				
H	2.1961	-6.6401	-0.0547				
H	3.3106	2.2200	-0.1526				
H	4.5663	4.3238	-0.5136				
H	7.0599	4.3006	-0.6737				
H	8.2752	2.1240	-0.4689				
H	7.0048	0.0134	-0.1078				
H	-1.2573	0.2162	3.4837				
H	0.1881	-0.8077	3.3054				
H	0.1583	0.3016	5.5674				
H	1.5417	0.8927	4.6163				
H	0.0825	1.9094	4.7896				
N	-4.4034	0.2505	-0.1018				
N	-5.1486	1.4180	-0.1139				
N	4.4033	-0.2508	0.1004				
N	5.1484	-1.4184	0.1120				
C	-3.0639	0.4993	-0.3107				
C	-2.9497	1.9313	-0.4629				
C	-4.3127	2.4069	-0.3229				
C	-4.8984	3.7871	-0.3775				
C	-1.7211	2.6093	-0.7251				
C	-0.8258	4.9210	0.1056				
C	-1.6650	4.1125	-0.9379				
C	-1.2222	4.5363	1.5435				
C	0.6841	4.6917	-0.0907				

Model 26

99

Cd -0.1177	-0.0295	-0.1107	H -1.0145	-0.7623	3.4309
C -3.2156	3.2948	1.6414	H 0.7159	-1.0346	3.1186
C -3.5008	2.9521	0.1560	H 0.3460	-0.2441	5.4851
C -2.9520	4.0549	-0.7705	H 1.2842	0.9642	4.5737
C -3.4970	5.4371	-0.3879	H -0.4564	1.2320	4.8721
C -3.1988	5.7723	1.0792	H 2.3217	-3.5831	1.0158
C -3.7428	4.6864	2.0165	H 5.1633	-2.5116	1.4465
C -2.8852	1.5909	-0.1532	H 3.8480	-2.5099	2.6185
C -0.0376	-0.2615	3.3526	H 5.4179	-4.4607	2.9392
C 0.3017	0.4666	4.6434	H 3.7558	-4.9770	2.6227
C 2.8740	0.7987	-0.0488	H 6.0451	-4.9010	0.5667
C 3.4204	-0.5389	-0.1098	H 5.3308	-6.3528	1.2800
C 4.7969	-0.3279	-0.5241	H 4.4097	-5.9124	-1.0206
C 2.6466	-1.6901	-0.2624	H 3.1398	-5.8545	0.2106
C 3.9443	3.0677	-0.4218	H 4.5340	-3.4495	-1.0926
C 5.1830	3.6995	-0.6303	H 2.8566	-3.9476	-1.3412
C 5.2540	5.0907	-0.6925	H -4.5900	2.9031	0.0239
C 4.1036	5.8724	-0.5486	H -1.8521	4.0525	-0.7067
C 2.8759	5.2394	-0.3431	H -3.2066	3.8199	-1.8183
C 2.7825	3.8465	-0.2782	H -3.0664	6.2054	-1.0521
C 5.8970	-1.2687	-0.9221	H -4.5913	5.4631	-0.5516
C 3.2127	-3.0707	0.6156	H -2.1044	5.8566	1.2171
C 3.6692	-3.9129	-0.5965	H -3.6253	6.7546	1.3439
C 4.0457	-5.3352	-0.1540	H -3.4797	4.9135	3.0636
C 5.1008	-5.3222	0.9611	H -4.8482	4.6847	1.9670
C 4.6350	-4.4880	2.1628	H -2.1250	3.2436	1.8056
C 4.2571	-3.0567	1.7520	H -3.6644	2.5269	2.2940
C -0.2261	0.5402	-3.4791	H 6.2241	5.5666	-0.8548
C -0.5413	-0.0375	-4.8490	H -6.3753	1.7844	-0.4126
C -3.1049	-0.9293	-0.3024	H -7.1066	0.4987	0.5834
C -5.0632	0.1485	0.1402	H -6.0117	1.6981	1.3255
C -3.6547	0.3888	-0.1004			
C -4.2010	-3.2162	-0.3012			
C -5.4520	-3.8580	-0.3028			
C -5.5225	-5.2457	-0.4197			
C -4.3598	-6.0134	-0.5372			
C -3.1199	-5.3706	-0.5327			
C -3.0269	-3.9813	-0.4150			
C -6.1948	1.0909	0.4249			
O -1.6456	1.6043	-0.4140			
O -0.1689	0.6489	2.2462			
O 1.7082	1.2271	0.2629			
O 1.3873	-1.6280	0.3991			
O -0.0657	-0.4962	-2.4904			
O -1.9111	-1.3180	-0.5537			
N 5.0640	0.9496	-0.6734			
N 3.9121	1.6465	-0.3692			
N -4.1664	-1.8002	-0.1761			
N -5.3500	-1.1310	0.0885			
H -0.9103	-0.9771	-2.3918			
H -2.0595	-3.4878	-0.4110			
H -2.2004	-5.9545	-0.6199			
H -4.4204	-7.0999	-0.6297			
H -6.5021	-5.7299	-0.4198			
H -6.3511	-3.2528	-0.2075			
H 0.7346	1.0766	-3.4904			
H -1.0043	1.2525	-3.1530			
H -0.6057	0.7682	-5.5987			
H -1.5085	-0.5687	-4.8451			
H 0.2405	-0.7462	-5.1643			
H 0.6890	1.0899	2.0901			
H 6.1578	-1.9962	-0.1418			
H 5.6279	-1.8359	-1.8278			
H 6.7876	-0.6678	-1.1514			
H 1.8248	3.3604	-0.1176			
H 1.9659	5.8338	-0.2310			
H 4.1644	6.9618	-0.5971			
H 6.0721	3.0832	-0.7452			

OP3 Protocol

Model 1

93

Cd	-0.052506	0.074621	0.031076	H	0.631312	-3.282546	4.796021
C	0.913429	1.375913	-2.869708	H	-7.147366	0.579102	-0.730043
N	0.102718	0.490065	-2.299471	H	-6.576749	1.276215	0.800576
C	-0.595409	-0.120093	-3.327820	H	-6.073341	2.002341	-0.723972
C	-0.192146	0.411577	-4.529355	H	-4.744698	1.562798	2.523132
N	0.771466	1.366908	-4.225993	H	-5.765023	3.567249	3.577147
O	-1.861842	-1.313288	-0.399597	H	-5.377226	5.825903	2.599856
C	-3.077198	-0.944385	-0.396014	H	-3.930097	6.067988	0.584803
C	-3.710257	0.318968	-0.047945	H	-2.857808	4.061206	-0.423154
C	-5.122001	0.103465	-0.304898	H	7.016794	-0.583106	-0.808602
N	-5.362650	-1.118750	-0.734258	H	6.425363	-1.681768	0.454599
N	-4.128869	-1.787300	-0.767746	H	5.856517	-1.879081	-1.201532
C	-3.017589	1.488060	0.382127	H	4.605424	-2.369090	2.054562
C	-3.757156	2.675162	0.959777	H	5.509780	-4.652559	2.428152
C	-4.574031	2.547694	2.094919	H	4.958583	-6.489443	0.837719
C	-5.147051	3.678619	2.688946	H	3.463696	-6.035076	-1.104564
C	-4.925458	4.948002	2.143292	H	2.506411	-3.760876	-1.430569
C	-4.110409	5.083619	1.011263	C	-2.923557	-3.911434	-1.161173
C	-3.516544	3.957305	0.435361	C	-2.954107	-5.245241	-1.581735
C	-4.104613	-3.142542	-1.190480	C	-4.139545	-5.835650	-2.031862
C	-6.292890	1.047944	-0.232658	C	-5.310916	-5.068537	-2.056555
C	1.505180	2.201810	-5.180874	C	-5.301441	-3.735894	-1.642220
O	1.860666	1.405115	0.235845	H	-2.003357	-3.463609	-0.812848
C	3.051401	0.986193	0.098850	H	-2.034465	-5.825753	-1.550977
C	3.610835	-0.355114	0.023611	H	-4.152278	-6.873696	-2.355434
C	5.030397	-0.149492	-0.194617	H	-6.244420	-5.508335	-2.401172
N	5.341710	1.130668	-0.233888	H	-6.206183	-3.140750	-1.656903
N	4.150934	1.843494	-0.023422	C	3.085702	4.045866	0.337406
C	2.849933	-1.559394	0.091052	C	3.189170	5.441032	0.336255
O	1.579639	-1.620793	0.032780	C	4.386270	6.077544	-0.008056
C	4.202762	3.262428	-0.016735	C	5.494939	5.294799	-0.353910
C	6.141491	-1.133720	-0.450622	C	5.411715	3.901520	-0.361182
C	3.518267	-2.905356	0.268700	H	2.158686	3.561907	0.612039
C	3.185114	-3.956593	-0.604185	H	2.319539	6.031323	0.616820
C	3.714347	-5.235450	-0.410917	H	4.456980	7.162577	-0.001736
C	4.556086	-5.491173	0.680276	H	6.437068	5.769742	-0.619283
C	4.869274	-4.457915	1.570717	H	6.268978	3.292446	-0.620881
C	4.361223	-3.170097	1.360591				
N	-0.175707	-0.302874	2.379139				
C	0.179264	-1.431659	2.983128				
N	-0.059217	-1.365499	4.325221				
C	-0.598664	-0.110186	4.581786				
C	-0.664273	0.532623	3.368628				
C	0.193421	-2.422558	5.307281				
O	-1.753543	1.642021	0.345556				
H	1.600047	2.025760	-2.346249				
H	-0.493754	0.206068	-5.546143				
H	-1.329748	-0.887546	-3.132260				
H	2.191434	2.848624	-4.630158				
H	2.082776	1.575479	-5.868484				
H	0.810970	2.824622	-5.754399				
H	-1.028291	1.523872	3.140750				
H	-0.876384	0.199651	5.578767				
H	0.604119	-2.297130	2.494278				
H	0.891866	-2.071448	6.073921				
H	-0.742396	-2.732050	5.784224				

Model 2

79

Cd	0.073478	0.271888	0.116940
C	-4.688701	-0.741243	2.083432
C	-4.379889	-0.937536	0.725679
C	-5.052691	-1.945736	0.016834
C	-6.022072	-2.734899	0.648329
C	-6.343385	-2.512842	1.992020
C	-5.675007	-1.509944	2.707468
C	-3.234022	-0.160006	0.110835
C	-3.399207	0.597737	-1.082954
C	-2.303234	1.215246	-1.826967
N	-2.912742	1.832947	-2.895703
N	-4.301916	1.715601	-2.878644
C	-4.595887	0.986021	-1.814447
O	-1.040576	1.268326	-1.648528
C	-2.256794	2.558560	-3.966298
C	-6.054356	0.754543	-1.516840
O	-2.138082	-0.277306	0.748889
N	0.109069	-1.880390	-0.945287
C	-0.586467	-2.933301	-0.533214
N	-0.320814	-4.030015	-1.302497
C	0.604975	-3.637705	-2.262996
C	0.859343	-2.307345	-2.026553
C	-0.894448	-5.367193	-1.139534
O	2.268915	0.563358	-0.637148
C	3.357566	0.095383	-0.167808
C	4.511303	0.146521	-1.147218
C	5.183146	-1.017674	-1.553158
C	6.160799	-0.963015	-2.554079
C	6.491314	0.259927	-3.148397
C	5.823856	1.426304	-2.750487
C	4.829397	1.366055	-1.770451
C	3.509488	-0.446496	1.139345
C	2.406885	-0.702603	2.063306
N	3.009114	-1.204250	3.194156
N	4.399962	-1.244886	3.103546
C	4.701629	-0.807026	1.891821
O	1.141780	-0.546346	1.985915
C	6.161917	-0.689779	1.541818
C	2.347935	-1.625042	4.413956
N	-0.024913	2.394156	1.213336
C	0.485770	2.747425	2.449711
C	0.182918	4.062896	2.710604
N	-0.529628	4.520721	1.607461
C	-0.626279	3.476135	0.733363
C	-1.075464	5.866503	1.419533
H	-1.129974	3.538509	-0.220612
H	0.401415	4.701367	3.554383
H	1.026998	2.035643	3.055263
H	-1.603852	5.903221	0.464336
H	-1.780022	6.107894	2.222236
H	-0.270588	6.609119	1.409722
H	1.524935	-1.637001	-2.550977
H	0.984295	-4.325132	-3.005156
H	-1.280803	-2.941522	0.295440
H	-1.427528	-5.667683	-2.047658
H	-0.107477	-6.097766	-0.924183
H	-1.599210	-5.349991	-0.305294
H	1.272311	-1.509261	4.264178
H	2.580010	-2.674205	4.632583
H	2.672541	-1.009146	5.261943
H	6.749184	-0.842080	2.452846
H	6.474055	-1.435635	0.801874
H	6.401723	0.294761	1.124378
H	4.924718	-1.970154	-1.096703
H	6.662235	-1.875486	-2.869495
H	7.255953	0.303930	-3.920946
H	6.071328	2.379773	-3.212320
H	4.285485	2.262326	-1.482988

H	-2.478660	2.094800	-4.934794
H	-2.595437	3.601874	-3.990906
H	-1.181283	2.522019	-3.779903
H	-6.647451	1.401957	-2.170410
H	-6.356573	-0.283630	-1.695845
H	-6.297954	0.983241	-0.473089
H	-4.804432	-2.121601	-1.027177
H	-6.526306	-3.520918	0.090183
H	-7.102734	-3.119435	2.480594
H	-5.915576	-1.335092	3.753946
H	-4.143524	0.014034	2.643918

Model 3

113

Cd	-0.033697	-0.218769	-0.175439	H	4.040405	5.530420	0.746893
C	-2.975376	0.443171	-1.816693	H	2.366211	5.897417	1.210634
N	-2.189041	0.667876	-0.698919	H	3.253439	4.651551	2.084736
C	-2.974626	1.257055	0.195788	H	-0.077995	5.294001	1.126449
N	-4.237941	1.429010	-0.295109	H	-0.710910	6.770564	3.021826
C	-4.248355	0.905212	-1.583463	H	-0.476436	5.961256	5.366252
O	0.135370	1.575085	1.338823	H	0.360210	3.654060	5.799722
C	0.765666	2.676687	1.248523	H	0.926765	2.158986	3.891062
C	0.494911	3.636980	2.384571	H	-1.518035	-1.455288	3.458901
C	0.592754	3.177382	3.709909	H	-1.944447	-1.176021	5.880780
C	0.262221	4.015238	4.778347	H	-3.107381	-2.963997	7.177137
C	-0.205974	5.313772	4.535242	H	-3.838508	-5.041923	5.996781
C	-0.333029	5.769708	3.218233	H	-3.411259	-5.313439	3.567458
C	0.025012	4.939554	2.149312	H	1.765293	1.253854	-3.647682
C	-5.401686	1.921598	0.476158	H	2.759571	0.786294	-5.865152
O	1.139614	1.275700	-1.520650	H	4.862030	1.928761	-6.576513
C	1.754565	2.292925	-1.072821	H	5.947445	3.558487	-5.024903
N	2.754833	2.956359	-1.792730	H	4.944292	4.023462	-2.801523
N	3.311865	4.011087	-1.052517	C	-6.311541	2.853521	-0.306604
C	2.654297	4.061099	0.089397	H	-5.974001	1.057383	0.831536
C	1.643865	3.024501	0.178331	H	-4.993499	2.430446	1.355012
C	3.297898	2.662122	-3.071199	C	6.688816	-1.576254	0.684612
C	4.482098	3.312284	-3.475435	H	5.758773	-2.721690	-0.885395
C	5.035031	3.045214	-4.729007	H	5.677432	-0.974755	-1.131548
C	4.428099	2.131990	-5.600438	C	-7.608302	2.445091	-0.653447
C	3.251005	1.491609	-5.198610	C	-8.461909	3.300709	-1.361666
C	2.679147	1.747862	-3.947735	C	-8.023559	4.576247	-1.730551
C	3.099510	5.092002	1.093264	C	-6.730377	4.993486	-1.387263
O	-0.521240	-1.954411	-1.655250	C	-5.880898	4.138663	-0.679163
C	-1.247530	-2.988435	-1.499063	H	-7.954710	1.453520	-0.365823
C	-1.733528	-3.466932	-0.248215	H	-9.464364	2.970031	-1.622481
C	-1.592462	-2.772788	1.024151	H	-8.683899	5.243121	-2.280003
N	-2.223265	-3.598399	1.959921	H	-6.385554	5.985457	-1.668941
N	-2.692573	-4.783166	1.369739	H	-4.877125	4.469136	-0.417165
C	-2.412643	-4.705710	0.084823	C	7.585620	-2.616391	0.970294
O	-1.037034	-1.673705	1.335546	C	8.592390	-2.448789	1.930015
C	-2.772060	-5.894800	-0.766689	C	8.708268	-1.235778	2.615751
C	-2.436928	-3.405878	3.350297	C	7.816640	-0.191047	2.336492
C	-2.022787	-2.233230	4.014408	C	6.815224	-0.358840	1.376049
C	-2.269525	-2.087596	5.383707	H	7.500085	-3.562488	0.437560
C	-2.921262	-3.087542	6.112961	H	9.280879	-3.263839	2.139643
C	-3.329955	-4.251140	5.449351	H	9.487998	-1.102385	3.362084
C	-3.094182	-4.415683	4.083614	H	7.903973	0.755438	2.864584
N	2.082511	-1.184545	0.317627	H	6.127696	0.458098	1.164190
C	3.215977	-0.948617	-0.335473				
N	4.233329	-1.716311	0.153701				
C	3.703109	-2.490424	1.180388				
C	2.375007	-2.149314	1.268117				
C	5.613773	-1.763080	-0.375191				
C	-1.582640	-3.693663	-2.797148				
C	-2.905137	-3.790857	-3.257733				
C	-3.181207	-4.339201	-4.516133				
C	-2.139018	-4.812932	-5.320724				
C	-0.816176	-4.717011	-4.868702				
C	-0.539520	-4.146037	-3.623220				
H	3.336969	-0.254650	-1.154688				
H	4.308942	-3.179930	1.749154				
H	1.617251	-2.524412	1.940225				
H	-2.576274	-0.030080	-2.701957				
H	-5.131613	0.930401	-2.203890				
H	-2.674265	1.561985	1.188077				
H	-3.079939	-6.711948	-0.107294				
H	-3.595226	-5.675641	-1.455561				
H	-1.924089	-6.227543	-1.375599				
H	-3.717112	-3.421918	-2.635460				
H	-4.209381	-4.395643	-4.866779				
H	-2.353690	-5.245921	-6.295193				
H	-0.000346	-5.077827	-5.491292				
H	0.487879	-4.042888	-3.282852				

Model 4

99

Cd	0.209861	-0.070071	-0.054993	H	-0.638844	2.827638	-4.397318
C	-2.586656	-3.867291	-1.856157	C	-5.557988	0.423673	0.888231
C	-2.838856	-4.376461	-0.565632	H	-5.588759	-0.552718	0.394451
C	-3.849832	-5.344377	-0.393031	H	-5.822513	0.265944	1.939560
C	-4.593403	-5.785251	-1.489108	C	-6.553449	1.377337	0.244620
C	-4.351800	-5.276292	-2.771362	C	-7.574232	1.954522	1.014205
C	-3.345539	-4.319693	-2.940917	C	-8.517308	2.807936	0.426796
N	-2.100314	-3.943678	0.567163	C	-8.445350	3.093085	-0.940062
C	-1.209751	-2.868374	0.694335	C	-7.428157	2.521467	-1.716661
C	-0.814793	-2.870731	2.091706	C	-6.489876	1.668543	-1.129063
C	-1.532876	-3.986404	2.673154	H	-7.635470	1.734045	2.079053
N	-2.285343	-4.610505	1.787807	H	-9.303187	3.246913	1.036764
O	-0.903483	-2.110366	-0.276501	H	-9.175689	3.755190	-1.399347
O	0.636836	-0.971860	2.088524	H	-7.368370	2.738177	-2.780603
C	0.077690	-1.934540	2.699594	H	-5.702808	1.228758	-1.739313
C	0.428481	-2.050264	4.187679	C	5.307379	-2.966839	0.143725
C	-1.543185	-4.521291	4.081519	C	6.703185	-2.463072	-0.195166
N	-1.954068	0.787651	0.504269	H	5.139339	-2.927543	1.225267
C	-3.103816	0.140965	0.343826	H	5.207590	-4.013841	-0.163141
N	-4.152225	0.873694	0.821141	C	7.641572	-3.333761	-0.768859
C	-3.625771	2.061412	1.318775	C	8.942645	-2.897242	-1.050480
C	-2.268843	1.992364	1.112745	C	9.315052	-1.580468	-0.763360
O	0.123968	0.719530	-2.249969	C	8.382762	-0.702916	-0.193105
C	0.381485	1.873064	-2.717503	C	7.086380	-1.141281	0.091294
C	0.899427	2.964184	-1.955272	H	7.355775	-4.359832	-0.996256
C	1.197815	2.938229	-0.534105	H	9.658776	-3.583966	-1.495410
N	1.688193	4.216010	-0.240870	H	10.323436	-1.237555	-0.983091
N	1.708534	5.035660	-1.379349	H	8.665414	0.322852	0.030580
C	1.247588	4.306333	-2.375787	H	6.367986	-0.450541	0.529332
O	1.072971	2.029854	0.347017				
C	1.169914	4.965207	-3.728483				
C	2.128818	4.760495	0.994658				
C	2.206275	3.981687	2.167270				
C	2.647327	4.565061	3.359832				
C	3.017566	5.912772	3.413365				
C	2.941629	6.681928	2.245459				
C	2.502617	6.119383	1.045887				
N	2.295723	-1.078437	-0.653266				
C	2.836118	-1.246690	-1.917016				
C	4.021548	-1.935402	-1.822658				
N	4.212015	-2.189308	-0.468642				
C	3.141573	-1.655069	0.191705				
C	0.098957	2.038472	-4.215197				
H	-3.217243	-0.838388	-0.097699				
H	-4.251860	2.831240	1.745053				
H	-1.505203	2.717835	1.352347				
H	2.337894	-0.861608	-2.794448				
H	4.737903	-2.246067	-2.568739				
H	3.012281	-1.710920	1.262792				
H	1.527555	5.994852	-3.634720				
H	1.789799	4.450369	-4.472235				
H	0.144135	4.988510	-4.115375				
H	-2.229178	-5.372320	4.126269				
H	-0.549756	-4.862716	4.396879				
H	-1.875431	-3.767789	4.805333				
H	1.924060	2.938755	2.133943				
H	2.700688	3.950120	4.255875				
H	3.359199	6.356015	4.345808				
H	3.225736	7.732003	2.264235				
H	2.444424	6.711835	0.141030				
H	-1.806211	-3.132540	-1.997041				
H	-3.137053	-3.918267	-3.930358				
H	-4.934211	-5.622569	-3.621831				
H	-5.368291	-6.533438	-1.336390				
H	-4.031519	-5.739256	0.599285				
H	1.161759	-1.276170	4.426539				
H	-0.458709	-1.900307	4.813523				
H	0.843261	-3.033590	4.434217				
H	1.007173	2.301780	-4.768703				
H	-0.291092	1.091157	-4.595162				

Model 5

99

Cd	-0.101089	0.117692	0.220897	H	0.758461	-7.462148	-1.243064
C	-2.964090	-1.100274	1.622134	H	1.993389	-7.093473	-3.375139
N	-2.382672	-0.510250	0.512513	H	2.865688	-4.823203	-3.920780
C	-3.377144	-0.199911	-0.309976	H	2.477399	-2.933251	-2.346582
N	-4.584019	-0.566824	0.216395	C	-6.833306	-1.481874	-0.462588
C	-4.327741	-1.141272	1.457923	H	-6.386350	0.511951	0.216519
O	0.713232	-1.946262	-0.580317	H	-5.713707	0.130443	-1.369689
C	1.199257	-2.954387	0.021755	C	-8.072385	-1.465459	0.194880
C	1.476125	-4.141912	-0.872012	C	-8.951463	-2.551414	0.091526
C	2.136771	-3.934715	-2.096327	C	-8.595390	-3.667946	-0.670962
C	2.338952	-4.994166	-2.984349	C	-7.358354	-3.694036	-1.329522
C	1.849147	-6.271062	-2.677822	C	-6.484016	-2.608378	-1.227472
C	1.161235	-6.479202	-1.477068	H	-8.354351	-0.597977	0.789952
C	0.984157	-5.423317	-0.575462	H	-9.908652	-2.523216	0.606705
C	-5.906895	-0.278161	-0.372344	H	-9.275129	-4.512955	-0.752994
N	2.169291	0.904522	0.210025	H	-7.076137	-4.559475	-1.924318
C	3.233906	0.195039	0.567538	H	-5.523689	-2.638350	-1.739422
N	4.366569	0.959102	0.547120	C	6.812347	0.826162	-0.035616
C	3.986536	2.238420	0.153869	H	5.948750	0.991312	1.930722
C	2.628843	2.184962	-0.051425	H	5.640171	-0.557789	1.144773
C	5.711954	0.520700	0.969975	C	7.909055	1.615374	0.341028
O	-0.634779	2.347698	0.819045	C	8.944824	1.879497	-0.564641
C	-1.121657	3.307394	0.142318	C	8.889487	1.357730	-1.860580
C	-1.215880	3.311273	-1.282624	C	7.796638	0.569324	-2.246139
C	-0.995282	2.134501	-2.117761	C	6.766608	0.303469	-1.339715
N	-1.154975	2.586201	-3.408023	H	7.956113	2.025234	1.348967
N	-1.402582	3.955724	-3.481754	H	9.788446	2.492752	-0.257199
C	-1.451687	4.388096	-2.231074	H	9.690365	1.562972	-2.567076
O	-0.746094	0.909613	-1.854919	H	7.748308	0.160568	-3.252612
C	-1.648585	5.866077	-2.016023	H	5.919965	-0.307461	-1.648204
C	-1.013714	1.803618	-4.621444				
O	0.219675	-0.979005	2.253555				
C	0.964809	-2.006767	2.377130				
C	1.469428	-2.991802	1.424365				
C	2.273890	-3.896198	2.229227				
N	2.273756	-3.543316	3.506024				
N	1.459430	-2.415913	3.595668				
C	3.136029	-5.066440	1.832220				
C	1.229137	-1.781280	4.879705				
C	-1.610517	4.471576	0.975495				
C	-2.910120	4.986069	0.840787				
C	-3.373762	5.985952	1.703632				
C	-2.536293	6.497481	2.701150				
C	-1.238988	5.987346	2.845737				
C	-0.787602	4.969859	2.001386				
H	3.230901	-0.847784	0.854686				
H	4.702887	3.038440	0.039858				
H	1.959689	2.970251	-0.370870				
H	-2.358472	-1.444781	2.447168				
H	-5.119128	-1.529068	2.082160				
H	-3.264509	0.282935	-1.269833				
H	-0.779126	0.778381	-4.327101				
H	-1.944738	1.819599	-5.201091				
H	-0.204594	2.204467	-5.243429				
H	-1.536955	6.374135	-2.979018				
H	-2.641552	6.101141	-1.616079				
H	-0.916151	6.275061	-1.310850				
H	-3.566296	4.585712	0.072032				
H	-4.388957	6.362421	1.598487				
H	-2.893712	7.279591	3.367460				
H	-0.585449	6.374141	3.624670				
H	0.203169	4.543272	2.134583				
H	0.679227	-2.452367	5.551119				
H	2.183265	-1.516691	5.350093				
H	0.641640	-0.878178	4.700680				
H	3.787557	-5.319863	2.674510				
H	2.543074	-5.952396	1.578467				
H	3.756082	-4.838773	0.957490				
H	0.439979	-5.585552	0.351476				

Model 6

71

Cd	0.000033	-0.001341	0.002114
C	-2.867055	2.748011	-2.481280
C	-1.549493	2.366635	-2.133650
N	-1.589281	1.367469	-1.226872
N	-2.918861	1.096635	-0.982330
C	-3.694494	1.922383	-1.732667
N	1.589918	-1.366446	1.228932
N	2.919259	-1.096875	0.982234
C	3.695260	-1.927775	1.726509
C	2.868206	-2.755491	2.473178
C	1.550454	-2.369846	2.130928
B	-3.396398	0.000525	0.008717
N	-2.916184	0.309693	1.452624
N	-1.586054	0.383569	1.807394
C	-1.543660	0.667751	3.126230
C	-2.860232	0.779722	3.632655
C	-3.689827	0.546670	2.544425
B	3.396180	0.000375	-0.007759
N	2.918214	1.405591	0.448300
N	1.588594	1.751289	0.563860
C	1.548380	3.035215	0.978534
C	2.865805	3.527956	1.133322
C	3.693587	2.468336	0.788844
N	-1.589390	-1.751179	-0.561191
N	-2.919001	-1.405163	-0.446917
C	-3.694218	-2.465578	-0.794828
C	-2.866308	-3.524113	-1.142524
C	-1.548959	-3.033313	-0.981585
N	1.585831	-0.385633	-1.805775
N	2.916080	-0.308074	-1.451969
C	3.689605	-0.538049	-2.545267
C	2.859928	-0.770377	-3.633620
C	1.543421	-0.665417	-3.125649
H	-4.597018	0.000963	0.010097
H	4.596779	0.000563	-0.009313
C	0.254163	-2.933268	2.644360
H	4.773283	-1.870125	1.670649
H	3.169087	-3.529244	3.167325
H	-4.772338	-2.389957	-0.770521
H	-3.166348	-4.511932	-1.467042
C	-0.252076	-3.758608	-1.213009
C	0.245324	-0.825684	-3.867754
H	3.158318	-0.985747	-4.651301
H	4.767839	-0.519974	-2.469641
C	0.251592	3.757888	1.218445
H	3.165877	4.517760	1.451708
H	4.771685	2.393668	0.761166
C	-0.245311	0.822753	3.869083
H	-3.158821	0.999710	4.649308
H	-4.768062	0.532520	2.467993
C	-0.252940	2.933602	-2.642599
H	-3.167536	3.517642	-3.180181
H	-4.772581	1.862561	-1.679753
H	-0.179171	1.812605	4.337649
H	-0.161960	0.078431	4.671002
H	0.610053	0.701885	3.200366
H	0.184696	4.657741	0.594240
H	-0.605304	3.119157	0.992480
H	0.172213	4.082087	2.263748
H	-0.194083	2.853409	-3.735186
H	-0.165546	3.997995	-2.390501
H	0.603955	2.409490	-2.213183
H	-0.149300	-4.606636	-0.524081
H	-0.207414	-4.161889	-2.232195
H	0.603884	-3.095635	-1.067485
H	0.171149	-0.099108	-4.686543
H	0.171114	-1.825362	-4.313948
H	-0.610573	-0.682848	-3.204164
H	0.171993	-2.798830	3.730344
H	-0.603128	-2.446328	2.173998
H	0.190696	-4.010432	2.445848

Model 7

91				H	0.278788	3.056974	-3.424741
				H	0.716883	1.402488	-2.944930
Cd	0.000007	-0.000994	-0.018829	H	-0.225839	1.687875	-4.420231
C	2.965869	3.520211	-0.131834	H	-0.477035	-4.646210	0.737460
C	1.639324	3.046697	-0.021042	H	-0.168253	-4.355154	-0.976610
N	1.637687	1.698526	-0.019382	H	0.486458	-3.241695	0.236011
N	2.953531	1.286202	-0.137105	H	-0.275136	-2.964075	-3.511320
C	3.757746	2.386598	-0.198630	H	-0.715380	-1.325240	-2.981968
N	-1.637226	-1.698167	-0.063748	H	0.230126	-1.564766	-4.463502
N	-2.953177	-1.283068	-0.169263	H	0.052456	-1.639094	4.309329
C	-3.757402	-2.381679	-0.257536	H	-0.691216	-1.576288	2.700165
C	-2.965163	-3.516498	-0.221853	H	-0.008537	-3.093680	3.311304
C	-1.638691	-3.045695	-0.099115	H	0.469695	4.606826	0.879002
B	3.427748	-0.210638	-0.058681	H	0.183567	4.401769	-0.851342
N	2.837631	-1.062690	-1.237013	H	-0.489374	3.231435	0.296685
N	1.554793	-0.885311	-1.721427	H	-7.940530	-0.445752	2.238507
C	1.350583	-1.845363	-2.648297	H	-8.955434	0.450720	1.088470
C	2.496161	-2.667434	-2.751482	H	-8.784652	-1.301666	0.928639
C	3.400045	-2.150787	-1.836511	H	8.786074	1.275327	0.956601
B	-3.427806	0.211243	-0.054544	H	7.943673	0.386948	2.245776
N	-2.837802	1.092380	-1.211615	H	8.957171	-0.480481	1.072478
N	-1.553736	0.929529	-1.698096				
C	-1.349316	1.913655	-2.599339				
C	-2.495657	2.736929	-2.682706				
C	-3.400928	2.194620	-1.784166				
N	1.596153	-1.014318	1.510680				
N	2.955569	-0.855913	1.282549				
C	3.652137	-1.405411	2.316325				
C	2.747029	-1.922060	3.230147				
C	1.468882	-1.654597	2.691104				
N	-1.597137	0.971916	1.537423				
N	-2.956503	0.824039	1.301980				
C	-3.654040	1.358613	2.342842				
C	-2.749851	1.856316	3.267875				
C	-1.471007	1.591917	2.728830				
N	4.963292	-0.206528	-0.223728				
N	-4.963317	0.210010	-0.218850				
C	-0.377152	-3.859539	-0.020097				
H	-4.830583	-2.287415	-0.324057				
H	-3.297758	-4.545035	-0.268505				
H	4.729341	-1.357818	2.324543				
H	2.976867	-2.419518	4.163310				
C	0.129678	-2.005339	3.278642				
C	-0.132476	1.918380	3.331514				
H	-2.980790	2.339777	4.208089				
H	-4.731454	1.316126	2.346839				
C	-0.070688	2.019036	-3.384430				
H	-2.643902	3.603145	-3.314429				
H	-4.399626	2.511017	-1.523358				
C	0.073441	-1.927633	-3.438582				
H	2.644723	-3.516498	-3.405983				
H	4.397840	-2.475218	-1.582182				
C	0.378500	3.858833	0.082049				
H	3.298708	4.549515	-0.151804				
H	4.830805	2.293845	-0.269139				
N	5.834793	-0.055519	0.842799				
C	7.042913	0.173966	0.311260				
C	6.972888	0.202320	-1.108652				
C	5.644135	-0.032732	-1.404746				
H	5.137798	-0.073173	-2.357772				
H	7.777116	0.366039	-1.814631				
C	8.248552	0.349209	1.195517				
C	-5.645101	0.063786	-1.403064				
C	-6.973641	-0.178106	-1.111444				
C	-7.042151	-0.184704	0.308828				
N	-5.833546	0.032112	0.844554				
C	-8.246746	-0.381831	1.189898				
H	-7.778573	-0.324694	-1.820383				
H	-5.139572	0.126901	-2.355274				
H	-0.016560	1.429576	4.306705				
H	0.690060	1.596085	2.689679				
H	-0.035397	2.998527	3.498122				

Model 8

53

Cd	0.000861	-0.000193	0.000076
C	0.007040	3.881447	2.538800
C	0.013573	3.250710	1.282119
N	0.003010	1.916926	1.446558
N	-0.012700	1.676428	2.799805
C	-0.011287	2.855995	3.477883
N	0.066814	-1.915843	-1.445751
N	0.069210	-1.675291	-2.799071
C	0.108978	-2.854277	-3.476941
C	0.132586	-3.879476	-2.537680
C	0.103439	-3.249142	-1.281117
B	-0.031983	0.238527	3.395541
N	1.243553	-0.544114	2.966951
N	1.543596	-0.807728	1.651764
C	2.700131	-1.492107	1.639468
C	3.155156	-1.673951	2.957387
C	2.209583	-1.062034	3.773029
B	0.030744	-0.237922	-3.395248
N	1.283145	0.569624	-2.945423
N	1.556532	0.837857	-1.625353
C	2.698956	1.544982	-1.593951
C	3.171157	1.737675	-2.904266
C	2.251366	1.107644	-3.735465
N	-1.590801	-0.778380	1.619948
N	-1.312952	-0.520251	2.941102
C	-2.303448	-1.022268	3.727330
C	-3.241858	-1.619186	2.892532
C	-2.757390	-1.444619	1.584096
N	-1.578809	0.745367	-1.646171
N	-1.272551	0.495235	-2.962562
C	-2.259106	0.978365	-3.765391
C	-3.224295	1.554062	-2.946392
C	-2.759425	1.387202	-1.629850
H	-0.043174	0.322058	4.590186
H	0.041213	-0.321450	-4.589913
H	0.107835	-3.687463	-0.292846
H	0.117884	-2.888351	-4.556131
Br	0.191226	-5.755849	-2.893065
H	-2.278563	-0.925682	4.802474
Br	-4.854949	-2.493918	3.424775
H	-3.188085	-1.761566	0.644477
H	-3.212941	1.693566	-0.697481
Br	-4.845623	2.395883	-3.505946
H	-2.213270	0.884328	-4.840057
H	3.122136	1.876387	-0.655939
Br	4.748832	2.671039	-3.443075
H	2.225142	1.010746	-4.810519
H	3.144578	-1.816124	0.708725
Br	4.741975	-2.575797	3.522334
H	2.164308	-0.964833	4.847424
H	0.026464	3.689137	0.293964
Br	0.018981	5.758680	2.894256
H	-0.022214	2.890142	4.557017

Model 9

71

Cd	0.000001	0.000716	0.000952
C	-2.808805	-3.730861	-0.022443
C	-1.516446	-3.157755	-0.024464
N	-1.579423	-1.815024	-0.017878
N	-2.910417	-1.485128	-0.011659
C	-3.657397	-2.624772	-0.014316
N	1.580843	1.814980	0.043805
N	2.911558	1.483955	0.039764
C	3.659462	2.622410	0.076452
C	2.811781	3.728835	0.105678
C	1.518944	3.157201	0.083750
B	-3.407216	-0.010565	-0.001099
N	-2.917316	0.738416	-1.273992
N	-1.587864	0.916780	-1.558743
C	-1.530834	1.594282	-2.718345
C	-2.825732	1.871855	-3.213240
C	-3.669350	1.306360	-2.258186
B	3.407246	0.009495	-0.000253
N	2.916833	-0.695058	-1.298072
N	1.587265	-0.862037	-1.589158
C	1.529823	-1.500035	-2.770925
C	2.824530	-1.762175	-3.274601
C	3.668507	-1.230212	-2.300758
N	-1.589419	0.886019	1.576649
N	-2.918569	0.720057	1.282993
C	-3.671796	1.285048	2.267980
C	-2.829335	1.836012	3.232534
C	-1.533851	1.552994	2.742408
N	1.588661	-0.938672	1.545963
N	2.917991	-0.764210	1.258101
C	3.670650	-1.363084	2.223308
C	2.827597	-1.945268	3.168825
C	1.532399	-1.644694	2.688462
H	-4.607120	-0.014676	-0.001693
H	4.607159	0.012731	-0.000662
H	0.553661	3.649255	0.094494
H	4.740339	2.569862	0.079035
C	3.190150	5.188562	0.149538
H	-4.752408	1.257899	2.217274
C	-3.214593	2.560367	4.498554
H	-0.570875	1.798496	3.174172
H	0.569149	-1.903558	3.111740
C	3.212150	-2.711934	4.409896
H	4.751320	-1.335308	2.173557
H	0.566185	-1.741310	-3.203497
C	3.207834	-2.452521	-4.560071
H	4.749174	-1.197699	-2.254619
H	-0.567347	1.850886	-3.142353
C	-3.209465	2.605070	-4.474611
H	-4.749991	1.270998	-2.213530
H	-0.550776	-3.649123	-0.030538
C	-3.186062	-5.191525	-0.028887
H	-4.738314	-2.573209	-0.010397
H	-4.298654	2.668799	-4.576208
H	-2.817266	3.630630	-4.484100
H	-2.824140	2.101506	-5.371225
H	-4.303832	2.630818	4.595045
H	-2.837447	2.046102	5.392507
H	-2.815376	3.583096	4.519372
H	-4.274688	-5.316236	-0.020916
H	-2.802109	-5.707005	-0.919209
H	-2.787903	-5.718242	0.848538
H	4.296961	-2.517191	-4.661751
H	2.811443	-3.475465	-4.606160
H	2.826428	-1.916332	-5.439293
H	4.278883	5.312193	0.160100
H	2.805166	5.734927	-0.721697
H	2.793758	5.684723	1.045387
H	4.301349	-2.786131	4.504220
H	2.835022	-2.227764	5.320536
H	2.812412	-3.734579	4.396288

Model 10

91				H	-2.459984	4.396119	-3.842021
				H	-4.071836	4.486310	-3.118900
Cd	-0.000014	0.032082	0.000479	H	-2.713262	5.329269	-2.361727
N	5.823544	0.306378	1.033751	H	-3.995730	1.977855	4.908541
N	4.982067	-0.128205	0.030650	H	-3.003879	0.721011	5.661515
C	5.675096	-0.940769	-0.839293	H	-2.266864	2.249748	5.168787
C	6.994882	-1.021646	-0.423325	H	4.081890	-4.627725	2.705289
C	7.020343	-0.218778	0.748936	H	2.574589	-4.497258	3.621889
B	3.448797	0.026800	0.081613	H	2.600929	-5.370868	2.085031
N	2.963883	1.281839	0.883592	H	2.266013	2.244034	-5.171448
N	1.615925	1.577005	0.883854	H	3.995047	1.974757	-4.909489
C	1.473540	2.709216	1.591462	H	3.005388	0.715487	-5.661285
C	2.718037	3.180875	2.061779	H	2.713805	5.331314	2.357995
C	3.632201	2.242431	1.588287	H	2.460079	4.399478	3.839040
N	-1.615850	1.576293	-0.884092	H	4.072092	4.488772	3.116165
N	-2.963761	1.280926	-0.884106	H	8.617605	-2.459195	-0.367130
C	-3.631960	2.240803	-1.589857	H	7.773623	-2.372443	-1.919765
C	-2.717804	3.179101	-2.063630	H	8.904397	-1.094725	-1.452343
C	-1.473387	2.707925	-1.592577	H	-7.774934	-2.373858	1.916357
B	-3.448849	0.026506	-0.081325	H	-8.904918	-1.094907	1.450397
N	-4.982147	-0.128461	-0.031169	H	-8.618895	-2.458249	0.363578
N	-5.822989	0.306270	-1.034729				
C	-7.020197	-0.218164	-0.750279				
C	-6.995347	-1.021723	0.421520				
C	-5.675721	-0.941297	0.838098				
N	-1.643617	-0.057871	1.767961				
C	-1.516291	0.371077	3.034874				
C	-2.723539	0.922530	3.518373				
C	-3.594022	0.803091	2.438834				
N	-2.944588	0.195606	1.399028				
N	1.643230	-0.058875	-1.767327				
N	2.944251	0.194784	-1.398726				
C	3.593816	0.801116	-2.439138				
C	2.723212	0.919950	-3.518640				
C	1.515687	0.369878	-3.034274				
N	-1.527544	-1.498129	-0.926350				
N	-2.870774	-1.277612	-0.742768				
C	-3.570834	-2.302571	-1.318791				
C	-2.677876	-3.213054	-1.875739				
C	-1.410693	-2.653851	-1.597190				
N	1.527763	-1.497273	0.928313				
N	2.870925	-1.276910	0.744004				
C	3.571179	-2.301538	1.320395				
C	2.678442	-3.211702	1.878200				
C	1.411161	-2.652492	1.600084				
H	0.560518	0.270120	-3.536220				
H	4.627633	1.102738	-2.349686				
C	3.011949	1.491968	-4.884392				
H	-4.701754	2.166491	-1.713812				
C	-3.003642	4.410117	-2.888046				
H	-0.484584	3.129055	-1.730608				
H	0.484725	3.130396	1.729336				
C	3.003931	4.412560	2.885165				
H	4.702049	2.168371	1.711928				
H	0.425420	-3.026977	1.849464				
C	2.999046	-4.491796	2.609389				
H	4.651737	-2.316152	1.308757				
H	-0.424865	-3.028498	-1.845966				
C	-2.998115	-4.493433	-2.606565				
H	-4.651401	-2.317079	-1.307651				
H	-0.561323	0.271073	3.537153				
C	-3.012039	1.496284	4.883446				
H	-4.627625	1.105298	2.348900				
H	-5.183721	-1.412055	1.677649				
C	-8.130273	-1.774822	1.070497				
H	-7.862733	0.001330	-1.397358				
H	7.863215	0.000304	1.395712				
C	8.129363	-1.774633	-1.073209				
H	5.182698	-1.410964	-1.678926				
H	-4.080865	-4.628773	-2.704031				
H	-2.572108	-4.499813	-3.618404				
H	-2.601301	-5.372385	-2.081015				

Model 11

89				H	-0.126934	3.750511	-2.696839
				H	0.623915	2.175200	-2.378308
				H	-0.153022	2.497656	-3.941271
				H	-5.562436	2.488987	-2.689591
				H	-5.620333	0.797389	-2.164395
				H	-5.624191	2.093230	-0.963269
				H	-5.560913	1.068378	3.507144
				H	-5.622111	1.462740	1.780436
				H	-5.620530	-0.226461	2.298684
				H	5.563846	-2.500623	2.677212
				H	5.623383	-2.094892	0.953101
				H	5.621933	-0.806061	2.161733
				H	5.563382	-1.061331	-3.505286
				H	5.621632	0.231936	-2.294988
				H	5.623821	-1.458004	-1.779119
				H	-5.558238	-3.577455	-0.827718
				H	-5.619641	-2.281302	0.379274
				H	-5.620009	-1.882702	-1.342070
				H	5.554379	3.581582	0.830045
				H	5.617718	1.886887	1.344567
				H	5.617491	2.285363	-0.376825
Cd	-0.000007	0.000671	0.001874				
C	2.837964	-2.534641	2.709192				
C	1.532412	-2.166731	2.317042				
N	1.598176	-1.246134	1.337339				
N	2.938940	-1.009983	1.087136				
C	3.703400	-1.787246	1.914786				
N	-1.597681	1.246126	-1.336238				
N	-2.938632	1.010282	-1.086373				
C	-3.702625	1.781581	-1.920089				
C	-2.836713	2.524708	-2.717988				
C	-1.531388	2.160801	-2.321440				
B	3.411465	0.004813	0.002124				
N	2.935394	1.451068	0.337210				
N	1.593755	1.783419	0.412586				
C	1.524609	3.093144	0.714989				
C	2.828794	3.620020	0.837531				
C	3.696963	2.559216	0.593468				
B	-3.411565	-0.003086	-0.000097				
N	-2.937926	0.430970	1.420363				
N	-1.596905	0.531470	1.748461				
C	-1.530111	0.924643	3.033925				
C	-2.835243	1.082007	3.549093				
C	-3.701529	0.763023	2.506787				
N	1.598075	-0.532402	-1.747017				
N	2.938935	-0.429346	-1.418733				
C	3.703317	-0.758794	-2.505389				
C	2.837866	-1.078364	-3.548198				
C	1.532347	-0.924108	-3.033088				
N	-1.595580	-1.782736	-0.413453				
N	-2.936918	-1.449852	-0.334914				
C	-3.699608	-2.557032	-0.591957				
C	-2.832450	-3.617932	-0.839342				
C	-1.527744	-3.092039	-0.718065				
H	4.604468	0.006601	0.002565				
H	-4.604569	-0.003897	0.000125				
C	-0.222929	2.669384	-2.859738				
C	-5.207314	1.785779	-1.929825				
H	-3.116683	3.235679	-3.485542				
C	5.207969	-0.759541	-2.515101				
H	3.118298	-1.383154	-4.548923				
C	0.224280	-1.141165	-3.741794				
C	-0.218427	-3.811838	-0.885535				
H	-3.111249	-4.637265	-1.076367				
C	-5.204290	-2.568507	-0.594143				
C	-0.221520	1.140283	3.742141				
H	-3.114875	1.387867	4.549705				
C	-5.206198	0.765064	2.517179				
C	0.214642	3.811645	0.883054				
H	3.106641	4.640157	1.072390				
C	5.201591	2.572201	0.596435				
C	0.224284	-2.672265	2.859011				
H	3.118440	-3.251218	3.471366				
C	5.208064	-1.792835	1.922036				
H	0.113038	4.206443	1.902068				
H	0.147520	4.665465	0.197110				
H	-0.630673	3.147775	0.688458				
H	-0.134841	0.477880	4.612853				
H	0.625475	0.947329	3.079950				
H	-0.142305	2.170891	4.110712				
H	0.159380	-3.763637	2.765652				
H	0.123599	-2.432115	3.925221				
H	-0.622727	-2.231427	2.328576				
H	0.150886	-2.168994	-4.119148				
H	-0.623015	-0.958887	-3.077012				
H	0.132603	-0.471589	-4.606490				
H	-0.141247	-4.253387	-1.887196				
H	0.627777	-3.136018	-0.742930				
H	-0.128355	-4.632331	-0.162303				

Model 12

53

Cd	0.000009	-0.000286	0.000461
N	-1.583978	0.841811	1.603301
N	-1.578817	-1.812594	-0.070051
N	1.583508	-0.946005	-1.543872
N	-1.583465	0.963282	-1.532919
N	1.584368	-0.860642	1.593280
N	1.578407	1.813046	-0.049182
N	-2.911736	-1.480112	-0.059280
N	-2.915954	0.682160	1.307046
N	-2.915568	0.784107	-1.248700
B	-3.406365	-0.005466	-0.000383
H	-4.606242	-0.007606	-0.000584
N	2.916276	-0.697091	1.298811
N	2.915599	-0.769395	-1.257974
N	2.911419	1.480842	-0.042290
B	3.406387	0.005689	-0.000621
H	4.606250	0.008127	-0.001018
C	1.515734	3.154848	-0.087023
C	3.663145	2.614585	-0.075359
C	2.808999	3.712866	-0.105422
H	0.553221	3.649270	-0.098413
H	4.742710	2.559211	-0.074787
H	3.082449	4.758494	-0.134758
C	-1.525672	1.466486	2.791609
C	-3.671376	1.206666	2.309951
C	-2.820737	1.720956	3.283890
H	-4.750746	1.176883	2.259135
H	-3.097499	2.206755	4.209275
H	-0.564786	1.700685	3.230753
C	1.526367	-1.498532	2.774563
C	3.671942	-1.232400	2.295808
C	2.821556	-1.758380	3.263711
H	0.565590	-1.738233	3.210971
H	3.098572	-2.254880	4.183331
H	4.751288	-1.201697	2.245254
C	1.524692	-1.649056	-2.687515
C	3.670590	-1.361943	-2.222571
C	2.819547	-1.937765	-3.161069
H	0.563609	-1.909354	-3.111264
H	3.095933	-2.483524	-4.052512
H	4.749972	-1.330487	-2.173345
C	-1.524602	1.679914	-2.668110
C	-3.670523	1.388760	-2.205789
C	-2.819435	1.975505	-3.137457
H	-0.563511	1.944521	-3.089157
H	-3.095780	2.532272	-4.022086
H	-4.749915	1.357417	-2.156548
C	-1.516536	-3.153862	-0.124170
C	-3.663783	-2.613171	-0.106010
C	-2.809953	-3.711281	-0.148679
H	-0.554170	-3.648382	-0.141979
H	-3.083706	-4.756415	-0.190534
H	-4.743323	-2.557497	-0.105151

Model 13

67

Cd	-0.000361	0.000054	-0.027239
C	2.594083	3.688532	0.337751
C	1.408629	3.099150	-0.139753
N	1.581175	1.785422	-0.360041
N	2.891203	1.501902	-0.038327
C	3.504076	2.640776	0.402027
N	-1.580804	-1.818870	0.049479
N	-2.889154	-1.469156	0.306414
C	-3.496094	-2.474025	1.005254
C	-2.584257	-3.507458	1.179992
C	-1.403823	-3.044957	0.568870
B	3.442880	0.028503	0.016533
N	2.906178	-0.832260	-1.186885
N	1.569476	-1.084389	-1.396392
C	1.488329	-1.910340	-2.449707
C	2.771566	-2.218340	-2.939102
C	3.641122	-1.520498	-2.110764
B	-3.443324	-0.023572	0.023594
N	-2.906543	0.540588	-1.344167
N	-1.570511	0.748510	-1.601182
C	-1.489208	1.307620	-2.817356
C	-2.771726	1.481737	-3.370324
C	-3.640996	0.987962	-2.406008
N	1.607815	-0.605411	1.640171
N	2.963240	-0.599260	1.367668
C	3.639169	-1.125355	2.429754
C	2.716431	-1.483275	3.406274
C	1.465442	-1.140488	2.862462
N	-1.611996	0.960362	1.466420
N	-2.966351	0.896738	1.196089
C	-3.643949	1.658123	2.103151
C	-2.723295	2.228739	2.974911
C	-1.471842	1.764166	2.531684
N	4.977130	0.102591	-0.126658
N	-4.977282	-0.131530	-0.098991
H	-0.438898	-3.528035	0.483898
H	-4.524591	-2.391147	1.323058
H	-2.754069	-4.454016	1.674228
H	4.713177	-1.216499	2.389931
H	2.924996	-1.928771	4.369066
H	0.475854	-1.251914	3.286217
H	-0.483417	1.967274	2.922841
H	-2.933466	2.886185	3.807128
H	-4.717315	1.741980	2.037767
H	-0.519562	1.552538	-3.230825
H	-3.032970	1.907781	-4.328935
H	-4.719500	0.936591	-2.403641
H	0.518297	-2.237715	-2.800477
H	3.033059	-2.857884	-3.770560
H	4.720004	-1.478241	-2.113852
H	0.443503	3.551413	-0.328554
H	2.768441	4.723918	0.595857
H	4.535018	2.632186	0.722435
N	5.837843	-0.796735	0.473139
C	7.039137	-0.554851	-0.062888
C	6.987092	0.478999	-1.028735
C	5.658474	0.865028	-1.046364
H	5.152790	1.607482	-1.646043
H	7.794665	0.887443	-1.621183
H	7.895382	-1.130166	0.267735
C	-5.657692	-1.090944	-0.811675
C	-6.986115	-0.711495	-0.888401
C	-7.038892	0.522693	-0.196678
N	-5.838167	0.885216	0.267842
H	-7.895228	1.160528	-0.014170
H	-7.793137	-1.249186	-1.367591
H	-5.151719	-1.955276	-1.215988

Model 14

39

Cd	-0.007735	-0.917485	0.040310
C	-2.888044	-0.912998	0.912895
S	-2.348960	-1.997699	-0.355439
S	2.322672	-2.012235	0.459539
C	2.871984	-0.961675	-0.832948
N	4.162881	-0.988533	-1.232913
N	-4.179533	-0.917523	1.311919
S	-1.732741	0.173767	1.662206
S	1.727724	0.120899	-1.604920
C	4.690986	-0.160041	-2.346854
C	5.924854	0.651746	-1.902338
H	4.964142	-0.843209	-3.167096
H	3.893184	0.493412	-2.700501
C	7.014415	-0.258005	-1.296816
H	6.312717	1.196893	-2.773702
H	5.608789	1.402170	-1.163813
C	6.422434	-1.138740	-0.176443
H	7.431740	-0.903091	-2.086120
H	7.845006	0.346286	-0.909348
C	5.177325	-1.909959	-0.659820
H	7.164058	-1.867048	0.179169
H	6.141693	-0.514465	0.683737
H	5.459168	-2.624666	-1.449685
H	4.716296	-2.468632	0.154945
C	-4.700064	-0.059466	2.406957
C	-5.925810	0.754253	1.943836
H	-4.980134	-0.721604	3.241997
H	-3.896081	0.593871	2.746517
C	-7.023851	-0.158211	1.358006
H	-6.308735	1.322657	2.802495
H	-5.602192	1.484921	1.188954
C	-6.439984	-1.068911	0.257527
H	-7.447486	-0.781805	2.161106
H	-7.848557	0.445254	0.956947
C	-5.202570	-1.841366	0.758345
H	-7.188415	-1.797684	-0.082531
H	-6.152909	-0.466315	-0.615924
H	-5.491589	-2.536109	1.563290
H	-4.746622	-2.421951	-0.043866

(For models 15 and 16 contributions of several configurational isomers has been taken into account. The corresponding averaged weights are also given together the relevant coordinates. Models contributing up to 1% have been neglected)

Model 15A avgd weight 33%

45			
Cd	-0.008028	-0.863676	0.036512
C	5.216813	-1.716167	-0.399299
N	4.228304	-0.778082	-0.997344
C	4.772726	0.144166	-2.050542
C	6.033604	0.872023	-1.515377
C	7.093325	-0.079737	-0.923332
C	6.449434	-0.975861	0.152223
C	2.910696	-0.827088	-0.697323
S	2.310966	-1.945307	0.516601
S	-2.337936	-1.932884	-0.417884
C	-2.925767	-0.781538	0.770681
S	-1.777222	0.279644	1.567502
H	4.712684	-2.277946	0.387710
N	-4.242394	-0.712604	1.071122
C	-5.241585	-1.653991	0.496360
C	-6.467976	-0.913921	-0.069189
C	-7.100476	0.012631	0.987183
C	-6.029958	0.966854	1.555342
C	-4.775256	0.238610	2.104259
H	-4.744904	-2.238363	-0.278814
S	1.772793	0.225793	-1.520084
C	4.989825	-0.601395	-3.385716
H	3.996715	0.895108	-2.212895
H	6.457403	1.467773	-2.335371
H	5.715069	1.580422	-0.736926
H	7.529524	-0.707033	-1.715051
H	7.919454	0.502294	-0.493893
H	7.163910	-1.724688	0.520914
H	6.144624	-0.365491	1.014715
H	5.522730	-2.432268	-1.177206
C	-4.996793	-0.474438	3.456364
H	-3.991383	0.985169	2.248067
H	-6.445894	1.585235	2.362494
H	-5.706103	1.654192	0.760389
H	-7.541106	-0.592235	1.793767
H	-7.921737	0.593072	0.546405
H	-7.190747	-1.663614	-0.419471
H	-6.159014	-0.326197	-0.945821
H	-5.552920	-2.349341	1.290777
H	-5.302305	0.262976	4.209795
H	-5.774131	-1.246223	3.406640
H	-4.064858	-0.940789	3.795977
H	5.304280	0.115760	-4.154862
H	5.759274	-1.379606	-3.316840
H	4.053946	-1.065931	-3.716839

Model 15B avgd weight 35%

45			
Cd	0.037175	-0.746877	0.055848
C	-4.808674	0.423402	1.886994
N	-4.222837	-0.590888	0.968935
C	-5.184879	-1.621964	0.452477
C	-6.432110	-0.927263	-0.152835
C	-7.083068	0.106488	0.789363
C	-6.027240	1.125781	1.259628
C	-2.897508	-0.650528	0.706953
S	-1.797646	0.538010	1.384646
S	1.811295	0.057379	-1.669533
C	2.953509	-0.831058	-0.676277
S	2.366584	-1.686048	0.740340
H	-4.026989	1.142248	2.134803
S	-2.252648	-1.923023	-0.316387
N	4.266293	-0.857600	-1.000971
C	5.257328	-1.663520	-0.236776
C	6.522140	-0.851517	0.097560
C	7.145293	-0.233516	-1.168837
C	6.084101	0.592685	-1.924203
C	4.791359	-0.200611	-2.245566
H	4.769802	-2.019065	0.671628
H	-4.660191	-2.134077	-0.356915
C	4.946902	-1.226967	-3.389924
H	4.024040	0.516403	-2.545248
H	6.490023	0.979609	-2.868895
H	5.808918	1.464454	-1.313075
H	7.540382	-1.031840	-1.814623
H	7.997273	0.406576	-0.904130
H	7.234710	-1.518564	0.601910
H	6.259923	-0.056765	0.811007
H	5.521949	-2.545175	-0.840415
H	-5.102561	-0.085013	2.817824
H	-6.449179	1.813717	2.005160
H	-5.690435	1.735319	0.408532
H	-7.526523	-0.396242	1.661754
H	-7.904863	0.617644	0.270594
H	-7.153406	-1.706335	-0.435333
H	-6.126475	-0.422342	-1.080628
C	-5.508962	-2.671733	1.538648
H	5.245914	-0.704861	-4.307930
H	5.704840	-1.989562	-3.174289
H	3.991884	-1.729733	-3.580804
H	-6.139883	-3.458745	1.105857
H	-4.586280	-3.137942	1.902908
H	-6.044392	-2.244484	2.394931

Model 15C avgd weight 32%

45			
Cd	0.036302	-0.586123	-0.073602
C	-4.708422	0.165335	2.191762
N	-4.182733	-0.619287	1.041398
C	-5.173203	-1.534817	0.379666
C	-6.465845	-0.752897	0.028917
C	-7.055069	0.033949	1.217472
C	-5.976612	0.955139	1.819203
C	-2.874027	-0.611439	0.699594
S	-1.738800	0.438236	1.532033
S	1.824222	0.385997	-1.697379
C	2.946006	-0.662751	-0.845721
S	2.343190	-1.676884	0.453451
H	-3.917010	0.834111	2.531412
S	-2.284300	-1.657181	-0.580444
N	4.254297	-0.694605	-1.187615
C	5.231962	-1.612059	-0.509780
C	6.535836	-0.842411	-0.173731
C	7.135531	-0.085704	-1.676542
C	6.070003	0.839890	-1.994343
C	4.790391	0.061746	-2.352047
H	4.761064	-1.899302	0.432554
H	-4.706182	-1.845751	-0.557051
H	4.998141	-0.656728	-3.159861
H	4.008392	0.735565	-2.703344
H	6.446399	1.320430	-2.907737
H	5.815754	1.642556	-1.286862
H	7.494143	-0.796394	-2.136113
H	8.009577	0.495567	-1.054529
H	7.258878	-1.560044	0.237276
H	6.311855	-0.121453	0.625863
C	5.451040	-2.899436	-1.334979
H	-4.926745	-0.535471	3.012213
H	-6.346452	1.457376	2.723543
H	-5.710579	1.741231	1.097588
H	-7.424210	-0.657653	1.989516
H	-7.920506	0.621846	0.884417
H	-7.198934	-1.467421	-0.369523
H	-6.231253	-0.049803	-0.783450
C	-5.410891	-2.803850	1.227820
H	6.101057	-3.583959	-0.774891
H	4.494464	-3.405541	-1.508344
H	5.923225	-2.706091	-2.305611
H	-6.070535	-3.488941	0.679824
H	-4.461687	-3.320404	1.410657
H	-5.880434	-2.586417	2.194642

Model 16A avgd weight 33%

45

Cd	3.605132	-4.210370	1.944666
C	5.942225	-8.712768	3.555013
N	5.771692	-7.332973	4.074201
C	6.438355	-7.119010	5.382075
C	5.922589	-8.105569	6.457078
C	6.068705	-9.561334	5.957828
C	5.421985	-9.749639	4.570017
C	5.102262	-6.363485	3.411271
S	4.367562	-6.699790	1.854382
S	3.810799	-2.267057	0.222690
C	2.093086	-2.050773	0.503485
S	1.264234	-3.113177	1.626301
H	4.329993	-9.653147	4.647590
S	4.964680	-4.755505	4.097921
N	1.413761	-1.076295	-0.141611
C	2.039211	-0.153586	-1.120374
C	1.834164	1.328362	-0.724302
C	0.330267	1.622560	-0.520231
C	-0.314406	0.616301	0.455141
C	-0.041096	-0.840221	0.031443
H	0.079258	0.770467	1.469565
H	2.348693	1.480052	0.237406
H	-1.401490	0.766320	0.503333
C	2.476806	2.258252	-1.772034
H	5.419531	-8.792719	2.601715
H	3.100307	-0.395361	-1.194984
H	7.521074	-7.265648	5.232404
H	6.275169	-6.085276	5.689554
C	6.648090	-7.868556	7.796067
H	4.851053	-7.896076	6.600406
H	7.140709	-9.813884	5.899967
H	5.620279	-10.254168	6.683148
H	5.631325	-10.754496	4.178838
H	7.017392	-8.868049	3.372136
H	-0.528847	-1.052072	-0.933315
H	-0.422833	-1.546930	0.768447
H	-0.181059	1.566324	-1.495776
H	0.194758	2.648804	-0.151915
H	1.574064	-0.343419	-2.102133
H	6.266896	-8.547247	8.569063
H	7.728368	-8.045797	7.698807
H	6.505412	-6.840347	8.151883
H	2.357521	3.309612	-1.482430
H	3.550614	2.059079	-1.878854
H	2.009073	2.127998	-2.758006

Model 16B avgd weight 31%

45

Cd	3.623323	-4.203872	1.973446
C	2.030110	-0.185634	-1.133098
N	1.417738	-1.088577	-0.127129
C	-0.027875	-0.828902	0.080861
C	-0.287566	0.631564	0.522969
C	0.340359	1.614485	-0.491506
C	1.827608	1.291578	-0.743088
C	2.101157	-2.061756	0.515627
S	1.282318	-3.111862	1.657356
S	4.940878	-4.741438	4.151853
C	5.128031	-6.340997	3.456481
S	4.447398	-6.676287	1.875314
H	2.416889	1.504013	0.159946
S	3.814337	-2.287481	0.215522
N	5.792935	-7.304397	4.132525
C	6.387162	-7.100060	5.476236
C	5.840071	-8.120542	6.503498
C	6.051492	-9.561890	5.986359
C	5.483117	-9.739628	4.563388
C	6.025892	-8.668704	3.597074
H	4.386241	-9.674445	4.585280
H	5.740869	-10.730255	4.164778
H	2.229606	1.921895	-1.547958
C	-1.796739	0.874407	0.718616
H	0.215083	0.769454	1.493032
H	5.555056	-8.742442	2.616611
H	3.088367	-0.431713	-1.222535
H	7.479484	-7.217383	5.380879
H	6.182071	-6.077095	5.794403
C	6.484294	-7.892062	7.884695
H	4.757115	-7.941178	6.591378
H	7.131549	-9.785161	5.980562
H	5.584695	-10.280322	6.674293
H	7.112910	-8.791872	3.467142
H	-0.544345	-1.026140	-0.873308
H	-0.404038	-1.534538	0.822697
H	-0.214918	1.550623	-1.442296
H	0.231516	2.646892	-0.131513
H	1.545769	-0.391732	-2.100885
H	6.080641	-8.597233	8.621886
H	7.572911	-8.037648	7.844108
H	6.292924	-6.875922	8.252289
H	-1.983299	1.901462	1.056296
H	-2.347873	0.726067	-0.220623
H	-2.217766	0.192715	1.468531

Model 16c avgd weight 31%

45

Cd	3.685653	-4.126219	1.971125
C	2.008096	-0.151566	-1.143588
N	1.404262	-1.097970	-0.173820
C	-0.057103	-0.900652	-0.005574
C	-0.370805	0.543603	0.431437
C	0.253758	1.575866	-0.529820
C	1.765228	1.320613	-0.730662
C	2.109604	-2.049669	0.477689
S	3.828289	-2.234980	0.183147
S	4.485820	-6.602088	2.028662
C	5.273991	-6.146145	3.528379
S	5.140508	-4.494583	4.102405
C	2.389747	2.279678	-1.762994
N	5.978724	-7.059158	4.233719
C	6.125220	-8.477212	3.823268
C	5.628331	-9.444508	4.925166
C	6.347697	-9.146163	6.260659
C	6.238576	-7.654925	6.640060
C	6.703542	-6.741418	5.489264
S	1.313586	-3.112831	1.624220
H	4.552903	-9.251722	5.062708
H	2.271697	1.472438	0.235298
C	5.806383	-10.908412	4.477367
H	6.848668	-7.435557	7.526809
H	3.075033	-0.365305	-1.219219
H	5.574852	-8.628067	2.893694
H	-0.533108	-1.114582	-0.975657
H	-0.425020	-1.624733	0.721452
H	-1.461660	0.665335	0.474471
H	0.012805	0.696974	1.449803
H	-0.251846	1.518387	-1.508296
H	0.091781	2.594296	-0.150691
H	1.549111	-0.342499	-2.127846
H	7.777867	-6.891386	5.297217
H	6.543359	-5.689639	5.726752
H	7.410879	-9.422940	6.163965
H	5.930244	-9.773155	7.060559
H	7.194125	-8.659479	3.622709
H	2.242634	3.323831	-1.460167
H	3.468769	2.108988	-1.866298
H	1.930493	2.150959	-2.753012
H	5.198458	-7.405737	6.892581
H	5.430113	-11.596637	5.244357
H	5.260858	-11.111661	3.547183
H	6.865924	-11.145229	4.306729

Model 17

63

Cd	-0.002040	0.002283	-0.227365
C	1.633343	1.684390	2.229040
C	3.703429	1.682518	1.369738
C	2.969117	2.028038	2.508116
C	3.704370	-1.822977	-1.539627
C	2.969412	-3.007487	-1.657107
C	1.631448	-2.666889	-1.391265
C	5.181910	-1.616065	-1.727169
C	0.409992	-3.542985	-1.413956
C	5.178225	1.845425	1.124832
C	0.414871	1.861380	3.092081
C	-1.620039	2.660742	-1.427715
C	-2.956026	3.008080	-1.691813
C	-3.701413	1.832900	-1.545045
C	-5.181536	1.635925	-1.722503
C	-0.397435	3.535638	-1.429653
C	-3.706802	-1.680258	1.375325
C	-2.966559	-2.039993	2.505668
C	-1.631003	-1.701464	2.220625
C	-0.406754	-1.898645	3.070876
C	-5.183955	-1.833697	1.138773
N	1.563355	1.161100	0.986430
N	2.841462	1.155661	0.456752
N	1.560661	-1.342646	-1.134276
N	2.839941	-0.822728	-1.218564
N	-1.558985	1.340628	-1.147407
N	-2.843771	0.830846	-1.212653
N	-1.566458	-1.167146	0.981913
N	-2.848396	-1.150897	0.460839
B	3.069546	0.718649	-1.037406
B	-3.083438	-0.709629	-1.031504
H	2.247186	1.293293	-1.717675
H	4.194250	0.990452	-1.356848
H	3.355234	2.478831	3.413664
H	-0.482005	1.473470	2.599926
H	0.529392	1.341601	4.051243
H	0.244229	2.922117	3.315010
H	5.376438	2.503144	0.270708
H	5.651495	2.278986	2.011287
H	5.662845	0.884567	0.914817
H	3.355916	-3.986122	-1.911717
H	-0.311621	-3.247245	-0.645554
H	-0.101669	-3.483421	-2.383406
H	0.687423	-4.588517	-1.245204
H	5.390740	-0.889563	-2.520728
H	5.659273	-1.245543	-0.811939
H	5.653997	-2.566066	-1.996000
H	-3.334090	3.984545	-1.966454
H	-0.621265	4.495499	-1.905057
H	-0.046227	3.737482	-0.409649
H	0.431073	3.065656	-1.970877
H	-5.656523	1.278453	-0.800891
H	-5.647392	2.587078	-1.997955
H	-5.400728	0.903246	-2.507558
H	-3.348836	-2.497560	3.409440
H	-2.271260	-1.290186	-1.717864
H	-4.213388	-0.971097	-1.340971
H	-0.515884	-1.403656	4.043573
H	-0.233749	-2.964661	3.265240
H	0.486702	-1.497893	2.582847
H	-5.653438	-2.273539	2.024124
H	-5.665249	-0.868612	0.940905
H	-5.390611	-2.482247	0.279685

Model 18

63

Cd	0.321754	0.102304	-0.013942
S	2.571285	-1.330405	0.721611
S	2.525518	1.325632	-0.712095
B	-2.991967	-0.122364	0.042549
N	-1.073382	-1.392391	-1.119508
N	-2.428797	-1.247822	-0.885364
N	-1.342813	1.702322	-0.690960
N	-2.651809	1.287628	-0.528090
N	-1.115860	-0.136707	1.812790
N	-2.458536	-0.269997	1.504082
N	4.782672	0.005544	-0.057944
C	-0.912896	-2.430819	-1.958874
C	-2.175304	-2.972586	-2.276056
C	-3.111179	-2.205027	-1.584468
C	0.443977	-2.851043	-2.451417
C	-4.607640	-2.356744	-1.569068
C	-1.379095	2.949680	-1.193256
C	-2.720121	3.353153	-1.358507
C	-3.501580	2.281514	-0.928769
C	-0.126319	3.721444	-1.509250
C	-5.001926	2.180103	-0.887806
C	-0.988021	-0.291774	3.142903
C	-2.256853	-0.531755	3.709181
C	-3.163498	-0.511788	2.651014
C	0.340816	-0.171543	3.835751
C	-4.652772	-0.717871	2.700240
C	5.550011	1.093828	-0.713667
C	5.954895	2.222186	0.252136
C	5.603685	-1.070344	0.551509
C	5.963101	-2.194669	-0.436294
C	3.426897	-0.008863	-0.014589
H	-4.178697	-0.235890	0.073151
H	-2.383309	-3.815890	-2.922257
H	1.222706	-2.611537	-1.719502
H	0.466884	-3.929556	-2.641725
H	0.697224	-2.342789	-3.391723
H	-4.990531	-2.552916	-0.560473
H	-5.114694	-1.459676	-1.943871
H	-4.892948	-3.197842	-2.208323
H	-3.077234	4.301474	-1.739932
H	0.448028	3.243074	-2.312404
H	-0.379075	4.735930	-1.832841
H	0.531887	3.795810	-0.635765
H	-5.438521	3.110069	-1.264791
H	-5.375712	1.356029	-1.507337
H	-5.375346	2.020432	0.130913
H	-2.487313	-0.700236	4.753487
H	1.164401	-0.441193	3.166540
H	0.511133	0.856479	4.183706
H	0.377804	-0.827085	4.712738
H	-5.201152	0.155807	2.328414
H	-4.967394	-1.581695	2.102506
H	-4.959775	-0.894161	3.735703
H	4.940564	1.494570	-1.527336
H	6.442316	0.634185	-1.156285
H	6.541755	2.976131	-0.288654
H	5.066299	2.709096	0.668153
H	6.569543	1.844702	1.078791
H	5.047027	-1.477998	1.398600
H	6.514949	-0.597477	0.938063
H	6.593818	-2.938884	0.067285
H	5.056438	-2.694988	-0.792996
H	6.518393	-1.810729	-1.301183

Model 19

75				H	0.494205	0.056440	5.253010
				H	1.551494	0.361723	3.038504
				H	-4.750317	-0.528088	4.273160
				H	-5.544654	-0.747935	2.699985
				H	-3.879593	-1.333324	2.950113
Cd	0.310681	0.014856	-0.196569				
C	1.679554	-0.574908	3.571620				
C	2.455032	-1.597100	2.994660				
C	2.636752	-2.791061	3.721989				
C	2.056396	-2.958360	4.981751				
C	1.279608	-1.935832	5.540622				
C	1.093276	-0.745550	4.828636				
C	3.116189	-1.425556	1.686538				
C	4.605891	-1.441943	0.033639				
C	4.409302	-1.883557	1.330079				
C	-2.513057	0.608158	0.790460				
C	-4.021801	0.835256	2.754888				
C	-4.587184	-0.531518	3.187000				
C	0.334108	-2.213908	-2.861578				
C	1.166019	-2.408136	-3.991246				
C	2.315376	-1.679663	-3.729381				
C	-0.976556	-2.834589	-2.597697				
C	-1.850219	-3.119762	-3.665554				
C	-3.075945	-3.749907	-3.438325				
C	-3.453675	-4.106502	-2.137887				
C	-2.593990	-3.827781	-1.069060				
C	-1.366135	-3.201547	-1.295747				
C	3.389509	2.332999	-2.371681				
C	2.673649	3.486566	-2.097583				
C	1.620500	3.079349	-1.242759				
C	0.598532	3.940120	-0.617926				
C	0.132598	3.704826	0.688598				
C	-0.810941	4.553328	1.273210				
C	-1.303837	5.656713	0.567295				
C	-0.844814	5.904638	-0.732221				
C	0.096964	5.055469	-1.318056				
C	-4.794594	1.509050	0.438007				
C	-5.697742	0.451372	-0.224120				
N	2.562169	-0.752595	0.648900				
N	3.494832	-0.765396	-0.365270				
N	-3.722309	0.953441	1.305289				
N	2.178956	-1.073607	-2.521128				
N	0.957040	-1.394840	-1.979920				
N	1.703029	1.743819	-1.029884				
N	2.798914	1.292296	-1.726954				
S	-1.263025	-0.011740	1.869704				
S	-2.182164	0.773565	-0.899097				
B	3.233323	-0.197597	-1.780623				
H	5.453484	-1.548704	-0.628331				
H	3.223638	-1.563498	-4.303401				
H	4.279524	2.178298	-2.964553				
H	-3.094917	1.035457	3.300596				
H	4.253079	-0.253753	-2.409602				
H	0.971300	-3.037261	-4.847662				
H	5.111115	-2.416272	1.955556				
H	2.900146	4.491334	-2.423568				
H	-4.736150	1.631088	2.996554				
H	-4.307613	2.110859	-0.334874				
H	-5.393453	2.178378	1.066730				
H	-6.427911	0.956171	-0.870795				
H	-5.103804	-0.228277	-0.844094				
H	-6.250427	-0.135727	0.518372				
H	-1.571705	-2.830137	-4.675698				
H	-3.738496	-3.957305	-4.275567				
H	-4.407196	-4.598673	-1.960285				
H	-2.873715	-4.105668	-0.055808				
H	-0.694604	-3.018608	-0.461922				
H	0.522847	2.865014	1.255643				
H	-1.154975	4.354616	2.285515				
H	-2.036228	6.318007	1.024896				
H	-1.225328	6.755637	-1.292571				
H	0.434461	5.243456	-2.334209				
H	3.223764	-3.596088	3.286812				
H	2.204764	-3.889579	5.523937				
H	0.825890	-2.065710	6.520512				

Model 20

98

Cd	-0.744677	0.133757	0.107364	H	-2.638964	-0.476560	-4.279776
N	2.093290	1.221549	-0.434822	H	-3.120571	-0.730299	-2.603193
N	0.971913	1.752912	0.166487	H	-1.705566	0.276749	-2.966441
C	1.082461	3.133050	0.075691	H	-1.557757	-0.467950	4.699721
C	2.284713	3.438959	-0.659016	H	-0.803706	0.387188	3.333851
C	2.881193	2.235001	-0.927096	H	-1.986568	-0.890297	3.032612
O	-2.473925	-1.214268	0.676229	H	-1.006800	-3.129920	4.866009
C	-3.729323	-1.027972	0.512917	H	0.739378	-3.372506	4.695225
C	-4.336755	0.154973	0.031057	H	0.104839	-2.112403	5.776021
C	-3.705951	1.352830	-0.374287	H	-1.136806	4.365494	2.366638
C	-4.613537	2.536890	-0.864129	H	-1.700437	3.138073	1.214916
C	-5.483711	3.036910	0.324677	H	-0.406875	2.740352	2.347253
C	0.212322	4.024718	0.723934	H	-0.679067	5.924394	0.230624
C	-0.808482	3.545292	1.715681	H	0.621763	6.034726	1.411126
B	2.464451	-0.297010	-0.415241	H	1.003512	5.775763	-0.305100
N	2.165205	-0.922321	0.971823	N	4.937956	-0.199387	0.141552
C	2.907072	-1.883935	1.627645	C	6.127374	-0.152169	-0.555900
C	2.188416	-2.352690	2.690404	C	5.853897	-0.338385	-1.966240
C	0.946735	-1.612349	2.695399	C	4.496144	-0.500669	-2.060018
N	0.945026	-0.762898	1.589804	H	3.866043	-0.645987	-2.925104
C	-0.047054	-1.609895	3.677112	H	6.556944	-0.354251	-2.786849
C	-1.152628	-0.592211	3.686925	C	7.361407	0.052101	0.092922
N	0.339884	-0.798743	-1.788419	C	8.656842	0.101371	-0.665320
N	1.649073	-1.112474	-1.466223	C	7.438708	0.230538	1.581961
C	1.954258	-2.376550	-1.922047	H	7.942901	1.177721	1.839425
C	0.880579	-2.885986	-2.597785	H	6.449610	0.226177	2.044848
C	-0.146435	-1.868903	-2.549421	H	8.045914	-0.567082	2.045430
C	-1.370207	-1.849972	-3.221734	H	9.172619	1.064616	-0.507150
C	-2.242062	-0.628162	-3.263312	H	9.357097	-0.673048	-0.306040
O	-2.444286	1.571689	-0.371097	H	8.532801	-0.037209	-1.742718
C	-3.741746	3.707988	-1.375555				
C	-5.540211	2.068296	-2.021141				
C	-1.870017	-3.054113	-3.974076				
C	-0.036620	-2.610228	4.801349				
C	0.307022	5.507263	0.493588				
C	-4.661113	-2.231057	0.897813				
C	-5.503584	-2.663919	-0.335554				
C	-3.812943	-3.436085	1.367639				
C	-5.614464	-1.804552	2.050270				
H	3.910127	-2.110478	1.302182				
H	3.824771	2.024558	-1.407483				
H	2.928857	-2.806491	-1.742813				
N	3.958762	-0.435572	-0.785387				
H	2.524851	-3.075602	3.418890				
H	2.686013	4.414863	-0.889034				
H	0.841910	-3.834845	-3.112272				
H	-5.418939	0.140645	-0.034988				
H	-6.100225	3.888991	0.005026				
H	-6.153996	2.253486	0.696800				
H	-4.854560	3.368610	1.160793				
H	-4.390908	4.521710	-1.725566				
H	-3.092199	4.099987	-0.587059				
H	-3.098318	3.395831	-2.205109				
H	-6.140743	2.915391	-2.381041				
H	-4.953561	1.686051	-2.866101				
H	-6.231423	1.279221	-1.704944				
H	-6.243758	-2.655029	2.348197				
H	-5.046454	-1.478534	2.931199				
H	-6.275933	-0.982819	1.752852				
H	-6.131294	-3.527063	-0.073124				
H	-6.163460	-1.862241	-0.685888				
H	-4.855213	-2.958337	-1.170585				
H	-4.475993	-4.274028	1.621344				
H	-3.118017	-3.763975	0.587748				
H	-3.216953	-3.186952	2.251597				
H	-2.888450	-3.322062	-3.646149				
H	-1.946590	-2.846343	-5.055564				
H	-1.240493	-3.938518	-3.845458				

Model 21

89

Cd	-0.226671	-0.352720	0.204251	H	5.744798	-0.137231	0.828273
C	0.239066	-1.801899	-3.199231	H	4.498627	0.962640	1.465008
C	0.584958	-3.017212	-2.579025	H	4.114484	-0.750946	1.206773
C	1.553131	-3.832596	-3.198384	H	5.583186	-1.077823	-1.516597
C	2.157905	-3.443296	-4.395824	H	3.949936	-1.704243	-1.172448
C	1.808807	-2.228861	-4.998966	H	4.220477	-0.656707	-2.581189
C	0.847989	-1.410571	-4.393966	H	6.128299	1.362012	-1.113476
C	-0.064971	-3.462713	-1.332716	H	4.839436	1.820315	-2.234859
N	-0.502722	-2.606521	-0.380004	H	4.885022	2.513369	-0.595973
N	-1.092772	-3.361910	0.604821	H	1.239467	5.256019	-3.092214
C	-1.021568	-4.677873	0.271209	H	2.190023	4.667516	-1.718151
C	-0.372585	-4.790782	-0.947328	H	2.278160	3.836621	-3.288335
O	-0.241474	1.475687	-1.029849	H	-0.723043	3.957052	-4.004264
C	0.785292	2.152692	-1.430049	H	0.281197	2.497559	-4.158801
C	2.138688	1.806705	-1.267419	H	-1.234490	2.439667	-3.226279
C	2.683372	0.644501	-0.655246	H	-0.873666	5.204746	-1.793941
C	4.231423	0.408370	-0.649950	H	-1.415660	3.719130	-0.974315
B	-1.728297	-2.756236	1.886066	H	-0.010638	4.616567	-0.356416
N	-0.666484	-2.073333	2.799425				
C	-0.235395	-2.487238	4.019474				
C	0.633204	-1.534597	4.527940				
C	0.689350	-0.516189	3.544989				
N	-0.097042	-0.859740	2.497427				
C	1.404041	0.770159	3.624316				
C	0.886395	1.934128	3.024336				
C	1.553827	3.155498	3.144091				
C	2.745727	3.241666	3.872933				
C	3.267566	2.092437	4.479435				
C	2.604414	0.869483	4.355005				
C	0.399788	3.468905	-2.186711				
O	2.008694	-0.285868	-0.103796				
N	-2.670038	-0.666352	0.684724				
C	-3.835904	0.024028	0.702133				
C	-4.754974	-0.599016	1.582319				
C	-4.089444	-1.706506	2.077236				
N	-2.843189	-1.740359	1.534188				
C	-4.114902	1.196250	-0.150699				
C	-3.711793	1.237057	-1.497687				
C	-4.075687	2.308589	-2.317285				
C	-4.840007	3.364088	-1.806818				
C	-5.238372	3.340547	-0.464802				
C	-4.882142	2.265467	0.353617				
H	-0.592194	-3.415029	4.443603				
H	-1.447291	-5.432431	0.916892				
H	-4.413190	-2.477818	2.761572				
H	-2.213122	-3.658457	2.509753				
H	1.117225	-1.541071	5.493700				
H	-0.185437	-5.695613	-1.506990				
H	-5.777197	-0.305951	1.774368				
H	-0.056869	1.887590	2.487358				
H	1.134745	4.042979	2.676337				
H	3.261174	4.194373	3.969984				
H	4.195380	2.147043	5.044268				
H	3.026896	-0.021445	4.812351				
H	1.845143	-4.767226	-2.726332				
H	2.907561	-4.084351	-4.853885				
H	2.280103	-1.924215	-5.930539				
H	0.565026	-0.467898	-4.855781				
H	-0.524913	-1.169329	-2.756491				
H	-5.192131	2.253118	1.395737				
H	-5.827150	4.158324	-0.055417				
H	-5.124089	4.195099	-2.448312				
H	-3.769738	2.315472	-3.360417				
H	-3.135475	0.411759	-1.904563				
H	2.854777	2.504951	-1.672316				
C	4.510695	-0.838024	-1.538145				
C	5.058922	1.602689	-1.182435				
C	4.672292	0.101184	0.807515				
C	-0.537546	4.300967	-1.267274				
C	1.605970	4.350356	-2.590566				
C	-0.369490	3.060694	-3.475844				

Model 22

85

Cd	0.070518	-0.678435	0.278650	H	-4.221737	6.008904	0.451791
C	-4.007855	2.152629	0.826438	H	-6.224729	4.720501	1.184769
C	-2.873098	2.864449	0.392329	H	-6.073812	2.243624	1.430187
C	-2.972016	4.263798	0.263251	H	-3.928819	1.076195	0.937539
C	-4.168769	4.926958	0.549115	C	1.606432	3.040139	-1.808331
C	-5.292832	4.203981	0.965585	C	1.147851	3.989088	-2.742651
C	-5.206267	2.813268	1.104115	C	2.050453	4.782703	-3.457048
C	-1.608787	2.089265	0.104479	C	3.427562	4.651359	-3.240176
C	-0.584714	2.699962	-0.660675	C	3.894287	3.708976	-2.315424
C	0.666405	2.162233	-1.019097	C	2.993143	2.902635	-1.615019
O	1.128244	0.991944	-0.728329	H	0.082723	4.090017	-2.932565
N	-1.495057	-2.157966	-0.706962	H	1.678890	5.499841	-4.185565
C	-2.567243	-2.102307	-1.531983	H	4.129403	5.274780	-3.789771
C	-3.381290	-3.242915	-1.323744	H	4.962245	3.600541	-2.139687
C	-2.731330	-3.984879	-0.351119	H	3.350335	2.160369	-0.908400
N	-1.600345	-3.324538	0.013332				
C	-2.759079	-1.037661	-2.533909				
C	-1.663318	-0.441728	-3.186701				
C	-1.860804	0.527386	-4.173507				
C	-3.156629	0.915829	-4.532669				
C	-4.255121	0.328526	-3.893376				
C	-4.058317	-0.637849	-2.904170				
B	-0.524129	-3.802066	1.021363				
N	-0.519154	-2.973701	2.341255				
C	-0.609351	-3.478455	3.599791				
C	-0.320339	-2.470671	4.503236				
C	-0.048565	-1.324846	3.716438				
N	-0.174901	-1.641253	2.403960				
C	0.338131	0.010259	4.212674				
C	-0.112056	1.195036	3.602915				
C	0.265297	2.441715	4.111799				
C	1.088681	2.528476	5.239650				
C	1.535283	1.355085	5.860036				
C	1.164200	0.108499	5.351472				
N	1.505621	-2.630102	-0.088260				
N	0.891647	-3.772716	0.385446				
C	1.759776	-4.817384	0.333027				
C	2.962646	-4.366356	-0.179516				
C	2.765397	-2.987692	-0.439529				
C	3.754683	-2.074551	-1.044439				
C	5.119109	-2.215340	-0.716098				
C	6.089423	-1.417150	-1.326147				
C	5.715035	-0.463319	-2.280886				
C	4.363657	-0.311855	-2.611248				
C	3.391915	-1.107521	-1.998259				
O	-1.558101	0.907728	0.592528				
H	-0.870918	-4.514970	3.757255				
H	1.454155	-5.802365	0.655797				
H	-2.978628	-4.939201	0.091228				
H	-0.781241	-4.934908	1.317533				
H	-0.334032	-2.531770	5.581619				
H	3.848026	-4.949280	-0.387993				
H	-4.283533	-3.508965	-1.855139				
H	-0.777254	1.139871	2.747026				
H	-0.095877	3.346538	3.629670				
H	1.378186	3.500182	5.633391				
H	2.179159	1.410232	6.734896				
H	1.531964	-0.798361	5.825039				
H	5.414227	-2.947149	0.031671				
H	7.135753	-1.537990	-1.054685				
H	6.469257	0.154683	-2.763186				
H	4.062348	0.426274	-3.349522				
H	2.348888	-0.986680	-2.270893				
H	-4.916391	-1.077670	-2.402096				
H	-5.265849	0.628309	-4.160272				
H	-3.309492	1.667096	-5.304158				
H	-1.000775	0.970245	-4.670046				
H	-0.655195	-0.762065	-2.940115				
H	-0.772550	3.707569	-1.002499				
H	-2.109162	4.848791	-0.040371				

Model 23

71

Cd	-0.387350	-0.205688	0.290449
C	2.269494	1.884677	2.291447
C	2.406657	0.668151	2.987075
C	3.695775	0.257653	3.378404
C	4.814942	1.037853	3.077355
C	4.666925	2.243633	2.381055
C	3.390266	2.663245	1.989454
C	1.226393	-0.133954	3.359592
C	-0.288435	-1.323302	4.480246
C	0.992511	-0.804583	4.583442
C	1.555224	1.581487	-1.551887
C	-1.914033	-3.260115	-0.425937
C	-2.796162	-4.105589	0.287543
C	-2.924840	-3.532621	1.541110
C	-1.465225	-3.438493	-1.821085
C	-0.129704	-3.227615	-2.207375
C	0.267082	-3.434100	-3.532261
C	-0.658946	-3.860972	-4.490267
C	-1.989611	-4.082910	-4.114481
C	-2.389202	-3.874729	-2.792414
C	2.589892	-0.608686	-1.032794
C	-4.146912	0.384255	2.560699
C	-4.526369	1.422644	1.729794
C	-3.452828	1.590731	0.821357
C	-3.386723	2.588833	-0.264674
C	-4.556333	2.891608	-0.992402
C	-4.542306	3.858864	-1.999603
C	-3.358152	4.543620	-2.299677
C	-2.192509	4.252379	-1.583038
C	-2.206344	3.287061	-0.572319
C	2.617004	0.671817	-1.623304
C	3.846599	-1.520537	-1.234319
C	1.736736	2.954753	-2.274679
N	0.140027	-0.264941	2.561134
N	-0.792344	-0.996143	3.261894
N	-2.167817	-2.405737	1.585882
N	-1.536663	-2.229781	0.371690
N	-2.476775	0.690269	1.098471
N	-2.917794	-0.052197	2.178575
O	0.424642	1.475053	-0.983878
O	1.666238	-1.160263	-0.380023
B	-2.203065	-1.325084	2.709923
H	-3.496745	-3.842811	2.403800
H	-4.656282	-0.073535	3.396551
H	-0.882070	-1.882478	5.189135
H	-2.852195	-1.772105	3.612191
H	-3.239344	-5.025879	-0.063996
H	-5.429961	2.012080	1.784957
H	1.650608	-0.849485	5.438993
H	0.602433	-2.927487	-1.465666
H	1.305721	-3.273037	-3.809471
H	-0.346989	-4.023025	-5.519451
H	-2.718090	-4.411500	-4.852099
H	-3.427275	-4.031502	-2.510015
H	-5.474043	2.350188	-0.776694
H	-5.452861	4.071990	-2.554928
H	-3.344584	5.295517	-3.085341
H	-1.268265	4.778158	-1.806693
H	-1.298283	3.082069	-0.016699
H	3.819264	-0.685349	3.904783
H	5.803391	0.701498	3.381140
H	5.537936	2.851787	2.148587
H	3.263778	3.604447	1.459841
H	1.278303	2.234826	2.017034
H	3.512159	0.972555	-2.150698
F	4.234175	-2.093217	-0.067829
F	3.543935	-2.534849	-2.109041
F	4.927042	-0.860114	-1.749450
F	2.999682	3.161708	-2.753680
F	0.881390	3.060581	-3.329864
F	1.459827	3.988530	-1.420347

Model 24

70

Cd	-0.068273	-0.000162	0.526531
C	1.589326	-2.226224	-2.861772
N	0.964111	-1.280207	-2.118841
N	1.063933	-1.606764	-0.780408
C	1.760041	-2.768243	-0.701703
C	2.108308	-3.187780	-2.008152
B	0.270080	0.000634	-2.657275
N	0.964240	1.281030	-2.117975
N	1.063278	1.606862	-0.779331
C	1.759569	2.768058	-0.699656
C	2.108248	3.188523	-2.005698
C	1.590181	2.227199	-2.860099
O	-0.479099	1.117719	2.568014
C	-0.599470	0.000935	3.177241
C	-0.934916	0.000790	4.663741
C	2.072911	3.476236	0.620137
C	0.766965	4.064368	1.229802
C	2.074231	-3.477564	0.617339
C	3.062816	-4.644721	0.356546
N	-1.773229	0.000075	-1.061413
N	-1.251874	0.000767	-2.338399
C	-2.266391	0.000924	-3.237215
C	-3.470247	-0.000216	-2.546986
C	-3.123835	0.000005	-1.175165
C	-4.060984	0.000180	0.033470
C	-3.822782	-1.270435	0.898065
O	-0.471819	-1.116030	2.569582
C	2.731926	-2.496717	1.626820
C	0.768405	-4.064107	1.228790
C	2.727251	2.493590	1.630026
C	3.063718	4.641964	0.361488
C	-3.830371	1.276381	0.892006
C	-5.534735	-0.005309	-0.449669
H	1.624379	-2.145186	-3.938880
H	1.625711	2.146785	-3.937252
H	-2.060872	0.001465	-4.298170
H	0.384459	0.001041	-3.850784
H	2.665709	-4.067839	-2.293169
H	2.665517	4.068912	-2.289892
H	-4.460250	-0.000525	-2.978797
H	-4.520256	-1.279163	1.746868
H	-3.991245	-2.180204	0.307869
H	-2.805075	-1.310987	1.300307
H	-4.528538	1.285330	1.740236
H	-2.813284	1.324594	1.294786
H	-4.003623	2.182237	0.297196
H	-6.206091	-0.005700	0.417936
H	-5.764739	0.882290	-1.051701
H	-5.759244	-0.896557	-1.048370
H	3.300630	5.138905	1.310355
H	4.003299	4.283625	-0.077115
H	2.634466	5.395270	-0.310210
H	1.001947	4.612319	2.152919
H	0.292569	4.762756	0.528417
H	0.051225	3.277059	1.480980
H	2.999598	3.032174	2.547633
H	2.040269	1.690919	1.914497
H	3.636933	2.046103	1.210392
H	1.004028	-4.612916	2.151238
H	0.054244	-3.275844	1.481555
H	0.291816	-4.761386	0.527783
H	3.005076	-3.036516	2.543490
H	3.641611	-2.050426	1.205899
H	2.046817	-1.693189	1.913216
H	3.300476	-5.142509	1.304794
H	2.631366	-5.397034	-0.314863
H	4.002259	-4.287600	-0.083349
H	-0.544503	-0.898524	5.147204
H	-0.546033	0.900975	5.146843
H	-2.027216	0.000041	4.772046

Model 25

97

Cd	-0.000089	-0.000605	0.000051	C	-1.197670	6.551812	-0.514116
O	-2.209485	-0.398832	-0.230848	C	-5.115026	-0.958824	0.265221
O	-0.629746	2.072539	-0.705709	C	-4.438247	-2.193955	0.243262
O	0.083806	-0.647583	-2.418703	C	-5.154502	-3.379983	0.436057
O	2.209406	0.398861	0.224649	C	-6.535964	-3.362832	0.651321
O	0.632031	-2.071945	0.709925	C	-7.203758	-2.132291	0.673466
O	-0.089565	0.645732	2.419219	C	-6.507067	-0.937717	0.483322
H	-0.856406	-0.528977	-2.651760	C	0.899870	0.118775	-3.366025
H	-4.855764	4.301289	-1.158098	C	0.699773	-0.353442	-4.804500
H	-4.427578	4.502763	0.548785	C	3.088490	-0.530475	0.165555
H	-5.983237	3.768802	0.102767	C	2.982683	-1.969687	0.332296
H	-2.757829	4.542363	-1.034295	C	4.343145	-2.447522	0.157901
H	-1.330908	4.209176	-2.006056	C	4.930746	-3.835236	0.184197
H	-1.062273	3.911057	1.779549	C	1.765995	-2.654742	0.645144
H	-2.341154	5.130606	1.586188	C	0.890964	-5.098463	0.084923
H	-0.703109	5.627631	2.045707	C	1.746428	-4.144884	1.000989
H	0.935872	4.966994	-1.291134	C	1.282148	-4.932155	-1.405942
H	0.909383	3.830731	0.066748	C	-0.628496	-4.843669	0.254273
H	1.205008	5.561741	0.362089	C	1.202984	-6.550709	0.535533
H	-0.950867	6.704311	-1.573707	C	5.114286	0.959040	-0.276904
H	-0.609902	7.269540	0.073731	C	4.435986	2.193459	-0.264909
H	-2.260213	6.794031	-0.376365	C	5.150962	3.378780	-0.466605
H	-3.371069	-2.217718	0.076026	C	6.532541	3.361605	-0.681346
H	-4.617642	-4.325765	0.414441	C	7.201831	2.131756	-0.693517
H	-7.083775	-4.290527	0.798096	C	6.506477	0.937928	-0.494136
H	-8.278292	-2.097131	0.839012	C	-0.911441	-0.118054	3.363674
H	-7.021261	0.015361	0.497763	C	-0.715766	0.354226	4.802639
H	1.929490	-0.045403	-3.036545				
H	0.670561	1.187344	-3.259129				
H	1.356168	0.215232	-5.476798				
H	-0.335850	-0.194549	-5.135336				
H	0.939268	-1.418540	-4.904378				
H	0.849350	0.524391	2.656015				
H	4.862089	-4.292507	1.178837				
H	4.434493	-4.504654	-0.526970				
H	5.988829	-3.765516	-0.084985				
H	2.761712	-4.538344	1.049745				
H	1.334051	-4.203039	2.019492				
H	1.071018	-3.918047	-1.767591				
H	2.349354	-5.137086	-1.567614				
H	0.712100	-5.635487	-2.028541				
H	-0.932438	-4.963741	1.303405				
H	-0.904455	-3.832906	-0.058983				
H	-1.198722	-5.565288	-0.347741				
H	0.954316	-6.699635	1.595185				
H	0.616634	-7.270751	-0.050889				
H	2.265890	-6.792887	0.400543				
H	3.368794	2.217312	-0.097865				
H	4.612943	4.324037	-0.452230				
H	7.079298	4.288791	-0.835101				
H	8.276485	2.096532	-0.858360				
H	7.021841	-0.014610	-0.500983				
H	-1.939320	0.048774	3.030141				
H	-0.684427	-1.187242	3.258030				
H	-1.377563	-0.211257	5.472395				
H	0.317687	0.191302	5.138012				
H	-0.951356	1.420344	4.900714				
N	-4.433983	0.277140	0.067693				
N	-5.181347	1.462564	0.085369				
N	4.434713	-0.276208	-0.070744				
N	5.183479	-1.460796	-0.081266				
C	-3.087481	0.531200	-0.166802				
C	-2.980008	1.971135	-0.325886				
C	-4.339692	2.449601	-0.148145				
C	-4.925094	3.838346	-0.166187				
C	-1.763073	2.656441	-0.636971				
C	-0.885575	5.097834	-0.069142				
C	-1.742822	4.147818	-0.987592				
C	-1.274244	4.926364	1.421776				
C	0.633486	4.842872	-0.242006				

Model 26

99				H	-0.177417	-0.986572	5.597914
				H	0.975747	0.213893	4.981536
				H	-0.752650	0.626844	5.109097
Cd	-0.124225	-0.036634	-0.018780	H	2.354990	-3.704058	0.474492
C	-3.346309	3.690284	1.145300	H	5.221360	-2.806242	1.073579
C	-3.577907	2.985214	-0.226579	H	3.911629	-2.989252	2.230818
C	-3.041727	3.870609	-1.385404	H	5.439408	-5.003869	2.167255
C	-3.665495	5.284238	-1.357161	H	3.764953	-5.411682	1.793743
C	-3.447138	5.980528	0.004604	H	6.033256	-5.046564	-0.251606
C	-3.961137	5.108125	1.171225	H	5.269519	-6.571654	0.195816
C	-2.916439	1.598801	-0.220253	H	4.361424	-5.681389	-1.985085
C	-0.281798	-0.703448	3.454522	H	3.100104	-5.822888	-0.760339
C	-0.045124	-0.175489	4.869137	H	4.541292	-3.251563	-1.612707
C	2.893606	0.820232	0.040301	H	2.853167	-3.652201	-1.919610
C	3.454410	-0.508069	-0.163058	H	-4.655066	2.871431	-0.368349
C	4.831407	-0.244988	-0.557491	H	-1.950238	3.942757	-1.297860
C	2.690503	-1.705144	0.067778	H	-3.253711	3.384989	-2.348667
C	3.953830	3.136339	-0.116871	H	-3.237860	5.892274	-2.166592
C	5.189265	3.799101	-0.257319	H	-4.746543	5.213379	-1.558130
C	5.248535	5.192029	-0.188830	H	-2.371419	6.172232	0.143618
C	4.089112	5.948722	0.020136	H	-3.945626	6.959970	0.015256
C	2.864659	5.287872	0.158777	H	-3.736117	5.588626	2.133716
C	2.784356	3.892778	0.092215	H	-5.058490	5.031480	1.109045
C	5.952724	-1.131660	-1.036361	H	-2.263262	3.749407	1.324240
C	3.247358	-3.144868	0.161510	H	-3.768696	3.079876	1.955359
C	3.672164	-3.771197	-1.197326	H	6.210979	5.686729	-0.299221
C	4.014700	-5.270416	-1.026632	H	-6.438516	1.720792	-0.566666
C	5.080283	-5.496543	0.069448	H	-7.137847	0.593034	0.610528
C	4.648190	-4.873205	1.415965	H	-6.048391	1.888187	1.153067
C	4.304692	-3.370479	1.278087				
C	0.372524	0.754348	-3.438000				
C	0.361853	0.270120	-4.886918				
C	-3.123283	-0.939053	-0.082437				
C	-5.096423	0.191639	0.190055				
C	-3.679481	0.401430	-0.048936				
C	-4.236690	-3.221381	0.177881				
C	-5.481844	-3.857156	0.354135				
C	-5.554242	-5.249699	0.417519				
C	-4.398931	-6.032990	0.307522				
C	-3.164998	-5.398835	0.132874				
C	-3.071047	-4.004605	0.067005				
C	-6.238387	1.161216	0.355297				
O	-1.648723	1.611724	-0.364639				
O	-0.171476	0.353934	2.451538				
O	1.726355	1.208580	0.401957				
O	1.430832	-1.667542	0.275351				
O	0.052755	-0.323038	-2.499343				
O	-1.928217	-1.358548	-0.272293				
N	5.097503	1.047685	-0.576167				
N	3.928759	1.713602	-0.201612				
N	-4.196836	-1.798340	0.121107				
N	-5.393421	-1.088475	0.290966				
H	-0.845322	-0.652879	-2.691559				
H	-2.112450	-3.524436	-0.069047				
H	-2.256153	-5.990193	0.045675				
H	-4.460559	-7.117446	0.357123				
H	-6.523986	-5.723176	0.554081				
H	-6.373666	-3.248761	0.440257				
H	1.371283	1.088718	-3.143332				
H	-0.327754	1.587304	-3.289762				
H	0.645935	1.092708	-5.556893				
H	-0.638474	-0.073430	-5.184017				
H	1.070721	-0.554080	-5.028150				
H	0.741887	0.704068	2.450975				
H	6.195861	-1.937174	-0.339697				
H	5.712027	-1.589328	-2.003356				
H	6.841386	-0.507763	-1.170438				
H	1.833250	3.391952	0.203259				
H	1.952755	5.858459	0.320410				
H	4.140491	7.033513	0.073818				
H	6.083838	3.211184	-0.422396				
H	-1.300920	-1.085466	3.343585				
H	0.417198	-1.515165	3.210163				

Table S1 Et₂Cd $\delta(^{113}\text{Cd})$ [$\sigma(\text{CdMe}_2)_{(\text{g})} - \sigma(\text{CdEt}_2)_{(\text{g})}$, ppm] in gas phase calculated by using different NR-1[F/B] protocols. Geometries from OP2. Experimental value: -142.6 ppm⁵³

Basis set/ Functional	DZVP;cc-pvdz	DZVP;6-31G(d,p)	DZVP;6-311G+	Sadleji;cc-pvdz	Sadleji;6-31G(d,p)	Sadleji;6-311G+
B3PW91	-140.2	-142.9	-132.8	-111.8	-109.3	-106.9
BLYP	-153.0	-155.4	-148.2	-123.6	-120.6	-120.0
PBEPBE	-153.6	-155.8	-147.215	-122.8	-119.8	-118.5
VSXC	-146.3	-147.5	-140.2	-116.4	-112.8	-111.4
THCTH	-144.0	-145.3	-137.2	-117.2	-114.0	-112.1
M06L	-119.2	-123.7	-115.4	-88.5	-85.1	-84.5
B97D	-145.7	-147.5	-134.0	-118.4	-115.2	-113.8
B3LYP	-142.6	-145.2	-137.2	-115.6	-113.3	-111.8
mPW1PW91	-138.0	-140.6	-131.4	-110.0	-107.4	-105.6
PBE1PBE	-140.3	-142.9	-133.3	-112.5	-110.2	-108.0
HSEH1PBE	-140.3	-142.9	-133.5	-112.2	-109.9	-107.7
TPSSH	-140.9	-143.3	-133.9	-110.7	-107.6	-106.1
M062X	-132.1	-135.5	-125.2	-109.7	-108.6	-104.8
THCTHhyb	-142.7	-145.0	-135.9	-115.0	-112.1	-110.3
LC-WPBE	-130.7	-134.0	-122.5	-103.5	-102.0	-97.8
CAM-B3LYP	-137.9	-140.6	-131.8	-112.3	-110.5	-107.8
WB97XD	-134.3	-137.2	-127.5	-107.7	-105.3	-102.6

Table S2 Calculated $\sigma(^{113}\text{Cd})$ used for the $\delta(^{113}\text{Cd})$ of Table 2. In parentheses are given the spinorbit contributions according to the ZORA approximation.

	NR1-BLYP ^a	NR2-BLYP ^b	RS-BLYP ^b	SO1-BLYP ^b	NR3-BLYP	DC-BLYP
OP1						
Me₂Cd	2902.5	3007.8	2959.1	3370.5	2987.4	3671.8
	3073.0			(420.98)		
	2926.4			3352.7		
	3095.8			(414.63)		
			3286.6			
			(428.97)			
Et₂Cd	3057.9	3155.3	3102.4	3522.0	3132.3	3827.1
	3193.6			(429.18)		
	3079.4			3498.0		
	3219.4			(421.62)		
			3443.1			
			(439.07)			
OP2						
Me₂Cd	2905.97	3010.9	2961.8	3373.3	2990.8	3048.0
	3077.05			(421.48)		
	2929.87			3355.8		
	3099.30			(415.14)		
			3290.4			
			(429.60)			
Et₂Cd	3061.86	3159.2	3105.7	3525.7	3136.2	3183.3
	3197.99			(429.63)		
	3083.49			3502.2		
	3223.35			(422.27)		
			3447.8			
			(439.80)			
OP3						
Me₂Cd	2959.1	3065.2	3018.8	3431.3	3044.7	3738.7
	3128.2			(422.31)		
	2983.7			3414.8		
	3151.1			(416.33)		
			3351.8			
			(431.51)			
Et₂Cd	3109.5	3209.0	3159.2	3580.2	3185.9	3897.0
	3242.6			(430.69)		
	3131.6			3556.9		
	3270.7			(423.46)		
			3504.5			
			(441.52)			
	NR1-B3LYP	NR2-B3LYP	RS2-B3LYP	SO2-B3LYP	NR3-B3LYP	DC-B3LYP
OP1						
Me₂Cd	2974.1	3067.8	3013.2	3455.8	3044.7	3754.5
	3123.6			(452.21)		
	2993.8			3435.1		
	3144.2			(445.17)		
			3381.7			
			(466.18)			
Et₂Cd	3119.3	3205.6	3147.2	3597.6	3179.4	3900.3
	3236.9			(459.91)		
	3136.4			3569.7		
	3259.8			(451.81)		
			3527.5			
			(475.75)			
OP2						
Me₂Cd	2977.4	3070.9	3016.1	3458.9	3048.0	3756.0
	3127.6			(452.34)		
	2997.2			3437.8		
	3147.6			(445.31)		
			3385.1			
			(466.35)			
Et₂Cd	3123.1	3209.4	3150.6	3601.1	3183.3	3904.0

	3241.3			(459.95)		
	3140.5	3219.7	3135.2	3573.7		
	3263.7	3186.9	3085.6	(452.07)		
				3531.6		
				(475.98)		
OP3						
	3048.4			3514.8		
	3079.1	3122.6	3069.9	(455.67)		
Me₂Cd	3176.1	3135.4	3060.4	3495.2	3099.6	3819.74
	3196.7	3101.8	3005.9	(448.01)		
				3445.5		
				(469.99)		
				3654.1		
	3186.0			(462.60)		
	3308.3	3256.68	3201.1	3587.3		
Et₂Cd	3220.3	3266.50	3185.7	(454.89)	3230.4	3962.6
	3285.5	3234.66	3137.6	3626.9		
				(479.56)		

^a In the entry(are given the results obtained with, from top to bottom, DZVP (Cd)/6-31G(d,p) (H,C), Sadlej (Cd)/6-31G(d,p) (H,C), DZVP (Cd)/cc-pvdz (H,C) and Sadlej (Cd)/cc-pvdz (H,C) gaussian type basis, respectively.

^b In the entry are given the esultes obtained with Slater type basis set of DZP, TZ2P and QZ4P quality, respectively.

Table S3 Calculated $\sigma(^{113}\text{Cd})$, for different $d(\text{Cd-C})$ bond distances (pm) and $\phi(\text{Cd-C-C-H})$ dihedral angles ($^\circ$) for Me_2Cd at SO[B3LYP/TZ2P;DZP], SC[B3LYP/TZ2P;DZP], NR-2[B3LYP/TZ2P;DZP] levels

SO		B3LYP/TZ2P				
$d(\text{Cd-C}) \rightarrow$		217	221	225	230	235
$\phi(\text{Cd-C-C-H}) \downarrow$						
-20		3513.61	3592.88	3667.67	3755.04	3836.37
25		3513.00	3592.78	3667.64	3755.02	3836.37
55		3513.28	3593.06	3667.91	3755.25	3836.62
85		3514.04	3593.71	3668.49	3755.76	3837.06
145		3516.02	3595.61	3670.31	3757.55	3838.72
175		3515.92	3595.53	3670.25	3757.45	3838.65
		B3LYP/DZP				
		217	221	225	230	235
-20		3531.74	3610.18	3683.85	3769.92	3850.12
25		3532.21	3610.61	3684.23	3770.28	3850.43
55		3532.69	3611.04	3684.64	3770.61	3850.70
85		3532.75	3611.11	3684.73	3770.70	3850.82
145		3534.85	3613.07	3686.57	3772.41	3852.39
175		3535.02	3613.24	3686.70	3772.52	3852.47
		SC				
		B3LYP/TZ2P				
		217	221	225	230	235
-20		3076.97	3152.99	3224.15	3306.98	3383.80
25		3077.12	3153.12	3224.27	3307.11	3383.91
55		3077.48	3153.45	3224.59	3307.40	3384.22
85		3077.97	3153.90	3225.03	3307.75	3384.52
145		3079.86	3155.73	3226.76	3309.44	3386.12
175		3079.92	3155.76	3226.80	3309.47	3386.15
		B3LYP/DZP				
		217	221	225	230	235
-20		3085.94	3161.22	3231.70	3313.78	3389.93
25		3086.31	3161.54	3231.99	3314.03	3390.14
55		3086.73	3161.93	3232.35	3314.35	3390.43
85		3086.94	3162.14	3232.56	3314.54	3390.62
145		3088.93	3164.01	3234.33	3316.22	3392.20
175		3089.06	3164.15	3234.45	3316.32	3392.28
		NR				
		B3LYP/TZ2P				
		217	221	225	230	235
-20		3150.98	3222.47	3289.18	3366.54	3437.95
25		3151.56	3223.00	3289.67	3366.96	3438.33
55		3151.99	3223.38	3290.03	3367.32	3438.64
85		3152.04	3223.46	3290.10	3367.37	3438.71
145		3153.72	3225.04	3291.62	3368.78	3440.04
175		3153.95	3225.26	3291.79	3368.94	3440.16
		B3LYP/DZP				
		217	221	225	230	235
-20		3138.87	3210.55	3277.42	3354.97	3426.58
25		3138.97	3210.66	3277.54	3355.09	3426.70
55		3139.25	3210.93	3277.79	3355.32	3426.93
85		3139.75	3211.38	3278.19	3355.67	3427.21
145		3141.51	3213.07	3279.84	3357.27	3428.76
175		3141.48	3213.05	3279.82	3357.25	3428.74

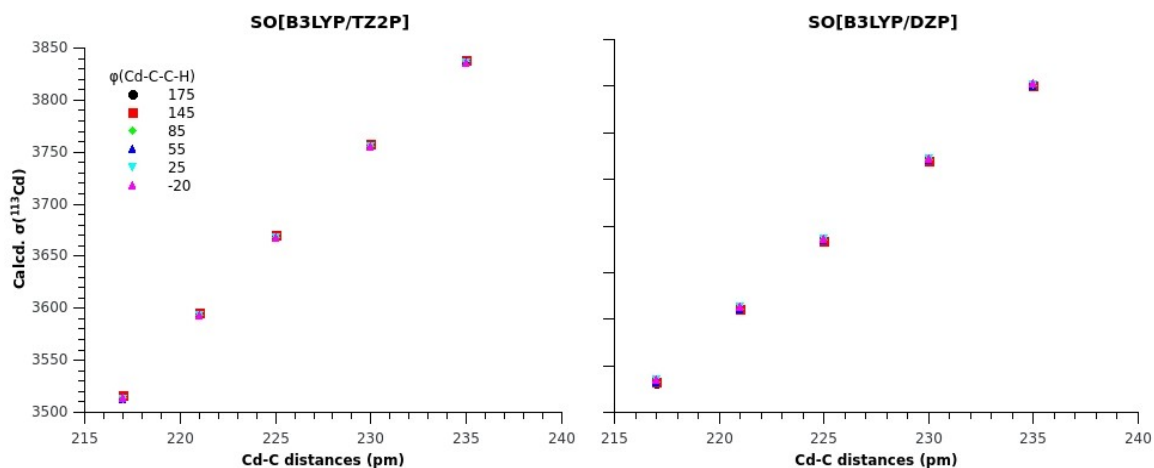


Figure S1 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SO[B3LYP/TZ2P;DZP]

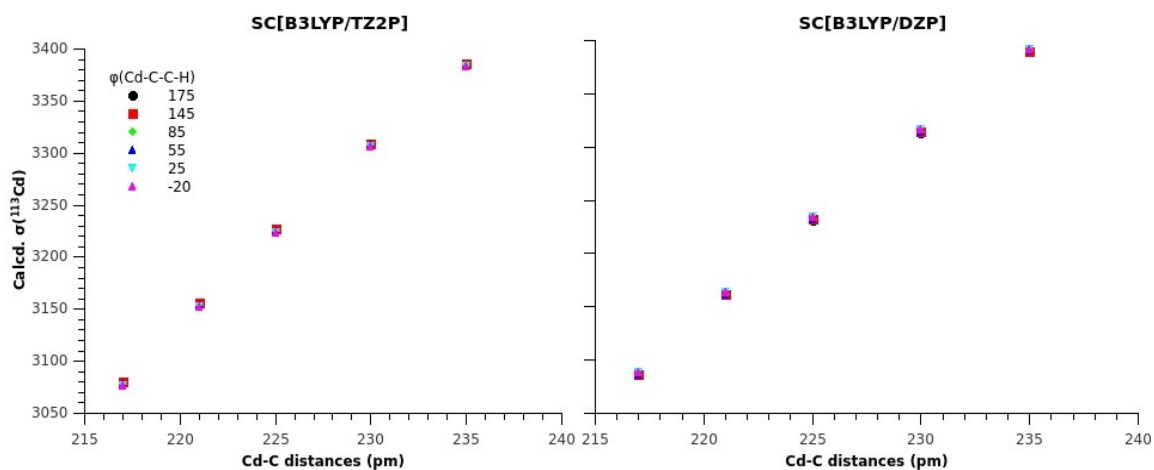


Figure S2 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SC[B3LYP/TZ2P;DZP]

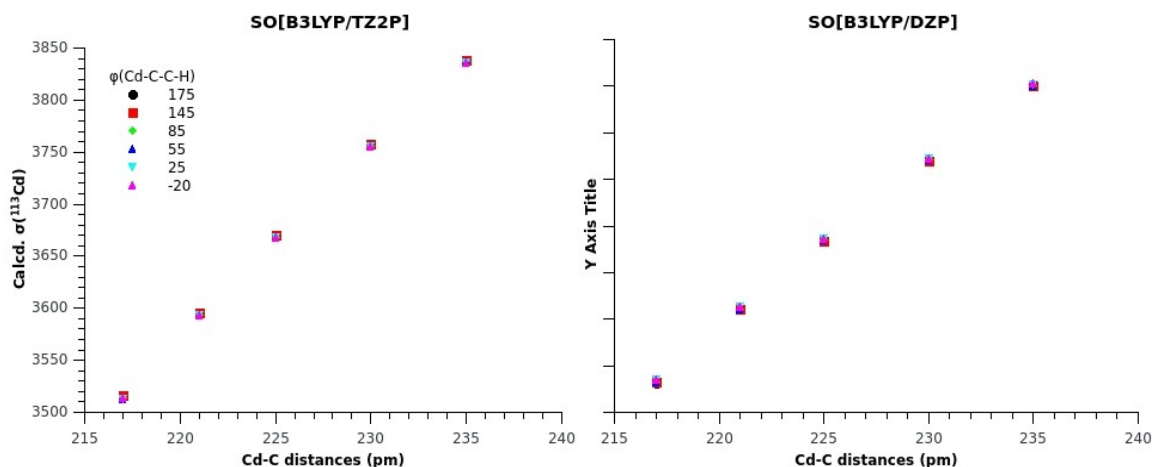


Figure S3 $\sigma(^{113}\text{Cd})$ dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd NR-2[B3LYP/TZ2P;DZP]

Table S4 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} B3LYP/Sadleji (Cd);6-31G(d) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3817.74	3705.99	3867.53	3879.71
2	3864.86	3814.09	3824.70	3955.78
3	3840.85	3759.12	3813.48	3949.95
4	3896.89	3829.96	3898.62	3962.08
5	3806.63	3700.96	3851.45	3867.50
6	3861.54	3812.88	3879.07	3892.66
7	3894.01	3813.34	3850.62	4018.08
8	3841.20	3748.99	3864.43	3910.18
9	3751.40	3690.70	3714.85	3848.66
10	3805.30	3703.80	3829.48	3882.61
11	3868.11	3757.31	3818.25	4028.78
12	3798.33	3743.36	3800.12	3851.51
13	3873.81	3846.75	3878.52	3896.16
14	3849.89	3723.96	3814.54	4011.16
15	3801.62	3700.94	3773.40	3930.52
16	3866.11	3783.70	3887.64	3927.00
17	3788.86	3761.35	3793.13	3812.10
18	3857.56	3806.44	3878.19	3888.05
19	3834.53	3760.18	3853.19	3890.22
20	3874.68	3769.31	3855.43	3999.31
avg	3839.70	3761.66	3837.3	3920.10
StdDev	38.373			

Table S5 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of Cd(ClO₄)₂ 1.0 M. B3PW91/Sadleji (Cd);6-31G(d) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3826.39	3711.26	3878.84	3889.08
2	3873.88	3821.41	3835.20	3965.03
3	3848.98	3765.17	3822.00	3959.77
4	3906.16	3837.72	3908.78	3971.98
5	3815.21	3708.19	3860.85	3876.59
6	3870.21	3819.95	3887.70	3902.98
7	3904.32	3823.03	3863.05	4026.89
8	3849.42	3755.36	3873.73	3919.17
9	3757.43	3695.43	3720.44	3856.43
10	3813.06	3710.43	3837.42	3891.33
11	3877.50	3764.76	3829.25	4038.50
12	3806.14	3752.04	3806.54	3859.83
13	3881.95	3854.71	3886.93	3904.21
14	3859.09	3732.80	3823.80	4020.68
15	3809.76	3710.32	3780.31	3938.64
16	3874.89	3790.99	3896.79	3936.90
17	3796.53	3768.30	3800.31	3820.98
18	3864.92	3812.41	3885.72	3896.63
19	3841.63	3764.60	3861.22	3899.06
20	3883.31	3776.51	3865.25	4008.18
avg	3848.04	3768.77	3846.21	3929.14
StdDev	39.064			

Table S6 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $\text{Cd}(\text{ClO}_4)_2$ 1.0 M. B3LYP/Sadleji (Cd);6-31G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3815.17	3704.78	3864.37	3876.35
2	3861.91	3811.61	3821.57	3952.54
3	3838.39	3756.75	3810.84	3947.58
4	3893.60	3826.79	3895.02	3958.98
5	3804.07	3698.06	3849.32	3864.84
6	3859.44	3811.10	3876.70	3890.51
7	3891.19	3810.75	3848.08	4014.75
8	3838.86	3746.17	3862.40	3908.00
9	3749.46	3688.02	3712.91	3847.47
10	3802.57	3701.11	3826.30	3880.29
11	3865.28	3754.14	3816.04	4025.66
12	3795.76	3740.72	3797.82	3848.74
13	3870.73	3843.23	3875.29	3893.68
14	3848.02	3721.94	3812.60	4009.52
15	3798.68	3698.32	3770.61	3927.10
16	3863.19	3781.03	3884.51	3924.02
17	3786.75	3759.08	3791.05	3810.11
18	3855.19	3804.12	3875.72	3885.72
19	3831.53	3756.90	3849.91	3887.77
20	3872.70	3767.54	3853.51	3997.05
avg	3837.12	3759.11	3834.73	3917.53
StdDev	38.219			

Table S7 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $\text{Cd}(\text{ClO}_4)_2$ 1.0 M. B3PW91/Sadleji (Cd);6-31G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3823.88	3709.66	3876.20	3885.77
2	3870.82	3818.78	3832.00	3961.68
3	3846.45	3762.76	3819.35	3957.22
4	3902.74	3834.40	3905.10	3968.73
5	3812.55	3705.18	3858.48	3874.00
6	3870.35	3819.82	3886.90	3904.32
7	3900.41	3817.04	3859.41	4024.78
8	3846.75	3752.31	3871.28	3916.65
9	3755.42	3692.74	3718.38	3855.15
10	3810.20	3707.63	3834.18	3888.79
11	3874.40	3761.35	3826.71	4035.13
12	3803.41	3749.24	3804.14	3856.86
13	3878.77	3850.96	3883.64	3901.70
14	3856.24	3730.09	3820.99	4017.63
15	3806.81	3707.26	3777.54	3935.64
16	3871.79	3788.14	3893.54	3933.70
17	3794.19	3765.78	3798.00	3818.78
18	3862.35	3809.91	3883.08	3894.07
19	3839.00	3761.57	3858.79	3896.65
20	3135.67	1711.43	3832.15	3863.42
avg	3843.50	3662.80	3841.99	3919.54
StdDev	38.99			

* Snapshot #20 has not been included in the average of the isotropic shielding.

Table S8 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $\text{Cd}(\text{ClO}_4)_2$ 1.0 M. B3LYP/Sadleji (Cd);6-31+G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3806.64	3692.53	3857.63	3869.77
2	3855.58	3802.73	3813.50	3950.50
3	3835.40	3755.58	3809.59	3941.03
4	3889.39	3825.33	3891.07	3951.75
5	3792.83	3680.23	3841.95	3856.32
6	3853.17	3801.52	3873.72	3884.27
7	3886.81	3804.31	3840.99	4015.13
8	3835.27	3742.51	3859.61	3903.69
9	3742.59	3683.14	3703.17	3841.47
10	3795.41	3692.14	3820.59	3873.50
11	3857.86	3746.65	3805.05	4021.88
12	3789.80	3731.83	3785.51	3852.05
13	3866.20	3836.89	3873.05	3888.67
14	3842.82	3719.36	3803.79	4005.31
15	3794.41	3694.50	3766.35	3922.38
16	3858.14	3776.71	3876.30	3921.41
17	3776.96	3746.88	3778.23	3805.75
18	3851.27	3802.43	3871.24	3880.15
19	3825.30	3751.25	3841.09	3883.55
20	3860.93	3756.43	3836.95	3989.40
avg	3830.84	3752.15	3827.47	3912.90
StdDev	39.02			

Table S9 Calculated and averaged σ_{iso} , σ_{xx} , σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $\text{Cd}(\text{ClO}_4)_2$ 1.0 M. B3PW91/Sadleji (Cd);6-31+G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3814.6314	3697.7229	3868.5894	3877.5818
2	3864.0154	3810.3265	3822.5278	3959.1920
3	3842.9164	3761.1961	3817.5326	3950.0206
4	3897.8275	3832.5224	3900.4005	3960.5595
5	3800.5122	3686.3902	3850.5369	3864.6095
6	3861.1355	3808.0461	3881.9608	3893.3996
7	3895.3402	3810.7806	3850.8535	4024.3865
8	3842.7312	3748.3432	3868.3565	3911.4940
9	3748.2746	3687.8386	3707.9242	3849.0609
10	3801.8354	3697.5732	3827.1263	3880.8066
11	3866.5637	3753.3001	3815.1760	4031.2149
12	3796.9637	3739.3868	3791.5979	3859.9065
13	3873.6447	3844.3479	3880.3969	3896.1893
14	3850.6909	3726.7121	3811.7333	4013.6274
15	3801.3802	3702.0367	3772.2303	3929.8735
16	3866.0390	3783.0782	3884.9230	3930.1157
17	3783.6401	3752.7595	3784.5248	3813.6359
18	3858.1287	3808.1294	3878.0407	3888.2159
19	3832.5849	3756.1940	3849.3296	3892.2310
20	3868.9092	3762.9631	3846.2184	3997.5462
avg	3838.39	3758.48	3835.50	3921.18
StdDev	39.63			

Table S10 Correlations at NR-1[F/B] [F=B3LYP,B3PW91; B=DZVP(Cd), 6-31G(d,p) levels of calculated $\delta(^{113}\text{Cd})$ (ppm), wrt $\text{Cd}(\text{ClO}_4)_2$ and Me_2Cd , respectively, on OP2 geometries, and relevant statistical data. For the complete set of calculated $\delta(^{113}\text{Cd})$ see Tables S14-S48.

Exptl. (wrt 1M $\text{Cd}(\text{ClO}_4)_2$)	Calcd		Exptl. (wrt $\text{Me}_2\text{Cd}_{(g)}$)	Calcd	
	B3LYP/ DZVP;6-31G(d,p)	B3PW91/ DZVP;6-31G(d,p)		B3LYP/ DZVP;6-31G(d,p)	B3PW91/ DZVP;6-31G(d,p)
77.1	-7.27	0.75	-629.03	-863.99	-847.18
82.1	-2.76	5.46	-624.03	-859.48	-842.46
76	-8.27	-0.14	-630.13	-864.99	-848.06
81.2	6.52	14.67	-624.93	-850.21	-833.26
59.1	-6.66	1.85	-647.03	-863.39	-846.07
200	111.52	129.38	-506.13	-745.20	-718.55
202.5	110.77	131.14	-503.63	-745.96	-716.78
193.8	142.18	156.15	-512.33	-714.54	-691.77
195.9	147.35	164.48	-510.23	-709.37	-683.44
218.3	188.54	203.42	-487.83	-668.18	-644.51
201.9	118.55	136.89	-504.23	-738.17	-711.03
198.3	152.17	166.89	-507.83	-704.55	-681.03
221.1	192.27	207.12	-485.03	-664.45	-640.81
353.6	252.65	253.84	-352.53	-604.07	-594.08
365.13	263.59	264.83	-341.00	-593.13	-583.09
352.13	253.45	254.71	-354.00	-603.27	-593.22
303.3	273.24	282.51	-402.83	-583.48	-565.41
265.67	199.92	209.96	-440.46	-656.80	-637.97
237.5	160.63	173.05	-468.63	-696.09	-674.87
168.2	168.00	135.78	-537.93	-688.72	-712.14
172.4	125.73	152.71	-533.73	-730.99	-695.21
155.2	143.75	151.78	-550.93	-712.98	-696.14
141.8	137.84	144.93	-564.33	-718.88	-703.00
148.1	132.39	144.67	-558.03	-724.34	-703.26
27.2	-37.09	-30.44	-678.93	-893.82	-878.37
26.3	-38.03	-31.71	-679.83	-894.75	-879.63
ME	101.54	100.30	ME	252.13	242.09
MAE	59.34	50.21	MAE	209.93	191.76
CMAE	28.19	28.66	CMAE	28.19	28.66
Slope	0.945	0.941	Slope	0.945	0.941
Int.	-49.35	-39.27	Int.	-238.77	-222.63

Table S11 Calculated Cd-N, Cd-O and Cd-S bond lengths (pm) for the models of Scheme 1 with OP2 and OP3 protocols. Averaged values.

Model	OPTIMIZATION PROTOCOL					
	OP2			OP3		
	Cd-N	Cd-O	Cd-S	Cd-N	Cd-O	Cd-S
1	238	232	-	238	234	-
2	239	231	-	240	233	-
3	238	231	-	239	234	-
4	238	230	-	239	234	-
5	240	231	-	239	234	-
6	240	-	-	243	-	-
7	240	-	-	242	-	-
8	238	-	-	241	-	-
9	238	-	-	241	-	-
10	237	-	-	239	-	-
11	239	-	-	243	-	-
12	238	-	-	241	-	-
13	237	-	-	239	-	-
14	-	-	261	-	-	261
15	-	-	259	-	-	260
16	-	-	259	-	-	261
17	226	-	-	228	-	-
18	235	-	267	236	-	270
19	238	-	264	242	-	265
20	234	225	-	234	225	-
21	236	222	-	241	224	-
22	235	222	-	239	226	-
23	235	227	-	237	231	-
24	232	233	-	235	236	-
25	-	245 _{ax} ;225 _{eq}	-	-	251 _{ax} ;226 _{eq} ; 228 _{eq}	-
26	-	243 _{ax} ;245 _{ax} ; 225 _{eq}	-	-	250 _{ax} ; 225 _{eq} ;227 _{eq}	-

Table S12 Calculated plane and dihedral angles for the models of Scheme 1 with OP2 and OP3 protocols.

Model	OPTIMIZATION PROTOCOL							
	OP2				OP3			
	<i>N-Cd-N</i>	<i>O-Cd-O-C</i>	<i>Cd-O-C-N</i>	<i>Cd-O-C-R'</i>	<i>N-Cd-N</i>	<i>O-Cd-O-C</i>	<i>Cd-O-C-N</i>	<i>Cd-O-C-R'</i>
1	179	158; -64; -111; -171	163; 155	168; 173	179	173; -54; -110; 155	175; 168	165; 172
2	178	171; -83; -95; 177	175; 168	165; 172	178	-176; -86; -84; 170	180	162; 166
3	179	-91; 164; -177; -98	155; 161	172; 170	178	-142; -173; -177; -56	161; -177	174; 166
4	175	177; -115; -81; 163	177; -171	-176; 179	176	168; -113; -93; 174	167; 178	-167; -175
5	173	150; -55; -82; -112	170; 149	167; 179	172	-166; 130; -163; 69	161; 169	174; 166
	<i>N-Cd-N (same ligand)</i>	<i>C-N-Cd-N</i>	<i>Cd-N-N-B (same ligand)</i>		<i>N-Cd-N (same ligand)</i>	<i>C-N-Cd-N</i>	<i>Cd-N-N-B (same ligand)</i>	
6	82	-42	0		82	-41	0	
7	80; 81; 82	-49	-12; -14; -29		80; 81; 83	-45	-9; -27; -28	
8	81; 82	-44	0		82	-43	0	
9	81	-40	0		81	-45	0	
10	80; 81	-41	10; 22; 6		80; 81	-39	10; 22; 7	
11	82	-42	0		81	-41	0	
12	81	-45	0		81	-44	0	
13	80	-40	10; 21; 5		81	-42	10; 23; 7	
	<i>S-Cd-S (same ligand)</i>	<i>S-Cd-S-C (same ligand)</i>			<i>S-Cd-S (same ligand)</i>	<i>S-Cd-S-C (same ligand)</i>		
14	71	128			71	128		
15	71	131			71	131		
16	71	130			71	130		
	<i>N-Cd-N</i>	<i>N-Cd-N-N (same ligand)</i>	<i>N-Cd-N-N</i>	<i>Cd-N-N-B</i>	<i>N-Cd-N</i>	<i>N-Cd-N-N (same ligand)</i>	<i>N-Cd-N-N</i>	<i>Cd-N-N-B</i>
17	112; 92	29; 30	-111; 29; 94; 145; -30; -149; 94; -110; 29; -150; 146; -30;	-12; 14	112; 92	25	-113; 25; 98; 142; -25; -146; 99; -114; 26; -145; 142; -26	-17; 16; -15
	<i>S-Cd-N</i>	<i>N-Cd-N-N (same ligand)</i>	<i>S-Cd-N-N</i>	<i>S'-Cd-N-N</i>	<i>S-Cd-S</i>	<i>N-Cd-N-N (same ligand)</i>	<i>S-Cd-N-N</i>	<i>S'-Cd-N-N</i>
18	69	37; -44; -46	-46; 46; 44; -37; 37; -44	180; 145; -146	68	-37; 44; -44	-43; 47; 43; -37; 39; -44	176; 143; -145
19	70	-51; -53; -30	-180; 129; -131	174; -159; 156	70	-53; 51; -29	171; 129; -132	-179; -157; 153
	<i>O-Cd-O</i>	<i>N-Cd-N-N (same ligand)</i>	<i>O-Cd-N-N</i>	<i>O'-Cd-N-N</i>	<i>O-Cd-O</i>	<i>N-Cd-N-N (same ligand)</i>	<i>O-Cd-N-N</i>	<i>O'-Cd-N-N</i>
20	82	-14; 61; -35	-153; 166; -159	121; 76; -108;	82	-18; 67; 28; -25; -60; 56	-133; 152; -140	136; -118
21	84	-26; 53; 30; -39; -52; 53	-148; 153; -168	126; -121; 35;	85	-22; 54; 28; -41; -52; 57;	-148; 155; -176	123; -118; 7
22	83	-52; 44; 55; -36; 35; -35;	-130; 138; -148	-130; 129; 147	83	-51; 58; 46; -24; 29; -49;	-154; -96; 159;	61; -61; -142
23	80	-29; 50; 35; -43; -48; 54	-153; 156; -162	128; -124; -18	80	-27; 49; 33; -45; -49; 2	-154; 157; -163	128; -122; -13
24	57	-48; 43; 48; -43; -41; 41	-159; -160; 148;	159; -148; 160	56	-47; 43; -47; 43; -42; 42;	-159; -159; 148	160; -148; 159
	<i>O-Cd-O_{ax}</i>	<i>O-Cd-O-C (same ligand)</i>	<i>O-Cd-O-C</i>		<i>O-Cd-O_{ax}</i>	<i>O-Cd-O-C (same ligand)</i>	<i>O-Cd-O-C</i>	
25	180	-32; 29; -29; 32	-107; -148; -102; 11		180	24; -24; -25; 24	-86; -156; -104; 155	
26	175	33; -27; 30; -29	149; -35; -109; -151		176	22; -23; 33; -30	155; 88; -146; 37	

Coordinates of the 20 snapshots obtained from MD simulation

Snapshot 1

296
O 3.626083 0.985525 2.357416
O 5.390150 -0.151843 0.859897
O 1.586494 -0.373843 1.512748
Cd 0.025060 0.184701 -0.038295
O -1.967493 1.032205 -0.969010
O -1.445252 -0.213500 1.582293
O 0.614407 2.450871 -0.389238
O 1.414305 0.029021 -2.057501
O -0.941487 -2.135535 -0.791287
O 1.287871 -2.384134 -2.452382
O 0.501961 3.465931 -2.689385
O 3.243383 -2.236192 1.147055
O 2.271411 -4.632966 1.160642
O 0.402211 -5.964217 0.548307
O -4.389510 1.303261 -0.094956
O -4.271471 2.173183 2.315446
O 2.711201 -4.548338 -2.187865
O 3.817606 -4.200262 -4.478200
O 1.796716 -2.786781 -5.264023
O 1.647088 -6.886728 -1.731171
O -2.548515 -2.401781 2.496573
Cl -3.030305 -3.419254 1.486279
O -3.916455 -4.518072 2.093278
O -1.756965 -4.117715 1.019592
O -3.725292 -2.781329 0.387218
O -1.625643 -6.405407 -1.054697
O -3.147075 -7.110869 0.728761
O 4.048694 1.101073 4.952992
O 4.815826 -3.030767 -0.811854
O 5.224239 -2.202690 -3.212352
O -0.512012 -7.714286 -3.052749
O -0.624459 -6.699227 -5.352895
O -0.499224 3.759751 1.608814
O -2.020657 3.054288 3.392272
O -1.685572 1.971324 5.423248
O 1.528631 4.200940 3.211818
O 3.397830 5.532191 3.824154
O 0.280161 1.345548 -4.256209
O -0.346250 0.388319 -6.442869
O 0.576833 -7.245346 2.857733
O 1.517199 -5.115344 3.803090
O 3.916957 -5.591510 4.512938
O 1.703252 2.919810 5.521244
O 2.643617 5.049813 6.466601
O 0.976290 5.790538 -3.869076
O -0.150129 -4.374620 -6.532586
O -2.173603 -3.582435 -7.427293
O -2.958506 -1.429304 -6.162496
O 2.773507 3.278430 0.932340
O 3.837620 5.616820 0.475646
O 4.944024 5.964895 -1.814688
O 2.923134 7.378377 -2.600510
O 2.414289 7.781023 0.211129
O -5.029122 4.592419 3.139644
O -0.472556 -3.475275 4.487720
O -5.628793 2.676697 -2.024787

O	-4.430073	2.822377	-4.213743
O	-3.302197	5.222786	-4.148211
O	-5.185364	6.622162	-4.014312
O	-2.373818	4.291503	-1.881730
O	-2.430133	5.793210	0.280101
O	-0.005588	-0.543366	3.824298
O	-2.543405	1.002629	-3.618571
O	-5.218352	6.401193	1.156486
O	4.823511	-1.396046	5.733978
O	3.268259	-3.066233	7.216008
O	4.780155	-3.203691	3.508379
O	-5.890848	4.010975	5.682300
O	-3.867375	3.218790	6.577005
O	-4.341704	0.894181	7.756695
O	-4.563501	-1.226203	6.189871
O	-5.189912	-2.183430	4.003210
O	-3.622562	-1.372926	-2.757504
O	-5.974489	-0.828746	-3.743169
O	-6.019180	-1.498172	-1.157785
O	-6.344769	-3.763964	-1.507025
O	-6.155539	-5.572738	0.476132
O	-6.139365	0.179553	2.945092
O	-1.295703	2.751303	-7.500988
O	3.158094	4.543072	-5.022834
O	4.283953	2.839679	-3.165307
Cl	4.652872	1.413716	-2.737980
O	3.902305	1.098997	-1.398281
O	6.174102	1.250969	-2.468764
O	4.163924	0.439363	-3.770453
O	4.371107	-0.903527	-5.958362
O	8.111926	-0.494485	-3.230074
O	-7.332480	4.877109	-2.052371
O	0.184932	8.029622	1.872224
O	6.969057	3.981701	-2.505108
O	4.634319	-6.235906	1.123232
O	5.760737	3.929250	3.786742
O	6.336875	2.791104	1.813120
O	8.050225	0.603529	1.968278
O	2.125391	1.409953	7.940974
O	-8.837751	-1.219319	-0.533349
O	-8.794395	0.588327	1.692250
O	7.598727	-3.482545	2.883945
O	7.643420	-2.813118	0.298560
O	-8.227757	1.832529	-3.181832
O	-3.556550	-4.371946	-2.383410
O	-3.500236	-5.873654	-4.545242
O	-2.496145	8.792231	-0.093992
O	4.838078	2.028384	-6.621784
O	0.380575	-4.774437	7.233730
O	-3.046948	-5.358528	5.182059
H	3.850658	0.951515	3.334023
H	4.419897	0.470513	1.901295
H	-7.552283	5.328779	-1.172672
H	-6.667408	5.406786	-2.584474
H	4.311433	-3.081435	2.687218
H	4.439206	-4.105908	3.875347
H	5.128934	-2.617148	-1.684870
H	5.672523	-3.241586	-0.450472
H	5.083822	0.232718	-0.028922
H	6.393921	0.104158	0.871144

H	-3.209200	1.740333	-3.827043
H	-1.636716	1.268840	-3.942703
H	6.907865	2.937534	-2.631270
H	7.730711	4.003992	-1.876756
H	3.155394	-5.162049	1.041377
H	1.542737	-5.017563	0.668319
H	-3.289029	-0.526568	-3.237873
H	-3.273417	-1.318146	-1.812820
H	0.241154	1.066899	-5.187358
H	0.895984	0.808606	-3.638895
H	2.908827	4.803056	-5.979283
H	3.184914	3.558913	-4.973809
H	-4.949507	0.500502	-0.072796
H	-4.273468	1.639327	0.890765
H	-2.054171	3.917434	3.822938
H	-1.394584	3.284287	2.613869
H	2.693675	-3.101615	1.076272
H	3.968553	-2.290143	0.347742
H	-3.594956	-4.925210	-3.268820
H	-3.028960	-3.592451	-2.424673
H	-4.784108	1.414254	2.789361
H	-3.417737	2.397284	2.767157
H	0.795666	4.375317	-3.043775
H	0.400472	2.768124	-3.481069
H	-4.544226	-2.262163	3.315246
H	-5.666212	-3.038751	3.999414
H	0.202855	-1.288461	4.361039
H	0.653627	-0.511493	3.079753
H	1.047681	-3.101451	-5.822827
H	2.382264	-2.078174	-5.769965
H	4.849441	-1.306922	-3.462621
H	4.913649	-2.950558	-3.796373
H	-2.707595	-6.396379	-4.812765
H	-3.934938	-5.535753	-5.311405
H	-5.047361	5.280747	2.419033
H	-4.844545	3.668402	2.883346
H	4.703330	-6.766630	1.962829
H	2.882947	-5.505905	4.467880
H	4.072603	-5.681908	5.520489
H	3.437461	-4.364919	-1.539674
H	3.124652	-4.403281	-3.134110
H	4.632691	1.586116	5.585653
H	3.141274	1.357741	5.096269
H	1.314872	-2.397505	-3.474540
H	1.804165	-3.257022	-2.197299
H	-1.077577	4.444324	1.123548
H	-0.128436	3.185602	0.890728
H	-0.991008	-4.164533	-7.011510
H	0.480958	-5.014847	-7.004093
H	1.009481	-6.010059	3.652209
H	1.628779	-4.881131	2.864825
H	1.606984	3.302294	4.549117
H	0.793173	2.552914	5.752512
H	-0.840728	-3.222517	3.602073
H	0.277393	-4.158743	4.241029
H	-6.122622	3.521821	-1.799687
H	-5.295006	2.203953	-1.158000
H	7.242780	-0.217018	-2.937560
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Snapshot 2

290			
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H	-5.955833	-0.318856	-2.539719
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H	-5.986294	-3.823892	0.446536
H	-7.487990	-3.980871	0.932549
H	-5.452467	-5.576411	-2.221366
H	-4.092902	-5.125587	-2.898905
H	-4.838501	-3.822259	-1.471025
H	-5.253609	-2.352256	-1.090778
H	-6.314333	-2.818367	-5.005908
H	-5.936678	-3.835896	-3.783120
H	-2.666550	8.487219	-3.430371
H	-2.380965	7.294404	-2.511822
H	-3.095144	5.606849	-4.187202
H	-3.558353	4.101889	-4.535310
H	-4.014111	7.671029	2.062617
H	-4.916951	6.810222	1.159082
H	-4.930192	5.726053	-1.049203
H	-4.076320	5.246284	-2.306604
H	0.246804	5.241743	7.000244
H	0.089892	3.619015	6.446255
H	1.501383	-1.035111	8.421733
H	2.738445	-1.857281	8.903438
H	-3.812905	2.731168	5.679102
H	-3.490546	1.785984	6.810797
H	0.153196	2.443494	4.185292
H	-0.702459	1.308475	4.637721
H	-7.616400	-0.059355	4.561401
H	-6.178050	0.015983	4.820617
H	-3.090117	-2.193090	7.075705
H	-4.635974	-2.671516	6.667120
H	-0.731524	-3.416527	7.668643
H	-0.107928	-4.360623	6.504371
H	-6.348024	-3.463661	5.181129
H	-6.474031	-1.824743	5.494659

Snapshot 3

302

O	3.407254	-0.654321	2.796691
O	3.617835	1.729648	1.795842
O	1.409498	1.890312	0.424020

Cd	-0.037907	0.096113	0.148818
O	1.049973	-1.450962	1.733126
O	-1.706442	0.168734	1.758203
O	1.119012	-0.096943	-1.793969
O	-0.911808	-2.043036	-0.887380
O	-1.217263	1.916473	-0.811327
O	1.272396	3.051563	-1.853085
O	2.158340	-3.466043	0.603935
O	-0.735820	-1.537379	3.647433
O	3.533656	-1.529345	5.272105
O	4.894028	-2.146908	1.219631
O	5.695587	3.358156	1.900794
O	6.662871	4.683570	-0.068694
O	4.701070	6.482687	-0.339908
O	3.712005	-0.333897	-1.155635
Cl	4.496616	0.775431	-1.741654
O	5.958678	0.750324	-1.264726
O	3.953945	2.134333	-1.429929
O	4.548697	0.575135	-3.231492
O	1.940910	0.582820	5.710794
O	2.343364	2.534773	4.021258
O	4.078398	3.092591	5.450483
O	2.719490	2.692804	7.727063
O	0.218657	3.282894	2.560655
O	0.504652	-5.522616	0.085999
O	-1.230382	-6.080434	-1.343226
O	-1.632836	-8.032387	0.346309
O	-0.854255	-5.922403	2.362578
O	-2.393590	-4.063161	3.330729
O	1.198501	-7.390640	3.245859
O	-3.355090	-5.332312	-2.803828
O	0.044091	-6.885558	-3.568643
O	-2.164248	-6.724894	-4.940465
O	2.121841	-5.257050	-3.463691
O	3.089125	-3.931638	-5.433178
O	1.127326	-2.132520	-5.704392
O	0.715069	-2.596395	-2.962823
O	-5.351428	-6.258741	-1.231065
O	-7.142125	-4.246593	-1.375028
O	-7.509472	-4.638012	1.238248
O	-1.777682	2.356465	4.133420
O	-1.098649	0.415048	5.692156
O	-3.903535	2.172405	2.596073
O	-3.568379	4.368613	3.989455
O	-3.895446	2.360610	-0.027962
O	-4.124931	4.397505	-1.626575
O	-3.935726	3.977195	6.602731
O	3.006495	-5.011048	2.671405
O	3.129484	-4.231600	5.128654
O	-5.803916	2.070885	6.057296
O	-6.175695	1.119267	3.676925
O	-6.188062	-1.486807	3.384159
O	-4.699921	-2.677952	5.043453
O	3.892580	-3.657543	-1.488458
O	4.797479	-2.538899	-3.786955
O	2.480709	5.517977	-1.928449
O	7.115443	-1.219996	-2.803698
O	6.246735	-4.982349	-0.946954
O	-6.761223	3.760345	-2.264881
O	7.530320	-1.509747	1.857936

O	-4.140470	-2.371200	1.705605
Cl	-4.522246	-2.125054	0.250179
O	-3.906391	-3.278474	-0.544201
O	-3.839055	-0.841080	-0.226410
O	-5.967377	-2.042154	0.056232
O	5.674905	-5.133254	1.787604
O	4.765951	-7.462221	0.708660
O	1.464962	-5.477545	7.012872
O	4.288814	6.018813	2.401660
O	2.661938	6.572171	4.477104
O	8.115102	2.787615	-1.644402
O	8.412737	-2.749858	-0.744445
O	7.945269	1.264140	2.552263
O	-3.709982	7.171392	-0.932248
O	-1.789303	7.803653	-2.940637
O	-0.153432	6.328435	-3.759270
O	-0.525210	5.376816	-6.139639
O	-0.537577	2.770743	-6.432407
O	0.950561	1.579599	-4.773113
O	-1.505484	1.150848	-3.784415
O	-3.242516	3.157395	-4.228952
O	1.714758	8.234746	-3.213834
O	-2.673366	0.875785	-6.418893
O	-1.858986	-0.380462	-8.578320
O	-3.446342	-0.862445	-3.125947
O	-4.758761	-2.776895	-4.157551
O	-6.889301	-1.554968	-2.775851
O	-5.980347	0.773998	-1.696906
O	-5.408516	0.924905	-4.431464
O	-8.648758	0.896204	-0.813107
O	-8.525768	1.675653	1.644142
O	-1.093037	-3.097229	-7.292933
O	5.684331	0.819165	4.609851
O	2.110586	-7.796042	-0.754633
O	-1.217343	5.214234	-1.284659
O	-1.185018	5.838311	1.206936
O	0.127403	7.752761	2.238539
O	-3.315558	7.060240	2.588635
O	-5.970923	6.726418	1.125341
O	2.464619	-1.469932	8.172164
O	-3.169775	1.260430	7.888118
O	4.551834	4.672597	-4.124411
O	4.914665	2.720170	-6.169135
O	3.256892	0.194389	-6.485839
O	-4.523158	-6.390068	4.112178
H	3.570377	-1.014765	3.720289
H	4.009442	-1.145212	2.115350
H	-3.900034	6.907438	0.023053
H	-4.324127	7.901906	-1.168115
H	2.767550	-4.535436	1.747790
H	2.377873	-5.774400	2.760046
H	4.283783	-2.988117	-2.100579
H	4.579352	-4.381868	-1.417039
H	4.599664	-1.912831	0.354261
H	5.858033	-2.122446	1.327275
H	-1.921528	2.044755	-3.956983
H	-0.531607	1.185808	-3.976180
H	7.359398	2.085102	-1.772210
H	8.957058	2.375414	-1.240346
H	1.011698	-6.296840	-0.174169

H	-0.196369	-5.503616	-0.647516
H	-2.766437	-0.110343	-3.344039
H	-3.557460	-0.645390	-2.168531
H	0.432577	2.101389	-5.434338
H	1.791789	1.379861	-5.270542
H	4.238848	5.463706	-4.628190
H	4.531610	3.947523	-4.807332
H	-4.685913	1.744612	-0.284621
H	-3.914700	2.281754	0.971522
H	-2.154226	3.232106	4.464749
H	-1.043002	2.670590	3.501133
H	1.565558	-4.023563	0.041706
H	2.965622	-3.420905	0.046095
H	-7.540602	-4.069542	0.457039
H	-7.477853	-4.100045	2.017815
H	-4.864498	-2.904102	-5.221178
H	-4.111557	-2.040628	-4.064866
H	-4.699985	1.781968	3.112286
H	-3.029128	1.960183	3.071445
H	1.893725	3.758780	-2.148164
H	1.168458	2.468626	-2.614530
H	-5.684415	-1.543313	2.520069
H	-6.934935	-2.182156	3.308521
H	-1.065147	-2.497032	3.767825
H	0.109586	-1.710003	3.117048
H	0.421787	-2.264366	-6.420053
H	1.437260	-1.199731	-5.861070
H	5.017587	-1.534213	-3.787351
H	4.066700	-2.753334	-4.494130
H	-3.037894	5.153464	3.608667
H	-3.622252	3.634425	3.310808
H	3.058452	-7.692636	-0.411008
H	1.901388	-8.443928	0.041691
H	0.393614	-6.829651	3.052135
H	1.138653	-7.803539	4.188374
H	2.686754	-5.170959	-2.698597
H	2.540266	-4.812677	-4.265227
H	4.310441	-1.570181	5.913292
H	2.836879	-0.772081	5.505017
H	0.640071	-2.536485	-3.969577
H	1.256649	-3.385112	-2.740489
H	-0.001478	4.211839	2.300592
H	0.439217	2.912161	1.667398
H	-1.546046	-2.328687	-7.782757
H	-0.431852	-3.452905	-7.980074
H	-1.294555	-6.676293	1.909050
H	-0.332388	-5.495977	1.607059
H	1.959339	1.316509	5.046890
H	1.020880	0.515806	5.909675
H	-2.749480	-3.564421	2.574194
H	-1.820305	-4.688912	2.846601
H	-3.776767	5.326764	-1.657361
H	-3.826214	3.880348	-0.774042
H	6.843346	-0.461289	-2.264652
H	7.719135	-0.841875	-3.522811
H	-3.594860	1.205980	-6.642105
H	-2.524330	0.759034	-5.430015
H	6.940957	-4.242323	-1.110993
H	6.637524	-5.892929	-0.890486
H	-0.525388	6.075215	-4.635958

H	0.714008	6.777007	-3.848338
H	3.217505	-3.258637	5.307047
H	3.061012	-4.383315	4.168336
H	3.543925	-4.414654	-6.155303
H	2.304790	-3.365532	-5.709107
H	-6.413949	-0.936281	-2.131521
H	-6.180655	-1.958489	-3.313643
H	3.667622	0.794682	2.291989
H	4.528130	2.065997	1.847743
H	-3.476925	3.755457	-3.438330
H	-3.393736	3.832968	-4.928895
H	2.752222	2.203804	3.209556
H	1.545025	3.121140	3.661384
H	4.763170	-5.373368	2.085224
H	5.648570	-4.718265	0.901817
H	-6.985037	1.505202	3.309274
H	-6.311944	0.145960	3.578922
H	1.137332	-0.935474	-2.328475
H	-2.187850	2.047893	-0.549874
H	-1.824281	-2.296687	-0.973597
H	1.432660	-2.242181	1.209601
H	1.576849	2.239370	-0.571811
H	-1.459914	-0.520974	2.452877
H	2.302940	1.810442	0.859231
H	-2.543041	-0.254208	1.372917
H	-1.221756	1.768630	-1.802422
H	-0.460933	-2.419614	-1.707878
H	2.030075	0.068171	-1.498692
H	1.891641	-1.146893	2.262351
H	1.683627	8.803213	-3.995045
H	1.746377	8.772712	-2.434267
H	-1.890118	0.188006	-9.359531
H	-1.827367	0.157504	-7.798753
H	-0.033930	2.714236	-7.296496
H	-1.284450	2.075394	-6.508045
H	4.585335	1.760518	-6.048743
H	5.760070	2.547545	-6.699520
H	2.901002	0.693128	-7.242373
H	3.830178	-0.431363	-6.969967
H	-1.334554	5.762751	-6.507291
H	-0.661460	4.403508	-6.237643
H	7.755217	1.000186	3.507564
H	7.331123	1.994653	2.316396
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H	7.829037	-2.026904	2.710469
H	5.241304	-6.843533	1.352991
H	5.474596	-7.865743	0.170868
H	8.178329	-2.151797	0.046177
H	8.261517	-2.074285	-1.444386
H	4.585444	2.318367	5.190315
H	3.377376	3.111592	4.716968
H	0.807308	8.504864	2.020447
H	0.016283	7.969816	3.195956
H	-3.966857	4.545664	5.821521
H	-3.904108	4.515162	7.382298
H	-1.290755	5.711106	0.143309
H	-0.537815	6.574579	1.299622
H	3.995533	6.350840	-1.055569
H	5.011005	7.415476	-0.496586
H	-0.750130	4.377602	-1.491006

H	-0.962726	5.695315	-2.162538
H	6.632197	0.922572	4.953477
H	5.475135	0.171279	5.406175
H	6.260500	3.444249	2.665888
H	6.114011	3.802530	1.099257
H	4.213816	6.078722	1.394905
H	4.830394	5.230096	2.623995
H	2.027699	6.286516	-2.418272
H	3.141894	5.162301	-2.615590
H	2.279191	1.938913	7.273534
H	3.241357	3.119230	6.971542
H	7.117672	4.200554	-0.790817
H	5.878536	5.249675	-0.344622
H	-2.840205	7.678926	3.232966
H	-2.606912	6.656717	2.050844
H	1.749464	6.318520	4.390886
H	3.112814	6.195592	3.656605
H	-5.727973	-5.383100	-0.899734
H	-4.616749	-5.944616	-1.863350
H	-6.611640	-3.461741	-1.755817
H	-7.195998	-4.980781	-2.053675
H	-3.575224	-4.403366	-3.063891
H	-3.134530	-5.703044	-3.697087
H	-1.614405	-7.298698	-0.317594
H	-2.552865	-8.099401	0.545190
H	0.093877	-7.820525	-3.072497
H	0.954384	-6.549210	-3.516742
H	-0.821523	-6.411403	-2.154928
H	-2.028721	-5.494067	-1.703101
H	-1.996896	-6.375835	-5.936297
H	-1.270805	-6.804765	-4.505254
H	-5.023056	6.829826	1.468967
H	-6.180119	6.078532	1.921665
H	-8.887703	1.371817	-1.736720
H	-9.277379	0.132853	-0.724466
H	-2.399844	7.264357	-2.364288
H	-1.137001	7.117698	-3.277443
H	-7.055586	3.994422	-3.130251
H	-5.797217	3.784806	-2.157236
H	-4.714294	1.664930	-4.595503
H	-5.017728	0.014324	-4.374997
H	-8.437748	2.648615	1.822536
H	-8.594240	1.523938	0.683825
H	-6.892081	0.533884	-1.399288
H	-6.006681	1.188987	-2.582694
H	-3.622785	2.028970	7.398296
H	-2.508590	0.904753	7.200977
H	1.708914	-2.172445	8.044357
H	3.306575	-1.882133	8.576221
H	-5.217907	-2.156161	4.382227
H	-3.858695	-2.877689	4.546024
H	-1.411635	1.206156	5.188378
H	-1.118872	-0.310026	5.009235
H	-5.228695	-6.521915	3.396515
H	-4.213223	-5.457278	3.955498
H	1.192863	-4.718838	7.551918
H	2.068654	-5.099424	6.293759
H	-6.175872	1.817665	5.180607
H	-4.936475	2.519457	5.968229

Snapshot 4

287

O	-3.310084	-0.772217	-1.893975
O	-0.840947	-1.223125	-2.039842
Cd	0.268710	0.018448	-0.396876
O	1.595070	1.500427	0.853805
O	1.671342	0.794006	-2.137877
O	-1.448370	1.638768	0.119893
O	-0.133902	-1.101728	1.693286
O	1.983871	-1.676438	-0.458852
O	-1.075079	-3.506618	-1.027437
O	1.096575	-4.657232	-1.574298
O	3.061546	-5.167182	-0.365782
O	-1.561737	-4.636241	1.212951
O	-3.870840	1.534895	-0.944068
O	-5.953770	2.427959	-0.322510
O	-4.142926	-2.769379	-0.484340
O	-0.111805	-6.824523	-0.819543
O	2.099494	-4.798346	-3.978829
O	-3.505109	3.116953	-3.027761
O	-5.470080	3.626903	-4.236276
O	-6.678460	1.459612	-3.481523
O	-4.467160	3.485789	-6.640807
O	2.695815	-6.749242	1.717911
O	0.612884	-5.856177	2.339469
O	5.118283	-6.645367	2.781872
O	3.502791	-2.820396	-5.091845
O	-0.259798	-5.042353	4.754736
O	-6.826453	3.241782	2.092756
O	-1.587952	2.955064	2.467735
O	-0.196838	1.254835	4.056030
O	-0.050569	1.853264	6.323846
O	2.424625	1.632348	3.555846
O	-2.741416	-4.479057	3.780384
O	-3.130255	1.511954	-5.320870
O	-4.045893	-0.881452	-4.529423
O	3.436399	-6.772182	-2.658890
O	-2.133438	0.355973	-7.593478
O	3.292263	0.979052	6.072509
O	3.533450	-1.511392	7.156171
O	3.047132	-3.847864	6.436176
O	1.217041	-2.599340	4.966059
O	1.796448	-2.951811	2.344301
O	-3.519525	4.436269	3.774194
O	-3.033206	6.772740	4.494190
O	-5.349615	5.684793	2.304078
O	-4.770208	5.332322	-0.317682
O	0.841560	-1.053267	-4.255238
O	4.228288	-0.734754	-3.379828
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O	5.356927	-2.151178	-1.666161
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O	5.014124	1.285534	-5.057634
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O	-4.216998	-5.799148	1.440207
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O	3.896820	5.462217	1.034036
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O	6.636945	1.829254	1.316503
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O	6.863212	-1.978278	2.256932
O	4.717567	-0.369681	2.099636
O	8.627851	-1.919109	-1.295317
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O	7.163692	4.542439	-2.546202
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O	-1.877377	-8.381365	1.122858
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H	-0.590198	-6.588423	-5.052590
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H	-3.709766	-0.018828	-4.893176
H	1.649964	-2.859141	3.343853
H	1.496829	-3.913185	2.237421
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H	1.720950	-4.631517	-3.062529
H	-3.212835	2.142382	-4.542684
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H	-6.770907	-3.428212	5.140450
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H	1.686677	0.092385	-2.867193
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H	2.327022	-2.239234	0.276422
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H	-0.442155	-8.899271	-3.996966
H	-7.721698	-2.322472	-1.639474
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H	-6.992290	-3.626925	0.198960
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Snapshot 5

293			
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Snapshot 6

299			
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H	2.503586	9.492621	-0.207769
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H	-5.482313	7.498596	0.410431
H	-6.561859	1.890360	3.738968
H	-5.957459	0.501680	3.757457
H	-7.016003	-6.047821	2.101596
H	-6.270183	-4.779777	1.500137
H	-0.463583	-3.782654	7.195361
H	-1.094423	-3.895868	8.571755
H	-3.009032	-4.962226	1.577054
H	-4.558412	-5.134684	2.171761
H	-7.081457	-2.853295	-1.302089
H	-8.620201	-3.036630	-0.976720
H	-2.223123	-4.331384	-0.416495
H	-2.119595	-5.766625	-0.364805
H	-8.056560	3.266497	2.784527
H	-6.620779	3.911239	3.151657
H	-6.934854	1.641260	1.465854
H	-7.304959	0.514406	0.236452
H	-7.374161	-2.196119	0.995743
H	-7.209050	-0.928013	1.791960
H	-5.429371	-4.194871	-2.119130
H	-5.594681	-2.950408	-3.032611
H	-4.183553	2.006734	6.232558
H	-5.526961	1.535796	5.680133
H	-7.932868	0.644468	-1.766817

H	-8.270461	-0.816223	-0.993446
H	-3.453016	-6.503397	5.134181
H	-3.029223	-5.633668	3.899484
H	-6.231543	-2.458321	4.933100
H	-6.906622	-2.222411	3.533560
H	6.654192	-3.490237	-1.658017
H	7.524115	-4.735179	-1.740180
H	7.248020	1.342293	0.584675
H	7.304822	1.408527	-1.009860
H	7.572217	-1.677932	0.688195
H	8.942415	-1.073655	0.320115
H	5.872355	0.417479	-2.154675
H	6.481409	1.669538	-3.109238
H	5.502142	4.727900	-0.788357
H	6.699192	4.939148	0.239994
H	5.034303	5.275198	-3.669291
H	3.813319	4.436461	-4.131202
H	4.659588	3.613766	-2.326003
H	5.005065	2.440484	-1.296611
H	6.563953	2.016180	-5.341896
H	6.022658	3.289653	-4.422966
H	-2.035550	-8.123131	-0.152884
H	-2.250663	-7.778974	-1.611487
H	2.876812	-8.893635	-0.355268
H	2.474039	-7.415560	0.100763
H	1.913398	-8.519827	-3.134916
H	1.252959	-8.057186	-4.580746
H	3.883233	-5.145674	-2.626628
H	5.455700	-5.765517	-2.514878
H	4.740797	-6.487485	4.640947
H	5.744310	-5.739355	3.540390
H	5.062928	-5.356317	1.165188
H	4.614411	-5.193354	-0.320209
H	-0.671087	-1.977326	8.474886
H	-0.850143	-0.690174	7.556035
H	4.049201	-0.642006	6.311616
H	4.000894	0.831335	7.060368
H	-0.920604	-0.463051	5.543459
H	0.017539	0.786881	5.509983
H	0.690956	0.303383	8.840901
H	2.164335	-0.050582	8.130394
H	6.860752	2.245038	4.332437
H	5.322007	2.061703	4.657805
H	-0.080304	6.439676	6.240241
H	-0.740743	6.902317	4.794411
H	6.009341	5.742802	3.867709
H	5.671746	4.282110	4.641079

Snapshot 7

296			
O	3.417526	-2.346870	1.314855
O	4.100357	0.167488	1.278987
O	1.942478	1.463134	0.461376
Cd	-0.090823	0.165670	0.250443
O	-0.968426	2.216767	0.466195
O	0.727064	-1.979231	1.001168
O	-1.466551	-0.044839	2.346962
O	0.475469	0.081588	-2.065648
O	-1.699840	-1.420835	-0.594029
O	1.824696	3.156462	-1.441407

O	3.644656	4.776301	-2.122779
O	3.271249	7.002935	-2.057213
O	1.140631	2.763816	-3.882699
O	-0.326547	3.545952	-5.543469
O	0.566564	-3.926248	-0.703891
O	-0.859821	-2.432844	3.229560
O	4.025874	7.988077	0.259681
O	1.500687	2.325483	2.905849
O	-1.274301	-1.131264	-3.617578
O	-1.430406	-0.314678	-6.071981
O	-2.013577	-4.484159	-0.938682
O	-4.259657	-4.561771	-1.625414
O	-3.439919	2.298231	1.457073
O	-2.770755	2.653463	3.958013
O	6.562423	1.211105	0.881295
O	7.712300	2.036643	-1.309379
O	3.726736	-3.747772	3.616713
O	3.109060	0.359876	3.888749
O	5.355140	0.437487	4.575481
O	-5.868032	-2.596164	-2.608313
O	-5.426241	-3.458511	-5.052788
O	-3.268362	-4.754157	-4.235175
O	-0.806296	-3.710540	-4.632868
O	0.343581	-2.885003	-6.823542
O	-3.665182	-0.143312	-7.618938
O	-4.038590	2.083323	-7.553373
O	-3.283964	3.068465	-5.236479
O	5.879433	4.604936	-0.575821
O	6.035536	3.788348	1.878582
O	-0.295454	1.635340	4.839808
O	-0.518889	-0.524006	5.739695
O	-7.664172	-3.286307	-0.674355
O	3.088123	-0.715398	-1.914465
Cl	4.206184	0.017832	-2.669606
O	3.601153	0.647194	-3.954759
O	5.267493	-1.003724	-3.100993
O	4.804406	1.106321	-1.854580
O	2.916269	-1.723569	5.654525
O	5.044459	-0.778615	7.035085
O	-4.452450	-6.645216	0.140363
O	-2.324261	-5.700262	1.520922
O	-3.332244	-3.740540	3.056084
O	-0.743167	-7.871023	1.121316
O	-1.503279	-8.566926	-0.990661
O	2.595562	-4.040273	7.083945
O	4.249344	-3.304340	-1.140418
O	7.976402	-0.124380	-3.018381
O	2.749725	-1.905929	-4.744478
O	2.357081	-4.070259	-3.065010
O	3.892975	-6.087671	-3.724961
O	3.292434	-7.704555	-1.663061
O	1.765969	-6.565679	0.195744
O	-5.163296	-2.672866	0.545761
Cl	-5.235890	-1.210226	0.941192
O	-6.702251	-0.807072	1.008989
O	-4.422597	-0.910755	2.245203
O	-4.573089	-0.387911	-0.201051
O	-5.615811	-0.452186	4.711167
O	-4.148634	-1.234321	6.371937
O	6.099140	-3.431321	5.172837

O	-5.217199	2.032105	6.065463
O	0.245110	5.966638	-4.136985
O	-1.551073	3.084567	-2.210336
O	-2.791950	5.204172	-1.502641
O	-2.851016	5.392228	1.099801
O	-3.451132	1.350231	-2.774114
O	-6.025020	0.787776	-2.712121
O	-7.527660	1.432703	-0.677463
O	-6.093067	3.046184	-0.222303
O	-7.619532	4.185061	1.636502
O	-5.492524	4.663068	-2.284203
O	-1.935882	7.009400	3.078590
O	-0.217823	6.352315	4.818697
O	-2.024926	4.924450	5.707788
O	1.284817	5.707388	2.784038
O	3.858705	6.269842	2.722044
O	-7.058095	0.431337	-5.252437
O	0.251742	5.350949	0.243722
O	0.311715	7.132605	-1.336238
O	-0.106104	8.972802	0.064336
O	-1.760867	0.633269	8.076648
O	-2.073760	2.869321	8.015018
O	4.902738	3.786058	-4.526900
O	2.593851	-6.361858	3.118978
O	0.184631	-7.165073	4.476875
O	-0.156686	-6.097404	-3.054980
O	7.212033	-1.175759	2.459182
O	7.449618	-3.741337	1.637833
O	6.534485	-5.358508	-0.340957
O	5.609997	3.498776	4.902129
O	2.107478	0.177389	-7.028237
O	4.521020	1.483049	-6.872766
O	-2.689997	-5.823857	5.339847
O	-5.136155	7.446398	0.300340
O	5.565472	-3.249178	-5.625453
O	-6.870126	-4.232604	4.012343
H	3.620699	-2.800574	2.147863
H	3.825168	-2.808054	0.489977
H	-1.149256	6.896670	3.746626
H	-2.490532	7.743259	3.531867
H	1.385404	-5.751085	-0.175625
H	0.942046	-7.106297	0.353393
H	2.456583	-3.297404	-3.730666
H	2.960870	-3.718006	-2.372304
H	4.725861	-2.591264	-1.594082
H	4.889435	-4.038288	-1.075958
H	-1.921134	4.005437	-1.968360
H	-0.704492	2.973991	-2.669704
H	7.228862	-0.679570	-3.096948
H	8.541737	-0.644079	-2.430071
H	-1.979886	-5.317848	-1.404107
H	-3.092490	-4.286767	-1.042466
H	-2.830117	2.076740	-2.490917
H	-2.855033	0.625153	-3.014423
H	0.561883	3.113444	-4.620079
H	1.620251	1.903633	-4.132890
H	4.988433	4.730700	-5.018147
H	4.805251	3.120649	-5.237988
H	-4.358900	2.418267	1.060869
H	-3.331552	2.396839	2.498596

H	-0.050242	2.239835	5.617310
H	0.267456	2.003233	4.081223
H	-0.447891	-4.128862	-0.951326
H	0.929890	-3.892850	-1.656905
H	-6.452361	0.746528	-3.659077
H	-5.070720	0.940356	-2.830629
H	-3.314618	2.283634	4.659479
H	-1.848633	2.269369	4.062780
H	2.788167	3.492642	-1.640420
H	1.480325	2.981650	-2.402703
H	-5.416757	-0.505336	3.768916
H	-6.556490	-0.810843	4.830965
H	-1.653258	-3.091408	3.241164
H	-0.337116	-2.531286	2.443948
H	-2.234735	-0.308933	-6.622990
H	-0.831558	0.419680	-6.361408
H	2.995848	-0.951048	-4.658647
H	2.090620	-1.933219	-5.439873
H	-6.609692	-0.325981	-5.614876
H	-7.147750	1.109948	-6.007342
H	-1.069992	5.239718	5.450780
H	-2.473406	4.440801	4.987474
H	0.830426	-6.105342	-2.773627
H	-0.556081	-6.806979	-2.530896
H	-1.256566	-7.091910	1.499162
H	-0.889284	-8.595115	1.801836
H	-0.165143	-4.152068	-3.994326
H	-0.293175	-3.503528	-5.472390
H	4.745762	-3.694102	3.920909
H	3.260836	-3.163844	4.280323
H	-1.476727	-0.511474	-4.391427
H	-1.207087	-1.978118	-4.188035
H	1.520334	3.292979	3.001090
H	1.676887	2.123732	1.918391
H	-4.049069	0.746752	-7.657540
H	-3.245669	-0.286771	-8.545266
H	-3.157685	-6.274005	1.326901
H	-2.258243	-5.161453	0.692833
H	3.004971	-1.014252	4.965887
H	2.014115	-1.496869	5.987983
H	-3.960208	-3.217934	2.551420
H	-3.060656	-4.449322	2.393124
H	-2.418376	5.738839	1.914012
H	-2.824286	4.415159	1.215372
H	4.870746	-2.784921	-5.150309
H	6.152713	-2.592008	-6.102382
H	-3.971192	3.742990	-5.116334
H	-3.400191	2.361088	-4.609319
H	4.855620	-5.781199	-3.710068
H	3.377354	-5.256705	-3.669449
H	-0.182683	7.191356	-2.171965
H	1.289230	7.065823	-1.707131
H	2.976875	-5.472585	3.351545
H	2.191019	-6.197057	2.208194
H	0.284937	-3.533050	-7.573227
H	-0.126214	-2.091833	-7.072323
H	-6.983426	1.863887	0.073483
H	-6.879892	1.177858	-1.419371
H	3.916194	-0.838868	1.226132
H	5.020046	0.335113	0.959280

H	-2.579451	5.405282	-0.550780
H	-2.910860	6.042540	-2.006119
H	3.468643	0.209142	2.966633
H	2.685568	1.209253	3.925047
H	2.946043	-7.294849	-0.850302
H	3.541857	-6.954120	-2.310097
H	-5.552480	2.832758	5.603368
H	-5.412552	1.226283	5.503043
H	0.018465	-0.368286	-2.835872
H	-1.950287	2.067975	0.688573
H	-2.646377	-1.336914	-0.517266
H	0.625298	-2.690026	0.296517
H	1.839186	2.171435	-0.314992
H	-1.360125	-0.932247	2.811219
H	2.877200	1.046487	0.560385
H	-2.438884	0.099101	2.449579
H	-1.108383	2.690928	-0.397783
H	-1.593063	-1.682907	-1.576903
H	1.421120	-0.188708	-2.083969
H	1.668787	-1.979835	1.175981
H	3.564802	7.608314	-2.773497
H	3.933230	7.074560	-1.346257
H	-3.745035	2.688700	-8.269656
H	-3.376607	2.154946	-6.842417
H	-0.127494	3.492800	-6.485720
H	-1.267226	3.187294	-5.423671
H	3.727583	0.824484	-6.861163
H	5.043724	1.384606	-7.658379
H	1.479514	0.699994	-7.532901
H	2.379066	-0.531393	-7.691197
H	-0.052279	6.797213	-4.571376
H	-0.008818	5.188502	-4.714785
H	6.269352	-3.411885	6.187640
H	6.528919	-4.273263	4.762371
H	8.236245	-3.854068	2.305870
H	6.894968	-3.007478	2.091110
H	-1.396732	-8.719644	0.299612
H	-1.073499	-9.408868	-1.401127
H	6.967124	-5.011898	0.473254
H	6.561214	-6.335577	-0.225385
H	5.388832	-0.396202	4.110055
H	4.283860	0.649227	4.487599
H	4.479720	6.996352	3.005242
H	4.454804	5.544765	2.481736
H	-1.760433	3.425374	7.267790
H	-1.413439	2.962910	8.724967
H	0.857476	5.666140	1.837081
H	2.239117	5.859968	2.665530
H	5.075103	4.610681	-1.126830
H	6.478281	5.339294	-0.865249
H	0.700145	4.593631	-0.118717
H	0.162085	6.029561	-0.511183
H	8.199145	-1.183697	2.740536
H	6.812637	-1.885333	2.983267
H	7.203576	0.769578	1.519838
H	7.075544	1.418117	0.041773
H	5.833111	4.408138	1.104732
H	6.102750	2.941494	1.308125
H	3.260770	5.666365	-2.161381
H	4.064169	4.632842	-3.049108

H	4.211034	-1.352358	6.841064
H	5.110475	-0.239806	6.206996
H	3.338646	8.662602	0.379825
H	3.909647	7.280700	0.886840
H	7.653656	1.388595	-2.059064
H	7.242505	2.829812	-1.558161
H	0.326411	6.783498	5.569642
H	0.429945	6.097470	4.076787
H	4.663460	3.582697	4.978893
H	5.716773	3.236705	3.919257
H	-7.418961	-2.681811	0.103147
H	-7.101263	-2.918414	-1.432940
H	-5.848383	-1.628667	-2.513073
H	-5.691832	-2.797916	-3.595772
H	-4.363747	-5.935899	-0.548276
H	-5.354603	-6.418516	0.473820
H	-3.452525	-5.760513	-4.288031
H	-2.348672	-4.586532	-4.554882
H	-3.900076	-4.712506	-2.547529
H	-4.683150	-3.712394	-1.589115
H	-5.529532	-2.750210	-5.829156
H	-4.491519	-3.875159	-4.953778
H	-8.000096	4.999654	1.265132
H	-8.443453	3.644441	1.794152
H	-0.569343	8.527698	0.837842
H	-0.009902	8.227668	-0.615195
H	-4.659638	8.159472	-0.153325
H	-4.496065	6.712451	0.364801
H	-4.529881	4.969539	-2.269310
H	-6.008146	5.494035	-2.228692
H	-6.439458	3.455890	0.590457
H	-5.843642	3.796619	-0.869339
H	-2.120167	1.529778	7.985840
H	-1.341044	0.426745	7.162453
H	1.848023	-4.595463	7.005379
H	3.160897	-4.559972	7.672256
H	-4.719639	-0.880009	5.625686
H	-3.669013	-2.094504	6.121746
H	-0.447362	0.349720	5.222694
H	-0.616377	-1.189416	5.028606
H	-7.674455	-4.226859	3.461334
H	-6.271278	-3.498247	3.722915
H	-2.443873	-4.868977	5.425677
H	-3.349101	-5.851147	4.644451
H	-0.510095	-6.700816	4.952019
H	0.771872	-6.507903	3.999946

Snapshot 8

305

O	3.039184	-3.369644	0.448321
O	3.968612	-1.301167	1.436948
O	3.786926	-1.378638	4.004858
O	5.939248	-2.763978	4.172634
O	3.933553	-3.720632	-1.995016
O	5.418643	-5.736927	-2.062367
O	2.049655	-3.083156	-3.595983
O	2.649847	-1.060293	-5.157850
O	2.306002	-5.225739	2.182410
O	1.747824	-5.137217	-5.239452
O	2.118057	-3.435324	4.162776

O	3.922028	-3.950517	5.892751
O	4.345169	-5.572926	-4.809519
O	0.102543	-3.520390	-1.741791
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Snapshot 9

305

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O	0.835039	-7.853103	-1.195193
O	2.139280	-5.244038	4.739788
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O	-2.320380	7.479121	-1.823842
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H	0.907381	-7.575280	-2.113651
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H	0.391063	5.608056	-1.200378
H	-0.702344	6.563722	-1.953861
H	2.441194	3.433714	2.620936
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Snapshot 10			
296			
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Snapshot 11

275

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H	2.209654	7.493900	0.850513
H	3.600862	7.905845	1.608930
H	0.833422	8.498579	-1.614866
H	-0.118936	7.231513	-2.141099
H	1.498717	6.798488	-1.051819
H	2.727744	5.861959	-0.672025
H	8.635779	-2.249060	-1.799048
H	9.109234	-0.908678	-1.199399
H	5.437334	-5.408209	-5.021526
H	4.605644	-4.751340	-3.913033
H	6.463115	-6.204442	0.175889
H	8.081703	-6.365993	0.194237
H	5.047130	-0.900005	-4.637400
H	6.302593	-1.686617	-4.588042
H	8.688530	-3.378575	1.530495
H	8.318273	-2.150909	0.448367
H	6.773789	-0.911886	-1.398068
H	5.891887	-0.631660	-2.692622
H	3.544383	-3.941461	6.249953
H	2.639362	-2.648276	6.375327
H	5.281069	0.477637	4.123040
H	4.298026	1.253277	5.040692
H	1.501823	-2.410348	4.330810
H	1.613487	-0.755360	4.719396
H	4.281576	-1.979294	6.778062
H	5.105274	-0.512590	6.419966

Snapshot 12

284

O	2.804928	-1.770383	2.931084
O	2.301424	-1.653141	5.459637
O	4.722037	-1.546018	6.159173
O	0.472938	-0.745324	2.212646
Cd	-0.111370	0.340843	0.247510
O	-0.509055	2.240054	-1.016664
O	-1.295782	1.824826	1.852923
O	2.246934	1.271757	0.200425
O	0.647367	-1.259380	-1.101029
O	-2.000298	-0.811516	-0.126289
O	4.067800	0.217264	1.625212
O	-1.424632	-2.576604	-1.906803
O	-2.148534	4.179726	-0.488318
O	-4.233928	4.494488	-1.471524
O	-0.061833	-3.241672	1.721905
O	1.489223	-4.207307	-0.011049
O	-2.651759	-3.554864	1.590499
O	3.929832	-3.705835	0.865101
O	2.642072	2.085681	-2.299934

O	1.771523	4.449639	-2.309344
O	2.490245	5.206742	-4.688506
O	2.164176	0.572619	-4.459401
O	1.219334	0.752589	-6.874013
O	2.005291	3.308775	-6.667892
O	6.768072	0.205871	1.659947
O	7.843828	-0.086907	-0.685662
O	8.049976	-2.228122	-1.843289
O	-0.754681	5.396999	-2.541307
O	-2.112817	4.046686	-4.228696
O	-4.482003	4.745136	-4.178630
O	-0.856853	1.812029	-3.788027
O	-2.438728	-0.096913	-4.622822
O	-1.682409	0.543233	-7.061910
O	-4.597348	-0.215201	0.357339
Cl	-4.789617	0.768454	1.471907
O	-6.248723	0.652666	1.986934
O	-3.755467	0.548715	2.570550
O	-4.556901	2.154078	0.885576
O	-4.912798	-0.133568	-3.504918
O	-6.089945	-1.725593	-1.651376
O	-7.808775	-0.723990	-0.106033
O	-4.185346	-3.233740	3.818663
O	-5.102458	-3.307171	0.379827
O	-1.739691	-5.274377	-1.505682
O	-0.663936	-5.567155	-3.851291
O	1.536518	-4.449919	-2.907176
O	-4.439963	-5.262984	-1.540416
O	-6.260830	-4.208491	-2.965202
O	-5.865692	-3.394566	-5.465561
O	-6.736241	-1.030608	-5.474971
O	0.891056	-3.417256	-5.335669
O	7.083131	2.903644	1.258826
O	-6.665038	-4.120108	2.493984
O	1.080326	-6.874366	0.570584
O	3.449512	-7.572816	0.520519
O	4.807650	-6.222504	2.207907
O	1.328403	-7.125015	3.277689
O	-3.498033	-2.950598	-6.819526
O	-1.784666	-2.829807	-4.751726
O	5.009731	2.529647	-3.653897
O	5.278506	0.647218	-5.384173
O	5.101625	4.536730	-5.390151
O	6.723098	2.650439	-1.586097
O	0.503032	-3.535295	6.452421
O	-0.213682	-4.839753	4.095307
O	-2.762165	-5.641331	4.511184
O	-4.797818	-0.756804	4.953514
O	-4.152356	-1.789466	7.382006
O	6.069035	5.383334	-1.457194
O	3.594965	5.346681	-0.339289
O	2.417817	3.754653	1.514253
O	0.698987	4.756258	3.059595
O	-0.410371	3.307674	4.905007
O	-0.679145	5.190102	6.635282
O	-0.587251	7.197184	4.899030
O	-1.620354	5.507399	1.946176
O	-3.683585	5.969229	3.621288
O	-4.469542	3.413044	3.415167
O	-3.524700	3.233075	5.829779

O	3.405306	2.173075	3.545455
O	5.856003	1.925384	4.756127
O	4.322416	2.246508	6.984291
O	1.842724	1.360140	5.659611
O	0.026245	7.836899	2.276487
O	2.419570	7.526291	1.111363
O	-1.691788	-7.360840	0.394400
O	6.815975	-1.880592	3.560030
O	7.034125	-3.973039	2.789941
O	5.573540	-1.155518	-2.714101
Cl	4.406696	-2.021037	-2.280738
O	3.600274	-1.334448	-1.210836
O	5.011370	-3.307433	-1.751925
O	3.494056	-2.305437	-3.493039
O	4.295470	-2.097928	-5.866874
O	-1.393406	0.562526	4.422307
O	-6.088193	2.046044	-2.054265
O	-8.481517	2.356651	-0.889141
O	-7.371286	3.203689	3.227270
O	-2.050140	-3.789331	7.854625
O	3.638733	-6.449784	-2.434558
O	1.471795	7.646462	-1.959276
O	-7.035968	2.166215	-5.124904
H	2.508277	-1.580238	3.886633
H	3.342039	-2.564785	2.925957
H	1.171075	8.310879	-1.263658
H	2.087197	7.073762	-1.484004
H	-0.182038	-4.226161	3.237815
H	-1.193129	-5.075014	4.131952
H	1.478479	-4.151144	-0.983420
H	2.330399	-3.920619	0.400484
H	4.235283	-3.367528	0.041843
H	4.542184	-4.453247	1.106943
H	-1.409486	2.592333	-4.120043
H	-0.178515	1.765773	-4.506467
H	7.086035	-2.365573	-1.902340
H	8.404020	-2.915833	-1.195457
H	-2.699889	-4.484255	1.574582
H	-3.460283	-3.250944	1.078300
H	-1.788590	0.500444	-4.123129
H	-2.036127	-0.998814	-4.681775
H	1.939632	0.521308	-5.461403
H	2.239226	-0.378007	-4.215172
H	5.429663	1.270081	-6.136284
H	4.875482	-0.178990	-5.817554
H	-3.157680	4.339574	-0.651638
H	-1.876575	4.721339	0.301664
H	1.097157	5.393392	3.689518
H	1.385367	4.282713	2.507944
H	-1.002567	-3.247462	1.395904
H	0.438449	-3.703622	0.952819
H	-5.585872	-0.433276	-4.182248
H	-3.980631	-0.194440	-3.847281
H	-2.314772	5.666055	2.632609
H	-0.780991	5.143580	2.384424
H	3.529238	2.394882	-2.686433
H	2.321680	1.516894	-3.065267
H	-4.203427	2.935580	2.518217
H	-5.437672	3.114318	3.497750
H	-1.436786	0.069370	5.289338

H	-0.761189	0.078778	3.818242
H	-2.444166	-2.808829	-5.465644
H	-0.879195	-2.969053	-5.116549
H	1.735311	-3.537260	-3.327890
H	0.707237	-4.814281	-3.396851
H	-6.534843	-2.032697	-5.498279
H	-6.416995	-0.623103	-6.358157
H	0.938630	7.506381	1.954460
H	-0.516641	7.047480	2.094361
H	-0.747716	-7.270410	0.730181
H	-2.335311	-7.113600	1.136408
H	-3.299232	-4.842878	4.490343
H	-2.827837	-6.113866	5.426449
H	-1.480809	-5.924008	-0.723292
H	-1.328064	-5.564392	-2.422725
H	3.272446	-1.766666	5.735252
H	2.114991	-0.672923	5.595610
H	-1.675768	-2.629629	-2.877931
H	-1.497623	-3.552795	-1.648536
H	2.789024	4.368699	0.885016
H	2.169938	2.947401	0.969752
H	-2.876584	-2.378237	-7.370029
H	-3.513694	-3.788127	-7.283842
H	-5.014050	-3.623825	3.421762
H	-3.553016	-3.190952	3.091148
H	2.164048	1.464131	4.713157
H	1.054074	1.978560	5.668312
H	-4.572354	-0.264943	4.148147
H	-4.602059	-1.736043	4.757687
H	0.224837	5.056432	-2.559435
H	-1.150754	4.851952	-1.745112
H	2.818901	-5.918195	-2.495412
H	4.442167	-5.998144	-2.894185
H	-2.090116	1.546453	-7.151086
H	-1.896206	0.369285	-6.084072
H	1.941608	-7.277854	0.351735
H	1.217503	-5.860308	0.499274
H	2.041613	4.607087	-5.396303
H	3.429200	5.082345	-5.007233
H	0.978682	-2.730747	6.060871
H	0.345117	-4.040340	5.623922
H	-0.454869	-6.554727	-4.350668
H	-1.159801	-5.073568	-4.480203
H	-5.467431	2.484651	-1.359499
H	-5.436598	1.346640	-2.421819
H	3.639304	-0.620993	1.912011
H	5.066179	0.120011	1.576756
H	-1.445587	4.723971	-3.753829
H	-2.116069	4.322891	-5.218928
H	3.689811	1.491333	2.852095
H	3.090275	2.937644	3.028668
H	0.858226	-6.332986	3.656992
H	1.178448	-6.946453	2.290926
H	-4.215653	6.714358	3.160317
H	-4.178039	5.037789	3.444854
H	0.032637	-1.984738	-1.459038
H	-1.212875	2.904811	-0.834523
H	-2.883225	-0.342749	-0.053163
H	0.281981	-1.760411	2.047556
H	2.679654	1.554237	-0.747402

H	-1.965723	1.343675	2.389847
H	3.064371	0.913794	0.682015
H	-1.705653	2.433022	1.219330
H	-0.725009	1.999509	-1.935512
H	-2.050082	-1.415163	-0.912360
H	1.595737	-1.335127	-1.366725
H	1.467777	-0.831389	2.273422
H	5.367764	4.893984	-6.272880
H	5.673015	4.935300	-4.711546
H	1.485450	0.275126	-7.770963
H	0.251205	0.453863	-6.791431
H	4.252090	-2.591084	-4.999843
H	4.927687	-2.581676	-6.470939
H	1.116520	-2.925395	-6.141036
H	1.086814	-4.396495	-5.531496
H	1.473222	4.053903	-7.128863
H	1.510837	2.377334	-6.844326
H	5.061329	-1.019605	7.060260
H	5.004969	-2.484645	6.327226
H	6.733404	-3.308622	3.485559
H	7.649527	-4.545739	3.265212
H	5.787167	-6.563071	2.189779
H	4.411577	-6.767551	3.004102
H	4.116742	-6.895531	0.995385
H	3.446261	-7.296612	-0.469714
H	5.807873	0.995992	4.740210
H	5.047479	2.229304	4.243928
H	6.719172	5.980692	-0.957502
H	6.471636	4.481433	-1.516147
H	-0.321112	7.554438	4.016301
H	-0.015861	7.595754	5.577635
H	2.921891	5.046971	-1.016619
H	4.527131	5.285807	-0.681652
H	6.063599	2.671417	-2.300016
H	7.628569	2.511194	-1.950920
H	1.972921	3.447550	-2.332652
H	2.090769	4.857144	-3.192530
H	7.760046	-1.790163	3.895811
H	6.172452	-1.633352	4.302038
H	7.026953	-0.443760	2.442338
H	7.179700	-0.084145	0.742905
H	6.831995	2.850618	0.287698
H	7.010140	1.927453	1.517094
H	5.631181	3.102009	-4.204400
H	4.994072	1.692119	-4.118213
H	3.493712	1.856422	6.587390
H	4.954746	2.289296	6.256775
H	8.052895	-1.074480	-1.185038
H	7.347963	0.406680	-1.314573
H	3.040332	7.964898	1.806130
H	3.071165	6.826887	0.743809
H	-7.336689	2.830632	-4.429286
H	-6.420565	1.593515	-4.649633
H	-7.410605	-0.086855	0.523890
H	-7.122395	-1.197534	-0.657685
H	-4.978526	-3.085365	-5.852060
H	-6.186085	-3.963353	-6.230893
H	-7.569132	2.026134	-1.211169
H	-9.024403	1.567232	-1.071267
H	-5.718738	-1.111548	-2.280613

H	-6.337824	-2.532846	-2.195877
H	-6.343715	-4.016116	1.547530
H	-7.453689	-3.501687	2.502684
H	-4.868458	-6.101241	-1.253616
H	-3.441584	-5.360237	-1.588872
H	-4.817952	-3.988914	-0.313533
H	-5.417488	-2.542603	-0.136959
H	-5.828110	-3.926011	-3.913030
H	-5.443392	-4.566454	-2.483613
H	-3.620722	4.341648	-4.397480
H	-4.344828	5.759193	-4.249941
H	-4.704105	5.286516	-1.092221
H	-4.383882	4.673049	-2.458286
H	-0.057695	5.762463	6.084779
H	-0.694805	4.352575	6.170967
H	-3.749245	3.181763	4.827777
H	-3.449650	2.282449	6.074008
H	-0.259214	3.930535	4.152896
H	-0.813395	2.481465	4.471626
H	-3.953563	-0.876808	6.961292
H	-4.981637	-2.153827	6.892331
H	-2.869972	-3.257742	7.793771
H	-1.246706	-3.337690	7.394997
H	-7.778993	4.206909	3.138095
H	-7.585082	3.029741	4.205108

Snapshot 13

287

O	2.878477	-2.632785	2.181665
O	2.557051	-2.496026	4.694945
O	0.453525	-1.676667	1.408000
Cd	-0.019878	0.116621	-0.068804
O	-0.645007	2.170686	-1.118393
O	-1.105502	1.122951	1.773155
O	2.016439	1.289493	0.513777
O	1.053622	-0.432698	-2.186447
O	-1.789042	-1.131967	-0.984733
O	-3.999379	0.193604	-0.970813
Cl	-4.722726	0.039110	0.359416
O	-5.929840	-0.814359	0.277545
O	-3.764006	-0.462430	1.506166
O	-5.070711	1.492459	0.707488
O	-0.339068	-3.953203	0.437360
O	-2.672831	-4.204714	-0.759039
O	-4.678511	-3.151588	-1.851975
O	1.925941	3.265232	2.270034
O	3.331060	1.629403	3.837171
O	5.336741	0.576277	4.930106
O	-6.083630	-1.515759	-3.419111
O	-5.993133	-3.491498	-5.175368
O	2.643004	2.190876	-1.916687
O	-1.168175	2.050136	-3.767993
O	1.321275	1.638718	-4.211895
O	0.815162	2.437332	-6.459064
O	-1.614148	2.497457	-7.217713
O	-2.698239	0.886207	-5.508820
O	-1.766389	4.674187	-3.873456
O	-3.979445	5.522521	-3.771581
O	-0.782339	5.510329	-1.634508
O	-4.072250	4.223384	-1.514702

O	1.774594	4.824558	-1.454927
O	2.909192	6.353600	-3.033970
O	2.520854	5.705559	0.914521
O	1.984490	0.059233	5.592201
O	3.812201	0.741999	7.183618
O	-6.025082	-4.721757	-0.096943
O	-4.197370	-4.038993	1.494473
O	-7.984490	-1.067131	-1.528013
O	-8.460341	-2.870190	-0.450398
O	-0.918050	-2.009240	-3.415879
O	-1.021299	-1.412177	-5.944842
O	-0.985881	-4.668758	-3.694162
O	0.840720	-4.664368	-5.442480
O	1.817167	-2.740985	-6.169452
O	-0.636754	-6.711303	-1.927830
O	-0.165931	-5.818588	2.435030
O	0.641659	-5.067221	4.929714
O	-1.633433	-4.928885	6.174614
O	-3.771125	-3.450720	6.120522
O	4.041898	-0.139044	1.841130
O	-3.967674	-4.920036	-3.848014
O	-4.702443	-2.193773	3.494818
O	-5.678890	-4.117157	4.221792
O	2.748483	-3.997930	-3.543750
O	4.886176	-5.476094	-3.489658
O	3.907997	-1.544291	-3.433171
Cl	4.591445	-1.450377	-2.052133
O	3.415181	-1.656451	-1.008965
O	5.667563	-2.547755	-1.879595
O	5.208467	-0.085372	-1.916000
O	5.034735	-1.622972	-5.948276
O	2.202411	-4.439410	-0.864007
O	1.998939	-7.002465	-1.030125
O	1.906133	-8.301601	1.226753
O	4.702799	-4.339073	0.232968
O	-6.104499	2.532242	-2.355915
O	-2.887173	-6.401799	2.450290
O	-3.252180	-7.405511	0.827548
O	5.233369	2.950899	-2.630817
O	5.649422	5.003595	-3.555549
O	6.068839	1.363592	-4.425526
O	8.278499	-1.753548	-1.247091
O	8.850290	0.116625	0.246663
O	7.023688	0.112234	1.994981
O	7.091519	2.771752	2.273265
O	6.988270	3.368815	-0.255698
O	7.372817	-1.930311	3.761314
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O	-5.198334	2.185926	5.452378
O	-8.133756	3.044665	2.446559
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O	-5.488717	0.924567	-4.774624
O	-1.275585	8.185912	-2.508487
O	5.196045	-7.014657	1.106947

O	4.757391	-2.624519	6.516692
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O	-0.450770	1.910799	5.238747
O	1.905072	7.313233	3.333229
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O	-1.484874	-1.075761	3.715995
O	-7.540908	-0.864966	3.719430
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Snapshot 14

278

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Snapshot 15

299

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H	4.397175	-7.262788	-1.866569
H	5.307562	-6.652582	-0.580774
H	1.261315	-9.637423	-0.685791
H	1.073782	-8.219627	-0.433162
H	-0.641138	-6.880192	2.463039
H	-1.456090	-8.097369	1.920696
H	-2.910860	-6.436826	-0.513306
H	-2.252027	-6.365410	0.936685
H	-5.008669	-2.128182	-5.320473
H	-5.205494	-0.579926	-5.395574
H	-0.726704	-1.048171	-6.233341
H	-1.921878	-0.239728	-5.455802
H	-8.228614	0.229818	-1.421286
H	-6.792768	0.607239	-2.029764
H	-5.812887	3.499421	-4.683026
H	-6.901210	4.002861	-3.558145
H	-8.462121	-1.815763	-0.178465
H	-8.553222	-0.636281	0.600748
H	-5.133705	5.384168	-4.340768
H	-3.646802	5.706443	-4.026277
H	-7.385859	-4.783771	-3.031759
H	-7.821391	-3.160681	-3.108216
H	-7.893118	3.908772	-1.513428
H	-7.925063	2.473517	-2.142634
H	-6.185203	6.855018	-1.225230
H	-5.168318	6.658460	-2.442128
H	-7.682919	-0.933767	2.011596
H	-8.878092	-0.125323	2.789135

Snapshot 16

299

O	2.309845	2.761220	-2.388461
O	3.406007	0.471806	-2.411071
O	2.336587	0.032758	-4.740980
O	0.621762	1.687788	-5.653950
O	1.483263	3.854954	-4.609378
O	3.607529	4.163254	-5.762793
O	4.556902	0.952296	-5.738724
O	1.902019	-1.265276	-1.090817
Cd	-0.094678	-0.105106	-0.217425
O	-0.537643	-2.323430	0.418783
O	-0.051319	1.963701	-1.263733
O	-1.558225	-0.490012	-2.061223
O	1.584774	0.574607	1.284278
O	-1.926109	0.618310	1.266276
O	-1.538718	-4.355798	-0.792368
O	-3.341606	-4.895478	0.892861
O	0.170706	1.417576	3.283958
O	-3.185423	0.784443	-3.694933
O	-0.249404	-3.259150	2.881533
O	-0.266703	-5.846370	2.910763
O	-2.660661	-6.162723	3.139254
O	-0.078648	-6.327882	0.391085
O	2.221215	-2.359761	3.098643
O	2.363105	-3.106358	5.486945
O	3.082284	-3.217632	0.760506
O	2.822146	-5.796259	0.474221
O	4.028205	-7.398040	1.582949
O	2.973793	-5.645306	-2.073064
O	2.237317	-6.979772	-4.136299
O	0.023746	4.120297	0.281588
O	-0.031989	-3.715434	6.495473
O	-0.229481	6.177904	-1.405461
O	-0.143177	6.143687	-3.979963
O	-2.391825	6.343201	-5.115280
O	-2.687955	7.007707	-0.958515
O	-3.434634	7.506321	1.431017
O	-1.204683	-1.831057	4.983076
O	1.318164	-3.133796	-2.931668
O	0.908757	-2.533537	-5.303048
O	-1.007075	-1.631346	-5.819787
O	-0.803442	3.758941	4.248900
O	1.223033	2.988721	5.856938
O	0.191611	0.462967	6.124603
O	2.566306	0.773697	7.286069
O	-1.906213	-3.689045	-4.215214
O	-4.354023	-4.777629	-4.503444
O	-4.164316	4.230289	-5.287681
O	-2.485261	4.295364	1.455086
O	-4.705575	3.375826	2.452829
O	-6.420400	5.030854	1.539859
O	-3.636155	3.814874	4.782739
O	-5.140143	2.077792	6.102992
O	-5.723998	0.209272	4.262143
O	-6.133405	0.809530	1.890762
O	-8.049236	1.711721	1.374023
O	-8.710542	0.734849	-0.647136
O	-8.162829	-1.091781	-0.076995
O	-5.148425	1.733519	-1.935330
O	-4.832274	-0.287576	-0.358020

Cl	-4.542552	-1.879610	-0.175231
O	-3.610042	-1.995895	1.015219
O	-3.774880	-2.412263	-1.385621
O	-5.778166	-2.693636	-0.018516
O	-7.523120	1.422789	-3.096795
O	-6.491698	3.948542	-3.364462
O	-6.225406	5.374338	-1.513546
O	-4.025831	4.234279	-0.888177
O	4.529308	-0.175379	5.526464
O	4.130186	0.900487	2.978987
Cl	5.160839	1.147279	1.771629
O	4.261258	1.209949	0.520381
O	5.857642	2.484834	1.969381
O	6.051444	-0.082814	1.607247
O	3.550416	3.270466	3.933718
O	2.540695	4.206524	1.768329
O	4.251916	4.067224	-0.179104
O	2.196043	6.941837	1.899130
O	4.590000	7.258188	1.670640
O	4.778054	6.776677	-0.849038
O	1.515099	8.209081	-0.347261
O	5.322906	5.383379	4.106118
O	-0.287452	6.843471	3.123636
O	3.016332	0.891213	-8.081987
O	-0.995811	-0.224972	8.574262
O	-5.351625	-2.146538	-3.734454
O	-5.493516	-1.399942	-6.122757
O	-7.746720	-2.755613	-2.725926
O	-5.086186	-6.926654	-0.165338
O	-4.999881	-6.960872	-2.739841
O	-4.804847	-3.636703	3.057513
O	-4.068371	-2.302237	5.120746
O	6.238721	0.415874	-2.944910
O	8.265196	-0.354346	-1.336872
O	8.531489	1.071450	0.514044
O	7.212869	-1.925491	-3.909851
O	7.233776	-2.880099	-1.069207
O	6.046354	-3.568039	1.380453
O	6.594067	-5.394669	1.950593
O	6.707660	-2.591165	3.401610
O	6.154471	4.572752	-2.286410
O	6.754710	3.500403	-4.070174
O	5.837480	-5.174126	-2.210733
O	3.360710	-5.737449	4.717954
O	1.297768	-8.531808	-1.046287
O	-0.658720	-6.488854	-4.727994
O	-7.700884	-3.145784	2.465815
O	5.116053	-2.724757	-5.927533
H	2.067406	3.255967	-3.281947
H	2.926770	3.388454	-1.870599
H	1.207328	-8.806225	-1.992952
H	0.654926	-7.791812	-0.911091
H	-0.034471	5.284181	-0.942943
H	-1.114101	6.519118	-0.980126
H	2.969945	3.744527	2.571387
H	3.229549	4.233896	1.019694
H	5.030982	3.532572	0.155991
H	4.567359	5.006813	-0.302356
H	-0.128347	-4.272039	3.045004
H	0.687634	-2.889390	2.925728

H	7.901039	1.053593	1.270541
H	8.530520	1.985767	0.058925
H	-2.556513	5.129883	1.915124
H	-3.113306	3.650663	1.937945
H	-0.745734	-2.410272	4.193320
H	-0.658523	-1.042804	5.179978
H	2.531851	-2.870688	3.946638
H	2.501898	-1.398588	3.185356
H	7.589638	-3.129820	3.403212
H	6.503774	-2.387603	4.345899
H	-2.472142	-4.716471	-0.300012
H	-1.723107	-4.495853	-1.757435
H	1.602159	-2.539265	-6.018899
H	1.284594	-2.823121	-4.407371
H	-0.792676	4.031456	0.857327
H	0.832499	4.117212	0.896195
H	-7.368144	-1.264703	0.459477
H	-7.965724	-1.359924	-1.036358
H	-4.230003	-2.275141	6.139520
H	-3.097209	-2.174261	5.052921
H	-2.882983	-3.967735	-4.324225
H	-1.625186	-2.879137	-4.751308
H	4.090451	-3.205152	0.830200
H	2.755419	-2.677686	1.589333
H	-4.796642	-2.236329	-2.848050
H	-6.247019	-2.096990	-3.283814
H	-3.913465	1.075263	-3.143345
H	-2.986018	1.693439	-4.104723
H	-0.277349	0.330406	7.041395
H	1.137476	0.208695	6.409206
H	3.903077	2.266462	3.724550
H	2.903870	3.187923	4.650567
H	0.324373	-6.421318	-4.627171
H	-1.207654	-5.731368	-4.554057
H	0.479230	7.409783	2.710282
H	-1.118997	6.970898	2.569432
H	-3.171062	6.200116	-1.220201
H	-3.090211	7.697206	-1.584503
H	-0.487101	4.606907	3.825954
H	-0.039741	3.565965	4.906332
H	2.414393	3.874966	-5.081025
H	1.013903	3.074651	-5.126730
H	0.238351	0.986995	4.242548
H	-0.268044	2.297753	3.547613
H	2.060714	-3.834912	-2.847482
H	1.587732	-2.486526	-2.304195
H	-0.652015	-1.195772	8.739324
H	-0.745316	0.316911	9.357972
H	-4.841671	4.756826	-0.642284
H	-3.393943	4.201804	-0.103004
H	1.239281	1.105443	-5.175165
H	-0.316703	1.353531	-5.569772
H	-5.213440	1.132159	-1.160864
H	-4.766120	2.690045	-1.694622
H	0.866710	-6.167643	0.261359
H	-0.620796	-5.557876	-0.053304
H	4.758514	4.599737	4.136685
H	6.226182	5.083171	4.395034
H	-0.521312	-4.579470	6.649633
H	-0.646032	-3.196243	5.940100

H	3.174596	7.109008	1.780865
H	2.180776	5.903159	1.911096
H	3.705124	-7.194756	2.454027
H	4.866951	-6.918141	1.541646
H	0.349240	5.377907	-4.327722
H	-0.149839	6.183493	-2.882266
H	1.323244	3.416675	6.758008
H	0.572719	2.212624	6.079889
H	-4.228728	-3.142145	2.490203
H	-4.637744	-3.295555	4.005312
H	3.173603	1.454126	-2.215327
H	4.216912	0.439047	-2.887848
H	-0.162810	-6.110621	1.882424
H	-0.165567	-6.551469	3.609167
H	2.687422	0.194832	-3.722975
H	1.602024	-0.747630	-4.745027
H	0.926582	7.523567	-0.797334
H	1.703644	7.734525	0.523074
H	-4.685617	-5.451325	-3.812118
H	-4.987126	-3.992588	-4.470365
H	1.222599	1.148513	2.008438
H	-1.025413	-2.968159	-0.210818
H	-2.575370	-0.123505	1.173595
H	-0.057620	2.744155	-0.591109
H	2.328853	-1.749223	-0.348865
H	-2.149756	0.173331	-2.497721
H	2.556714	-0.612412	-1.474862
H	-2.098851	-1.276802	-1.880476
H	-0.661727	-2.612472	1.307583
H	-1.616493	0.635294	2.189646
H	2.327587	0.992914	0.850787
H	0.750953	2.184159	-1.824952
H	7.388752	-5.567590	2.487066
H	6.791172	-5.662811	0.991231
H	2.918089	-3.196146	6.373349
H	1.467712	-3.056811	5.937585
H	3.801266	0.115441	6.078053
H	4.728713	0.733618	5.116675
H	2.501292	0.172336	8.060533
H	2.948611	1.730222	7.526778
H	3.029114	-6.411145	5.409281
H	2.727607	-4.952408	4.751033
H	3.526051	3.996513	-6.712363
H	3.968851	5.136616	-5.599060
H	6.064032	4.298335	-3.233076
H	5.511629	5.312748	-2.151216
H	-3.516112	7.339581	0.481447
H	-3.073312	8.479682	1.594750
H	5.723412	6.936917	-0.978764
H	4.235908	7.546683	-1.293427
H	4.693895	6.993937	0.642301
H	4.691136	6.553089	2.369044
H	4.485649	1.786816	-5.278686
H	3.928855	0.307595	-5.255865
H	6.296429	-5.753340	-3.000489
H	6.383640	-4.385872	-2.013831
H	2.812161	-5.618211	-1.054290
H	3.944954	-5.517331	-2.140889
H	6.764815	-3.012660	-0.152414
H	8.179641	-3.134370	-0.784603

H	3.007753	-4.825465	0.795628
H	3.400675	-6.346828	1.056890
H	7.521392	4.066716	-4.483527
H	5.923165	3.627831	-4.624378
H	6.555063	1.263839	-3.367856
H	7.002423	0.222899	-2.287480
H	7.280515	-2.356072	-2.951262
H	6.774119	-1.045313	-3.646197
H	6.390150	-4.538838	1.545515
H	6.296850	-3.026154	2.164162
H	2.200492	1.413759	-7.836094
H	3.648220	0.858736	-7.296813
H	8.365408	0.073609	-0.435802
H	7.614882	-1.130441	-1.113922
H	2.813435	-6.485214	-4.703608
H	2.404419	-6.638624	-3.188499
H	4.466793	-3.466574	-6.020215
H	5.425669	-2.707774	-5.004163
H	-5.440003	0.803803	1.174911
H	-5.757568	0.519945	2.786439
H	-6.717790	-3.078249	2.566638
H	-8.249818	-2.388298	2.639752
H	-4.981447	-0.491845	4.346329
H	-5.454430	0.856541	4.889615
H	-5.802882	4.448511	2.018644
H	-7.358866	4.696598	1.624037
H	-3.868559	4.797194	4.978483
H	-2.825250	3.782114	4.305962
H	-4.354740	3.537899	3.470835
H	-5.440136	2.595437	2.448784
H	-4.713310	1.593844	6.844945
H	-4.485448	2.730657	5.718948
H	-4.891175	-7.820378	0.297180
H	-5.970804	-6.585441	0.259997
H	-1.682108	-5.995551	3.020988
H	-2.675927	-7.201401	3.151219
H	-4.507463	-7.726653	-3.087600
H	-5.006543	-6.921066	-1.642144
H	-3.930121	-5.580994	0.442788
H	-3.153060	-5.370035	1.763195
H	-5.182879	-1.910869	-5.274762
H	-5.212832	-0.438769	-6.036044
H	-0.125096	-2.169999	-5.818186
H	-1.210960	-1.427782	-4.875498
H	-7.992081	1.290228	-2.180005
H	-6.577255	1.168517	-2.812192
H	-3.811654	3.226284	-5.496849
H	-4.810862	4.147744	-4.570833
H	-8.366747	-0.235951	-0.482074
H	-8.460046	1.276734	0.136573
H	-2.956217	5.559559	-5.084714
H	-1.488549	6.042993	-4.826365
H	-8.236043	-3.619651	-2.571766
H	-8.360763	-2.236423	-3.281300
H	-6.391488	4.376497	-2.463392
H	-7.142013	3.172447	-3.141512
H	-6.855856	5.356481	-0.757049
H	-6.226374	6.288655	-1.968665
H	-7.167257	1.173067	1.375624
H	-8.253122	1.915285	2.318311

Snapshot 17

287

O	2.763541	-3.530914	1.214600
O	2.289642	-4.946293	3.421798
O	4.671340	-5.803134	4.416730
O	0.524556	-1.955506	1.012025
Cd	0.106536	0.219453	0.200842
O	2.162193	1.070452	0.606904
O	0.348479	-0.118857	-1.969598
O	-2.095920	-0.995525	-0.531395
O	-0.755272	2.284980	-0.253459
O	-1.301057	0.782769	2.184079
O	3.127161	2.671997	-1.097115
O	-3.795636	0.868940	1.619857
Cl	-4.882280	1.419407	0.602740
O	-4.120188	1.569673	-0.761783
O	-5.981034	0.256420	0.561597
O	-5.450719	2.639906	1.269557
O	-1.576702	-1.286299	-3.212269
O	-1.928263	-3.141563	-5.014035
O	-0.601169	3.544084	-2.562120
O	-1.242581	6.085480	-2.245612
O	-3.700634	6.641815	-2.467274
O	-2.546104	-0.957485	3.800464
O	3.864458	-0.915590	1.260462
O	3.516463	-0.941186	3.866673
O	5.657406	-1.836295	4.636623
O	-4.664312	-1.780965	2.331810
O	-7.140328	-1.699897	3.396584
O	-6.535118	-4.191424	3.048153
O	-5.837026	-5.370510	0.892679
O	-3.737657	-4.131487	0.905121
O	-6.829375	-4.800584	-1.483720
O	-4.404315	-4.645712	4.541572
O	1.722065	2.417162	-3.395771
O	1.674452	3.707732	-5.355633
O	2.957070	-0.854496	-1.901258
Cl	4.193243	-0.549535	-2.708612
O	4.850168	0.657578	-2.109015
O	3.633116	-0.229148	-4.116821
O	5.058242	-1.837085	-2.673496
O	3.940605	1.313875	-5.849759
O	3.699552	-3.926474	-1.710962
O	1.495645	-4.002021	-3.075265
O	0.947909	-6.408688	-3.945249
O	3.405963	-6.965023	-3.723587
O	2.082395	-2.374354	-5.108650
O	-0.048409	-1.920067	-6.602069
O	-0.653619	0.571460	-6.253637
O	-0.069411	-3.814003	-0.903652
O	1.822396	0.490393	-7.318412
O	-1.825277	2.485158	-4.756666
O	-0.897311	4.537826	-6.100210
O	-0.324987	-6.198019	0.354331
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O	-1.689122	-5.877532	-4.293733
O	6.560149	-0.975140	1.565778

O	6.911711	0.880125	3.367545
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O	-6.442579	-0.960676	-1.823719
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O	2.045834	1.205747	4.756096
O	0.046868	0.369233	5.632087
O	-0.357831	1.226526	8.068272
O	3.753730	4.906367	2.096312
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O	3.972283	7.278352	-1.600167
O	2.763853	5.524236	4.476784
O	6.392494	1.170898	6.048419
O	8.440005	0.246357	-0.022255
O	7.834796	2.737883	0.326177
O	6.128878	3.497884	-1.581950
O	6.533577	2.640590	-4.018135
O	6.663139	4.651583	1.823149
O	3.870199	-4.422075	-5.744400
O	0.403926	4.724068	5.736197
O	-8.084487	2.557644	-0.843618
O	-8.602542	1.215180	1.020480
O	1.659039	-2.634160	5.096094
O	2.651387	-3.204087	7.472493
O	4.750756	-1.965064	7.484935
O	-1.262784	3.462863	3.741967
O	-3.480664	3.945954	5.266936
O	-0.948992	9.124028	-0.232986
O	4.961964	-6.412663	-1.266034
O	6.799290	-3.711107	2.286080
O	6.397939	-4.448743	0.240519
O	1.749398	8.601761	1.718494
O	-4.812258	1.436373	4.294589
O	-4.764644	0.145803	6.254450
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H	4.189790	-3.129872	-2.055710
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H	1.351265	-2.079391	-5.680953
H	1.340018	4.794159	5.338921
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H	-3.189856	-6.570186	0.123936
H	-2.909485	-8.049643	0.586907
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H	-1.106937	-2.672849	-5.390277
H	3.232144	-5.272085	3.647939
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H	-1.890353	-2.057223	-3.764494
H	2.808201	3.544497	2.400183
H	1.988821	2.244606	1.939447
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H	-3.338736	-3.996363	-0.006257
H	2.381090	-2.125672	4.635887
H	0.953546	-1.900374	5.008490
H	-4.851128	-1.016601	1.739734
H	-4.338404	-2.636412	1.730335
H	1.282403	6.230061	0.107276
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H	4.742340	-3.941732	-5.809950
H	-1.370084	5.337803	-5.696014
H	-1.218108	3.759359	-5.551889
H	1.832426	-6.675480	-4.407138
H	1.033105	-5.468077	-3.658528
H	3.485421	7.123846	-2.425608
H	4.941690	6.922504	-1.759762
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H	4.913826	-0.868330	1.232108
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H	-1.150144	6.928646	-2.690537
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H	5.943794	-2.589184	4.063224
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H	6.787222	1.617321	2.686511
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Snapshot 18

296			
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H	-0.763336	-1.779308	2.404471
H	0.327610	-0.951812	-7.491227
H	1.541323	-0.586544	-6.596045
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H	-1.102185	3.983706	-6.972061
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H	3.336931	-7.123793	-2.669150
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H	2.805442	6.683416	-3.002033
H	3.914714	6.656891	-1.800987
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Snapshot 19

302			
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H	7.064221	3.511585	0.451759
H	0.321572	9.738655	1.328249
H	0.107765	8.157523	1.029878
H	0.178597	7.022893	3.434671
H	0.039346	7.722117	4.806341
H	3.842942	4.615012	-0.931341
H	4.811097	4.733327	0.393309
H	7.739956	1.658376	-0.869548
H	9.131879	2.070142	-0.186212
H	3.388236	2.563165	-2.292682
H	4.035987	3.715303	-3.266983
H	5.569350	-1.713115	6.873306
H	4.064386	-1.611475	6.893106
H	6.212904	-0.716518	4.173175
H	6.751471	-0.128745	2.807666

H	6.361571	2.869897	2.731001
H	6.391016	1.674417	3.719345
H	7.322055	1.935648	-3.011091
H	7.093550	0.320556	-2.671434
H	8.292351	-0.852499	1.283480
H	8.054974	0.775614	1.002096
H	3.636204	7.731567	1.467353
H	3.300266	6.611211	0.477814
H	5.149947	5.082710	4.366698
H	5.880836	3.702047	4.519969
H	-6.165512	-0.325230	-0.990387
H	-6.306794	-1.162287	-2.454265
H	-2.798998	-3.946930	-6.861928
H	-4.030788	-4.815018	-7.075295
H	-6.533209	1.512813	-3.708980
H	-7.908356	0.664611	-3.700778
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H	-6.625052	-4.024110	0.858528
H	-8.201625	-4.166556	1.365710
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H	-3.503159	-5.221344	-1.992319
H	-5.144729	-3.977669	-0.978192
H	-5.770660	-2.564081	-0.688717
H	-5.015477	-4.397916	-5.260332
H	-5.191897	-4.875982	-3.615873
H	-4.153632	6.782108	-3.755114
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H	-7.472392	5.910854	-3.048361
H	-6.951303	5.081186	-1.761927
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H	-7.713495	3.303693	1.987242
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H	-7.025247	-4.163077	4.581879

Snapshot 20

305

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O	1.175773	5.632209	4.444697
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O	6.514728	3.678198	2.859758
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O	4.951097	1.147437	1.334442
O	5.485497	-0.440471	-0.532335
Cl	4.668585	-1.653945	-0.922350
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Cd	0.182847	-0.207105	0.235607
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O	-1.320895	0.711894	-1.453266
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O	-3.153016	0.161282	2.169588
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O	0.023362	-4.927163	-4.336527
O	0.006868	-2.378157	-3.553216
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O	2.278749	-2.812720	6.770023
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O	-2.269116	-0.877822	4.717034
O	-3.142347	-2.736699	-1.248279
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O	-0.401645	-6.008150	-1.875268
O	0.382380	-8.562100	-2.026641
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O	5.011544	-6.906367	1.173739
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O	3.454127	7.198501	0.969800
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O	7.702068	-2.484738	1.175460
O	5.897578	-1.345864	4.704769

O	-2.870298	-0.762314	8.373180
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O	-5.862158	2.694100	3.921546
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O	-8.570927	-0.662479	1.809698
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O	-6.661842	-1.787359	-3.642539
O	-6.626634	-4.931735	-2.301442
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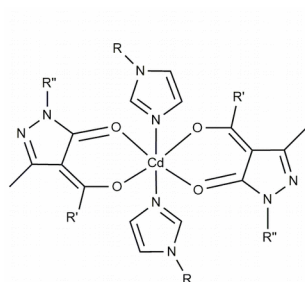
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H	7.013678	5.356497	0.587101
H	6.770764	6.295718	1.903130

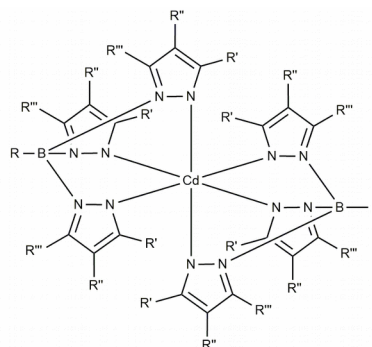
Calculated $\delta(^{113}\text{Cd})$ for the model systems investigated. (1)-(5)⁵³ (CDCl_3);(6)-(13)⁵⁴ (CDCl_3);(14)-(16)⁵⁵ (CD_2Cl_2);(17)-(24)⁵⁶ (CDCl_3);(25)-(26)⁵⁷ (CDCl_3).

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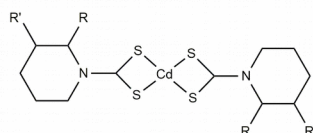


- (1) R=Me; R'=R''=Ph
 (2) R=Me; R'=Ph; R''=Me
 (3) R=PhCH₂; R'=R''=Ph
 (4) R=PhCH₂; R'=Me; R''=Ph
 (5) R=PhCH₂; R'=Ph; R''=Me

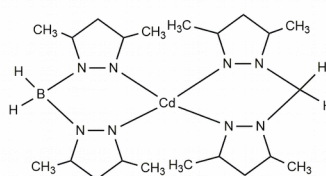


- (6) R=R''=R'''=H; R'=Me
 (7) R=3-MePz; R'=Me; R''=R'''=H
 (8) R=R'=R'''=H; R''=Br
 (9) R=R'=R'''=H; R''=Me

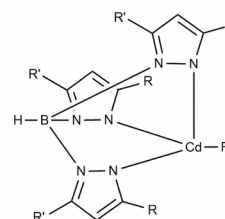
- (10) R'=R'''=H; R=4-MePz; R''=Me
 (11) R=R''=H; R'=R'''=Me
 (12) R=R'=R''=R'''=H
 (13) R=Pz; R'=R''=R'''=H



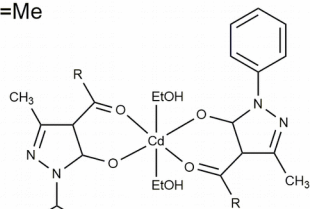
- (14) R=R'=H
 (15) R=Me; R'=H
 (16) R=H; R'=Me



(17)



- (18) R=R'=Me; R''=S₂CNEt₂
 (19) R=Ph; R'=H; R''=S₂CNEt₂
 (20) R=i-Pr; R'=H; R''=(t-BuCO)₂CH
 (21) R=Ph; R'=H; R''=(t-BuCO)₂CH
 (22) R=Ph; R'=H; R''=(Ph)₂CH
 (23) R=Ph; R'=H; R''=(CF₃CO)₂CH
 (24) R=t-Bu; R'=H; R''=CH₃CO₂



- (25) R=CH₂C(CH₃)₃
 (26) R=C₆H₁₁

OP2 geometry [G09; B3LYP/cc-pVDZ PP (Cd);cc-pVDZ (Light atoms)]

Table S14 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)] level. Data referred wrt 1 M Cd(ClO₄)₂. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	72.86	4.24	61.76	15.34
2	82.10	84.07	1.97	73.73	8.37
3	76.00	73.70	2.30	62.65	13.35
4	81.20	91.59	10.39	81.77	0.57
5	59.10	73.67	14.57	62.62	3.52
6	200.00	189.35	10.65	186.21	13.79
7	202.50	200.72	1.78	198.35	4.15
8	193.80	197.98	4.18	195.44	1.64
9	195.90	202.38	6.48	200.13	4.23
10	218.30	225.96	7.66	225.32	7.02
11	201.90	200.97	0.93	198.62	3.28
12	198.30	207.28	8.98	205.37	7.07
13	221.10	229.82	8.72	229.45	8.35
14	353.60	340.42	13.18	347.61	5.99
15	365.13	353.09	12.04	361.15	3.98
16	352.13	341.67	10.46	348.94	3.19
17	303.30	298.53	4.77	302.85	0.45
18	265.67	261.82	3.85	263.63	2.04
19	237.50	234.81	2.69	234.79	2.71
20	168.20	173.17	4.97	168.93	0.73
21	172.40	178.93	6.53	175.08	2.68
22	155.20	176.36	21.16	172.34	17.14
23	141.80	152.03	10.23	146.34	4.54
24	148.10	171.63	23.53	167.28	19.18
25	27.20	44.96	17.76	31.94	4.74
26	26.30	34.08	7.78	20.32	5.98

ME	23.53
MAE	8.53
CMAE	6.31
Slope	0.936
Int.	15.06

G09: B3LYP/Sadlej(Cd);6-31G(d)//OP2

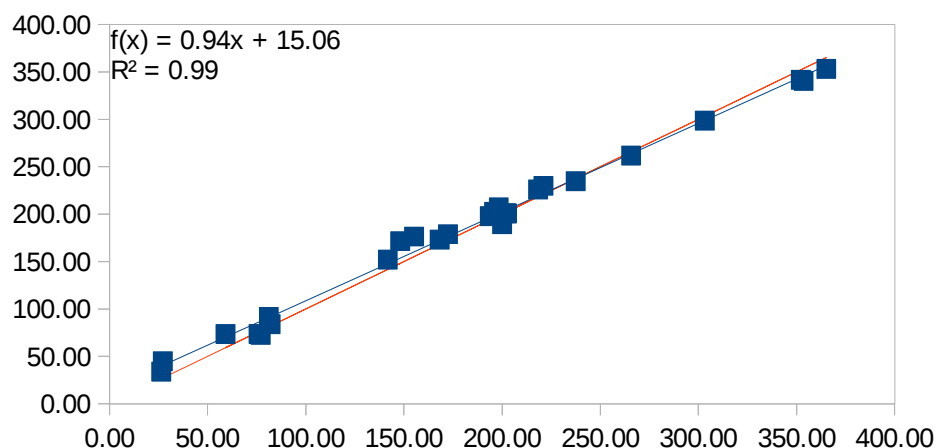


Table S15 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt 1 M Cd(CIO₄)₂. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	69.82	7.28	61.11	15.99
2	82.10	81.42	0.68	73.53	8.57
3	76.00	67.39	8.61	58.51	17.50
4	81.20	88.73	7.53	81.35	0.15
5	59.10	76.52	17.42	68.28	9.17
6	200.00	186.61	13.39	186.15	13.86
7	202.50	198.10	4.40	198.45	4.06
8	193.80	194.83	1.03	194.95	1.14
9	195.90	199.09	3.19	199.51	3.60
10	218.30	222.53	4.23	224.60	6.30
11	201.90	198.16	3.74	198.51	3.39
12	198.30	204.02	5.72	204.79	6.48
13	221.10	226.42	5.32	228.77	7.66
14	353.60	337.91	15.69	348.13	5.48
15	365.13	350.52	14.61	361.62	3.51
16	352.13	337.92	14.21	348.14	4.00
17	303.30	296.27	7.03	303.54	0.23
18	265.67	258.97	6.70	263.61	2.07
19	237.50	232.26	5.24	235.01	2.49
20	168.20	170.99	2.79	169.42	1.21
21	172.40	176.59	4.19	175.41	3.01
22	155.20	174.17	18.97	172.83	17.62
23	141.80	149.62	7.82	146.54	4.74
24	148.10	169.81	21.71	168.16	20.05
25	27.20	42.23	15.03	31.57	4.36
26	26.30	31.36	5.06	19.94	6.37

ME 21.71
 MAE 8.52
 CMAE 6.65
 Slope 0.934
 Int. 12.74

G09: B3LYP/Sadlej(Cd);6-31G(d,p)//OP2

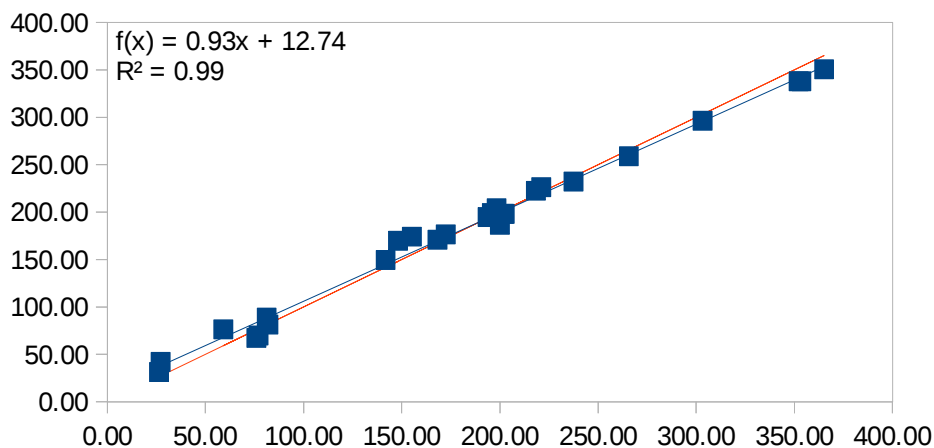


Table S16 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt 1 M Cd(CIO₄)₂. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	79.39	2.29	64.22	12.88
2	82.10	87.61	5.51	73.14	8.96
3	76.00	81.45	5.45	66.46	9.54
4	81.20	102.58	21.38	89.39	8.19
5	59.10	76.02	16.92	60.57	1.47
6	200.00	195.59	4.41	190.35	9.65
7	202.50	201.91	0.59	197.20	5.30
8	193.80	200.72	6.92	195.91	2.11
9	195.90	209.63	13.73	205.58	9.68
10	218.30	230.91	12.61	228.67	10.37
11	201.90	205.09	3.19	200.66	1.24
12	198.30	207.13	8.83	202.87	4.57
13	221.10	227.80	6.70	225.30	4.20
14	353.60	335.00	18.60	341.65	11.95
15	365.13	346.78	18.35	354.44	10.69
16	352.13	337.21	14.92	344.05	8.08
17	303.30	303.44	0.14	307.40	4.10
18	265.67	264.84	0.83	265.51	0.16
19	237.50	238.51	1.01	236.93	0.57
20	168.20	175.30	7.10	168.32	0.12
21	172.40	185.37	12.97	179.24	6.84
22	155.20	183.06	27.86	176.74	21.54
23	141.80	159.56	17.76	151.24	9.44
24	148.10	176.95	28.85	170.11	22.01
25	27.20	37.13	9.93	18.36	8.84
26	26.30	29.00	2.70	9.53	16.77

ME 28.85
 MAE 10.37
 CMAE 8.05
 Slope 0.921
 Int. 20.22

G09: B3LYP/Sadlej(Cd);6-31G+(d,p)//OP2

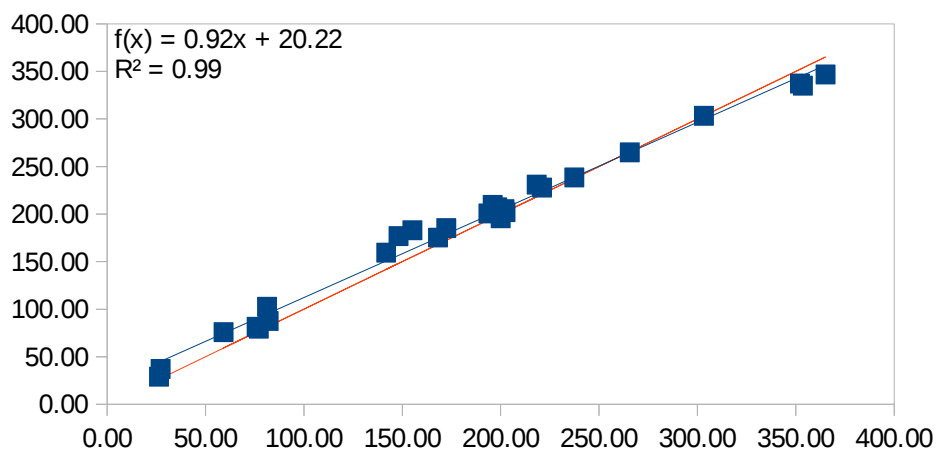


Table S17 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d)]level . Data referred wrt 1 M Cd(CIO₄)₂. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	72.24	4.86	59.82	17.28
2	82.10	83.96	1.86	72.37	9.73
3	76.00	73.20	2.80	60.84	15.16
4	81.20	91.18	9.98	80.10	1.10
5	59.10	73.31	14.21	60.97	1.87
6	200.00	195.97	4.03	192.35	7.65
7	202.50	209.94	7.44	207.32	4.82
8	193.80	201.12	7.32	197.87	4.07
9	195.90	206.24	10.34	203.35	7.45
10	218.30	230.16	11.86	228.98	10.68
11	201.90	208.00	6.10	205.23	3.33
12	198.30	211.12	12.82	208.58	10.28
13	221.10	233.99	12.89	233.08	11.98
14	353.60	334.56	19.04	340.80	12.80
15	365.13	348.60	16.53	355.85	9.28
16	352.13	335.57	16.56	341.88	10.25
17	303.30	299.42	3.88	303.16	0.14
18	265.67	263.10	2.57	264.26	1.41
19	237.50	238.88	1.38	238.32	0.82
20	168.20	174.36	6.16	169.20	1.00
21	172.40	178.00	5.60	173.10	0.70
22	155.20	175.20	20.00	170.10	14.90
23	141.80	149.54	7.74	142.62	0.82
24	148.10	174.49	26.39	169.34	21.24
25	27.20	42.65	15.45	28.12	0.92
26	26.30	31.54	5.24	16.22	10.08

ME 26.39
 MAE 9.73
 CMAE 7.30
 Slope 0.934
 Int. 16.40

G09: B3PW91/Sadlej(Cd);6-31G(d)//OP2

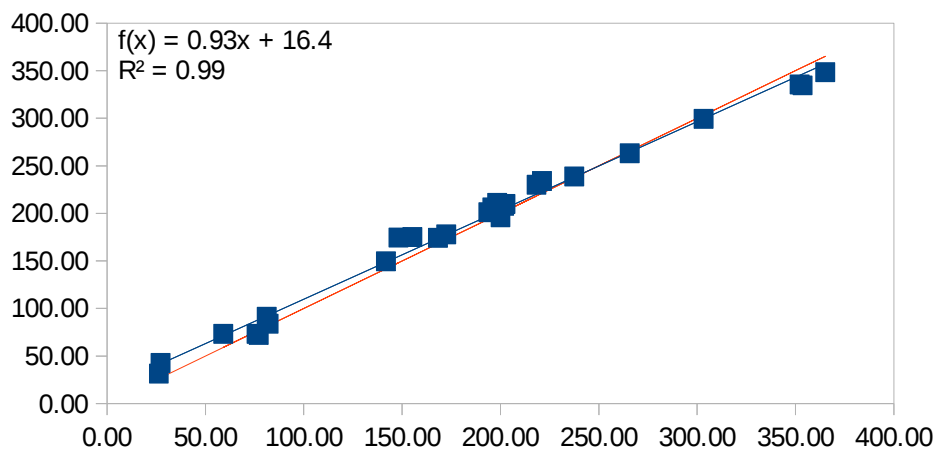


Table S18 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d,p)] level. Data referred wrt 1 M Cd(ClO₄)₂. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	67.34	9.76	60.05	17.05
2	82.10	79.05	3.05	72.59	9.51
3	76.00	68.35	7.65	61.12	14.88
4	81.20	79.31	1.89	72.88	8.32
5	59.10	67.83	8.73	60.56	1.46
6	200.00	191.27	8.73	192.91	7.09
7	202.50	205.45	2.95	208.10	5.60
8	193.80	195.99	2.19	197.96	4.16
9	195.90	200.96	5.06	203.29	7.39
10	218.30	224.76	6.46	228.80	10.50
11	201.90	203.22	1.32	205.72	3.82
12	198.30	205.89	7.59	208.58	10.28
13	221.10	228.64	7.54	232.97	11.87
14	353.60	329.25	24.35	340.82	12.78
15	365.13	339.92	25.21	352.26	12.87
16	352.13	330.08	22.05	341.71	10.42
17	303.30	295.24	8.06	304.36	1.06
18	265.67	258.27	7.40	264.72	0.95
19	237.50	234.37	3.13	239.11	1.61
20	168.20	170.22	2.02	170.33	2.13
21	172.40	173.73	1.33	174.10	1.70
22	155.20	171.08	15.88	171.26	16.06
23	141.80	145.19	3.39	143.50	1.70
24	148.10	170.82	22.72	170.97	22.87
25	27.20	37.94	10.74	28.53	1.33
26	26.30	26.84	0.54	16.63	9.67

ME 25.21
 MAE 8.45
 CMAE 7.96
 Slope 0.933
 Int. 11.33

G09: B3PW91/Sadlej(Cd);6-31G(d,p)//OP2

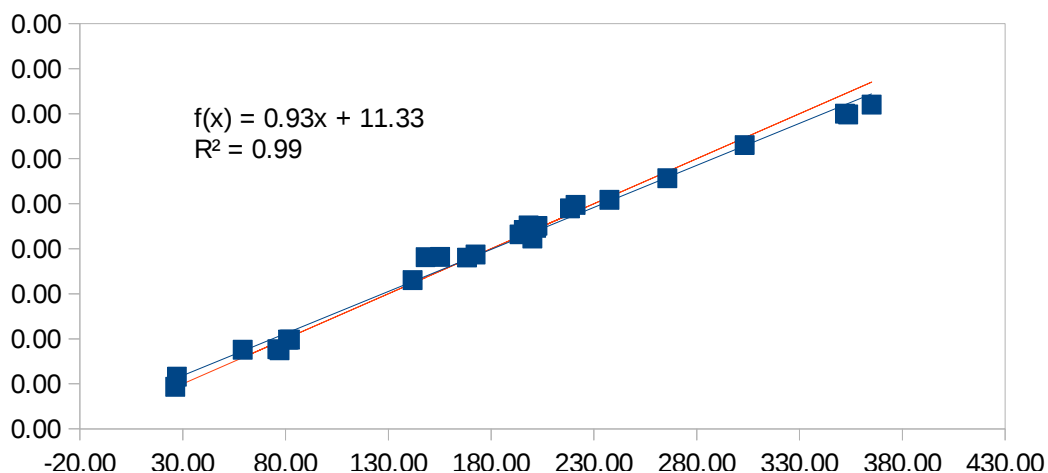


Table S19 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31+G(d,p)] level. Data referred wrt 1 M $\text{Cd}(\text{ClO}_4)_2$. Orange line=ideal correlation

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	77.10	31.73	45.37	19.43	57.67
2	82.10	42.46	39.64	30.72	51.38
3	76.00	81.69	5.69	71.99	4.01
4	81.20	102.94	21.74	94.35	13.15
5	59.10	76.72	17.62	66.76	7.66
6	200.00	200.97	0.97	197.49	2.51
7	202.50	209.74	7.24	206.72	4.22
8	193.80	203.75	9.95	200.41	6.61
9	195.90	213.60	17.70	210.77	14.87
10	218.30	235.31	17.01	233.62	15.32
11	201.90	210.46	8.56	207.48	5.58
12	198.30	211.20	12.90	208.25	9.95
13	221.10	232.12	11.02	230.27	9.17
14	353.60	329.85	23.75	333.08	20.52
15	365.13	345.10	20.03	349.12	16.01
16	352.13	332.01	20.12	335.36	16.77
17	303.30	303.30	0.00	305.15	1.85
18	265.67	265.79	0.12	265.69	0.02
19	237.50	242.03	4.53	240.68	3.18
20	168.20	182.85	14.65	178.43	10.23
21	172.40	184.96	12.56	180.64	8.24
22	155.20	182.38	27.18	177.94	22.74
23	141.80	157.64	15.84	151.90	10.10
24	148.10	179.97	31.87	175.39	27.29
25	27.20	43.49	16.29	31.81	4.61
26	26.30	32.63	6.33	20.37	5.93

ME 45.37
 MAE 15.72
 CMAE 13.45
 Slope 0.950
 Int. 13.26

G09: B3PW91/Sadlej(Cd);6-31+G(d,p)//OP2

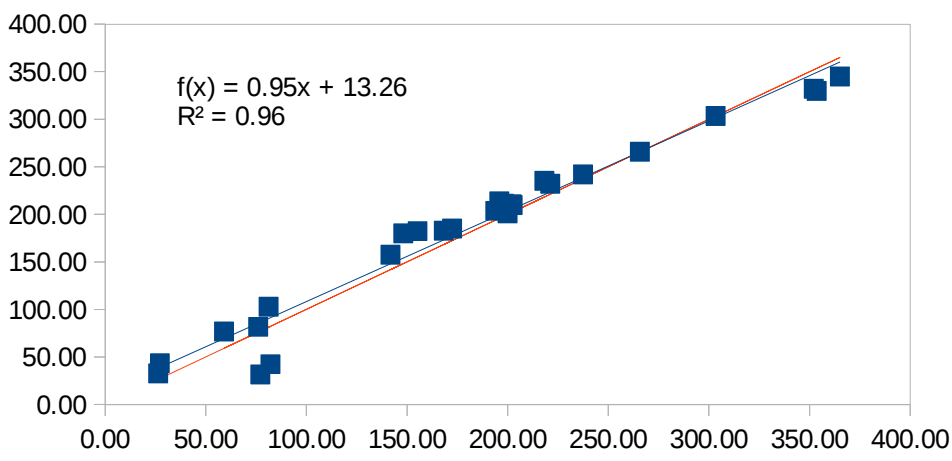


Table S20 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)]level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-643.11	14.08	-644.14	15.11
2	-624.03	-631.91	7.88	-632.17	8.14
3	-630.13	-642.28	12.15	-643.25	13.12
4	-624.93	-624.38	0.55	-624.13	0.80
5	-647.03	-642.31	4.72	-643.28	3.75
6	-506.13	-526.63	20.50	-519.70	13.57
7	-503.63	-515.26	11.63	-507.55	3.92
8	-512.33	-517.99	5.66	-510.47	1.86
9	-510.23	-513.60	3.37	-505.77	4.46
10	-487.83	-490.02	2.19	-480.59	7.24
11	-504.23	-515.01	10.78	-507.28	3.05
12	-507.83	-508.69	0.86	-500.54	7.29
13	-485.03	-486.16	1.13	-476.46	8.57
14	-352.53	-375.56	23.03	-358.31	5.78
15	-341.00	-362.88	21.88	-344.77	3.77
16	-354.00	-374.31	20.31	-356.98	2.98
17	-402.83	-417.45	14.62	-403.06	0.23
18	-440.46	-454.16	13.70	-442.28	1.82
19	-468.63	-481.16	12.53	-471.13	2.50
20	-537.93	-542.80	4.87	-536.98	0.95
21	-533.73	-537.05	3.32	-530.83	2.90
22	-550.93	-539.61	11.32	-533.57	17.36
23	-564.33	-563.95	0.38	-559.57	4.76
24	-558.03	-544.35	13.68	-538.63	19.40
25	-678.93	-671.02	7.91	-673.95	4.98
26	-679.83	-681.90	2.07	-685.57	5.74

ME	23.03
MAE	9.43
CMAE	6.31
Slope	0.936
Int.	-40.15

G09: B3LYP/Sadlej(Cd);6-31G(d,p)//OP2

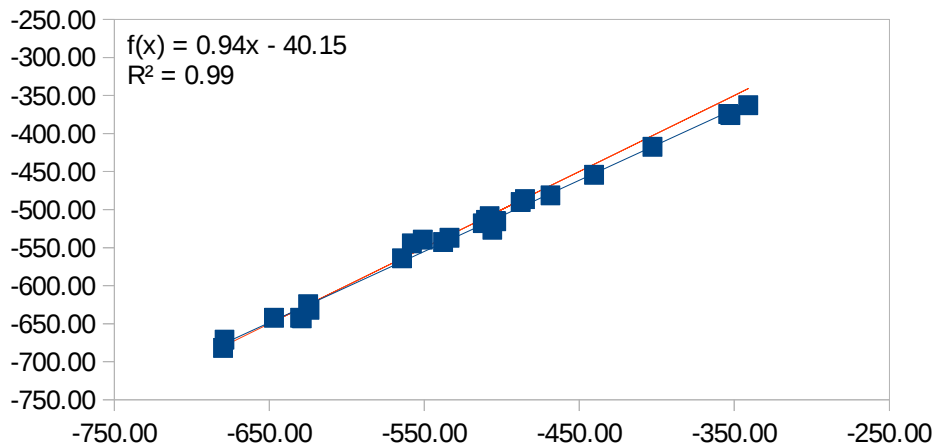


Table S21 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-639.72	10.69	-645.00	15.97
2	-624.03	-628.12	4.09	-632.58	8.55
3	-630.13	-642.15	12.02	-647.61	17.48
4	-624.93	-620.81	4.12	-624.76	0.17
5	-647.03	-633.02	14.01	-637.83	9.20
6	-506.13	-522.93	16.80	-519.93	13.80
7	-503.63	-511.44	7.81	-507.62	3.99
8	-512.33	-514.71	2.38	-511.12	1.21
9	-510.23	-510.45	0.22	-506.56	3.67
10	-487.83	-487.01	0.82	-481.46	6.37
11	-504.23	-511.38	7.15	-507.56	3.33
12	-507.83	-505.52	2.31	-501.28	6.55
13	-485.03	-483.12	1.91	-477.29	7.74
14	-352.53	-371.63	19.10	-357.89	5.36
15	-341.00	-359.02	18.02	-344.39	3.39
16	-354.00	-371.62	17.62	-357.88	3.88
17	-402.83	-413.27	10.44	-402.49	0.34
18	-440.46	-450.57	10.11	-442.44	1.98
19	-468.63	-477.28	8.65	-471.05	2.42
20	-537.93	-538.55	0.62	-536.66	1.27
21	-533.73	-532.95	0.78	-530.67	3.06
22	-550.93	-535.37	15.56	-533.25	17.68
23	-564.33	-559.92	4.41	-559.54	4.79
24	-558.03	-539.73	18.30	-537.92	20.11
25	-678.93	-667.31	11.62	-674.56	4.37
26	-679.83	-678.18	1.65	-686.19	6.36

ME	19.10
MAE	8.51
CMAE	6.66
Slope	0.934
Int.	-37.44

G09: B3LYP/Sadlej(Cd);6-31G(d,p)//OP2

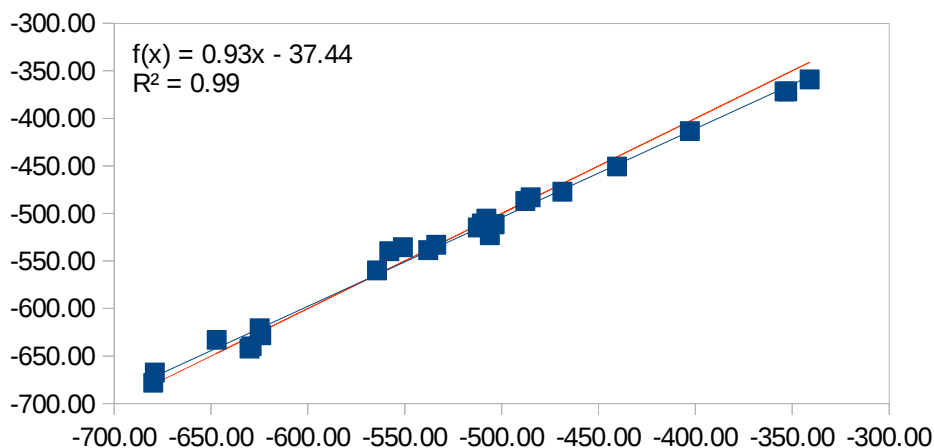


Table S22 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-604.82	24.21	-641.91	12.88
2	-624.03	-596.60	27.43	-632.99	8.96
3	-630.13	-602.76	27.37	-639.68	9.55
4	-624.93	-581.63	43.30	-616.74	8.19
5	-647.03	-608.18	38.85	-645.56	1.47
6	-506.13	-488.61	17.52	-515.79	9.66
7	-503.63	-482.29	21.34	-508.93	5.30
8	-512.33	-483.49	28.84	-510.23	2.10
9	-510.23	-474.58	35.65	-500.55	9.68
10	-487.83	-453.30	34.53	-477.46	10.37
11	-504.23	-479.11	25.12	-505.47	1.24
12	-507.83	-477.08	30.75	-503.27	4.56
13	-485.03	-456.41	28.62	-480.83	4.20
14	-352.53	-349.21	3.32	-364.48	11.95
15	-341.00	-337.42	3.58	-351.69	10.69
16	-354.00	-347.00	7.00	-362.08	8.08
17	-402.83	-380.77	22.06	-398.73	4.10
18	-440.46	-419.36	21.10	-440.62	0.16
19	-468.63	-445.69	22.94	-469.20	0.57
20	-537.93	-508.91	29.02	-537.81	0.12
21	-533.73	-498.84	34.89	-526.89	6.84
22	-550.93	-501.15	49.78	-529.39	21.54
23	-564.33	-524.64	39.69	-554.89	9.44
24	-558.03	-507.26	50.77	-536.02	22.01
25	-678.93	-647.08	31.85	-687.78	8.85
26	-679.83	-655.21	24.62	-696.61	16.78
		ME	50.77		
		MAE	27.85		
		CMAE	8.05		
		Slope	0.921		
		Int.	-13.40		

Table S23 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-623.03	6.00	-646.31	17.28
2	-624.03	-611.31	12.72	-633.76	9.73
3	-630.13	-622.07	8.06	-645.29	15.16
4	-624.93	-604.09	20.84	-626.03	1.10
5	-647.03	-621.96	25.07	-645.16	1.87
6	-506.13	-499.30	6.83	-513.78	7.65
7	-503.63	-485.33	18.30	-498.81	4.82
8	-512.33	-494.15	18.18	-508.26	4.07
9	-510.23	-489.03	21.20	-502.78	7.45
10	-487.83	-465.11	22.72	-477.15	10.68
11	-504.23	-487.27	16.96	-500.90	3.33
12	-507.83	-484.15	23.68	-497.55	10.28
13	-485.03	-461.28	23.75	-473.05	11.98
14	-352.53	-360.71	8.18	-365.33	12.80
15	-341.00	-346.66	5.66	-350.28	9.28
16	-354.00	-359.70	5.70	-364.25	10.25
17	-402.83	-395.85	6.98	-402.97	0.14
18	-440.46	-432.17	8.29	-441.87	1.41
19	-468.63	-456.39	12.24	-467.81	0.82
20	-537.93	-520.91	17.02	-536.93	1.00
21	-533.73	-517.27	16.46	-533.03	0.70
22	-550.93	-520.07	30.86	-536.03	14.90
23	-564.33	-545.73	18.60	-563.51	0.82
24	-558.03	-520.78	37.25	-536.79	21.24
25	-678.93	-652.62	26.31	-678.01	0.92
26	-679.83	-663.73	16.10	-689.91	10.08
		ME	37.25		
		MAE	16.69		
		CMAE	7.30		
		Slope	0.934		
		Int.	-19.65		

Table S24 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-619.64	9.39	-646.08	17.05
2	-624.03	-607.94	16.09	-633.54	9.51
3	-630.13	-618.64	11.49	-645.01	14.88
4	-624.93	-607.67	17.26	-633.25	8.32
5	-647.03	-619.16	27.87	-645.57	1.46
6	-506.13	-495.71	10.42	-513.22	7.09
7	-503.63	-481.53	22.10	-498.03	5.60
8	-512.33	-490.99	21.34	-508.17	4.16
9	-510.23	-486.03	24.20	-502.85	7.38
10	-487.83	-462.22	25.61	-477.33	10.50
11	-504.23	-483.76	20.47	-500.42	3.81
12	-507.83	-481.09	26.74	-497.55	10.28
13	-485.03	-458.34	26.69	-473.16	11.87
14	-352.53	-357.73	5.20	-365.31	12.78
15	-341.00	-347.06	6.06	-353.87	12.87
16	-354.00	-356.90	2.90	-364.42	10.42
17	-402.83	-391.74	11.09	-401.77	1.06
18	-440.46	-428.72	11.74	-441.41	0.95
19	-468.63	-452.61	16.02	-467.02	1.61
20	-537.93	-516.76	21.17	-535.80	2.13
21	-533.73	-513.25	20.48	-532.03	1.70
22	-550.93	-515.90	35.03	-534.87	16.06
23	-564.33	-541.79	22.54	-562.63	1.70
24	-558.03	-516.16	41.87	-535.16	22.87
25	-678.93	-649.04	29.89	-677.60	1.33
26	-679.83	-660.14	19.69	-689.50	9.67
		ME	41.87		
		MAE	19.36		
		CMAE	7.96		
		Slope	0.933		
		Int.	-16.97		

Table S25 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-635.97	6.94	-686.70	57.67
2	-624.03	-625.24	1.21	-675.41	51.38
3	-630.13	-586.01	44.12	-634.14	4.01
4	-624.93	-564.75	60.18	-611.78	13.15
5	-647.03	-590.98	56.05	-639.37	7.66
6	-506.13	-466.73	39.40	-508.64	2.51
7	-503.63	-457.95	45.68	-499.41	4.22
8	-512.33	-463.95	48.38	-505.72	6.61
9	-510.23	-454.10	56.13	-495.36	14.87
10	-487.83	-432.39	55.44	-472.51	15.32
11	-504.23	-457.23	47.00	-498.65	5.58
12	-507.83	-456.50	51.33	-497.88	9.95
13	-485.03	-435.57	49.46	-475.86	9.17
14	-352.53	-337.85	14.68	-373.05	20.52
15	-341.00	-322.60	18.40	-357.01	16.01
16	-354.00	-335.68	18.32	-370.77	16.77
17	-402.83	-364.39	38.44	-400.98	1.85
18	-440.46	-401.90	38.56	-440.44	0.02
19	-468.63	-425.67	42.96	-465.45	3.18
20	-537.93	-484.85	53.08	-527.70	10.23
21	-533.73	-482.74	50.99	-525.49	8.24
22	-550.93	-485.31	65.62	-528.19	22.74
23	-564.33	-510.06	54.27	-554.23	10.10
24	-558.03	-487.73	70.30	-530.74	27.29
25	-678.93	-624.20	54.73	-674.32	4.61
26	-679.83	-635.07	44.76	-685.76	5.93

ME 70.30
 MAE 43.32
 CMAE 13.45
 Slope 0.950
 Int. 16.725

G09: B3PW91/Sadlej(Cd);6-31+G(d,p)//OP2

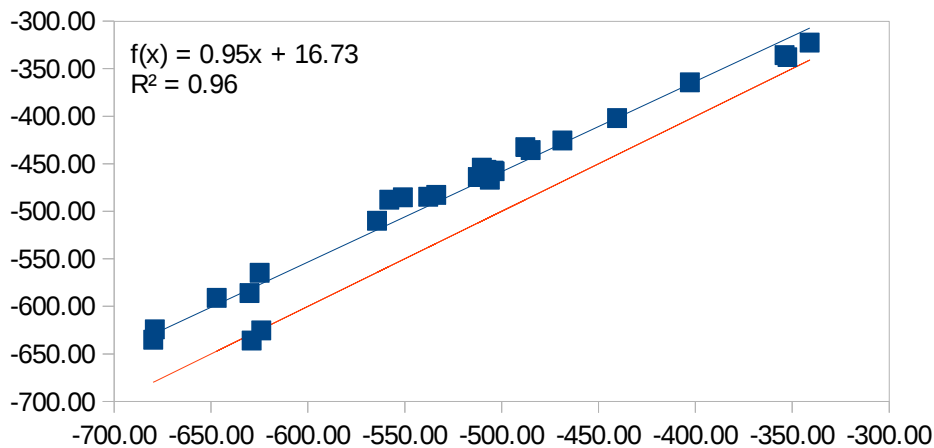


Table S26 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-2 [B3LYP/DZP]] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-707.28	78.25	-636.72	7.69
2	-624.03	-729.03	105.00	-658.29	34.26
3	-630.13	-706.12	75.99	-635.57	5.44
4	-624.93	-695.65	70.72	-625.19	0.26
5	-647.03	-708.80	61.77	-638.23	8.80
6	-506.13	-600.08	93.95	-530.44	24.31
7	-503.63	-578.95	75.32	-509.49	5.86
8	-512.33	-590.60	78.27	-521.04	8.71
9	-510.23	-588.22	77.99	-518.68	8.45
10	-487.83	-556.22	68.39	-486.96	0.87
11	-504.23	-589.60	85.37	-520.05	15.82
12	-507.83	-584.41	76.58	-514.91	7.08
13	-485.03	-557.72	72.69	-488.44	3.41
14	-352.53	-416.33	63.80	-348.26	4.27
15	-341.00	-405.38	64.38	-337.41	3.59
16	-354.00	-416.50	62.50	-348.43	5.57
17	-402.83	-466.55	63.72	-398.05	4.78
18	-440.46	-515.57	75.11	-446.65	6.19
19	-468.63	-532.51	63.88	-463.45	5.18
20	-537.93	-599.43	61.50	-529.80	8.13
21	-533.73	-595.68	61.95	-526.08	7.65
22	-550.93	-599.03	48.10	-529.40	21.53
23	-564.33	-626.52	62.19	-556.65	7.68
24	-558.03	-597.89	39.86	-528.27	29.76
25	-678.93	-734.91	55.98	-664.12	14.81
26	-679.83	-745.89	66.06	-675.00	4.83

ME	105.00
MAE	69.59
CMAE	9.81
Slope	1.009
Int.	-65.06

ADF: B3LY/DZP//OP2

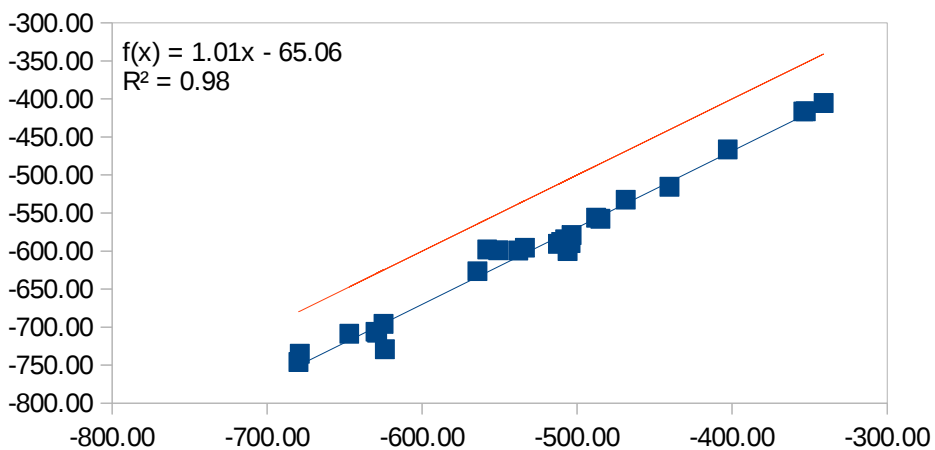


Table S27 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-2 [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-694.77	65.74	-635.75	6.72
2	-624.03	-715.88	91.85	-656.04	32.01
3	-630.13	-693.26	63.13	-634.29	4.16
4	-624.93	-681.69	56.76	-623.17	1.76
5	-647.03	-695.15	48.12	-636.11	10.92
6	-506.13	-584.51	78.38	-529.73	23.60
7	-503.63	-573.31	69.68	-518.96	15.33
8	-512.33	-581.58	69.25	-526.91	14.58
9	-510.23	-577.55	67.32	-523.03	12.80
10	-487.83	-543.40	55.57	-490.20	2.37
11	-504.23	-568.70	64.47	-514.52	10.29
12	-507.83	-574.19	66.36	-519.80	11.97
13	-485.03	-544.01	58.98	-490.78	5.75
14	-352.53	-397.52	44.99	-349.93	2.60
15	-341.00	-383.02	42.02	-335.99	5.01
16	-354.00	-395.16	41.16	-347.66	6.34
17	-402.83	-448.24	45.41	-398.70	4.13
18	-440.46	-491.90	51.44	-440.68	0.22
19	-468.63	-512.59	43.96	-460.57	8.06
20	-537.93	-582.17	44.24	-527.48	10.45
21	-533.73	-579.81	46.08	-525.21	8.52
22	-550.93	-581.51	30.58	-526.84	24.09
23	-564.33	-610.08	45.75	-554.31	10.02
24	-558.03	-591.27	33.24	-536.23	21.80
25	-678.93	-728.15	49.22	-667.84	11.09
26	-679.83	-737.54	57.71	-676.87	2.96

ME	91.85
MAE	55.05
CMAE	10.29
Slope	1.040
Int.	-33.59

ADF: B3LY/TZ2P//OP2

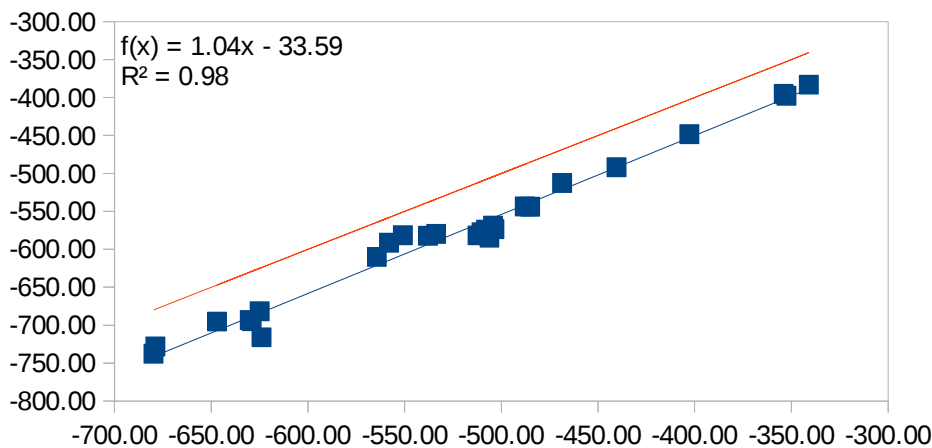


Table S28 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at RS [B3LYP/DZP] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-667.87	38.84	-632.65	3.62
2	-624.03	-692.02	67.99	-654.99	30.96
3	-630.13	-666.78	36.65	-631.64	1.51
4	-624.93	-648.73	23.80	-614.94	9.99
5	-647.03	-669.19	22.16	-633.87	13.16
6	-506.13	-556.72	50.59	-529.83	23.70
7	-503.63	-546.16	42.53	-520.06	16.43
8	-512.33	-550.21	37.88	-523.80	11.47
9	-510.23	-547.68	37.45	-521.46	11.23
10	-487.83	-518.37	30.54	-494.35	6.52
11	-504.23	-544.15	39.92	-518.20	13.97
12	-507.83	-543.33	35.50	-517.44	9.61
13	-485.03	-515.00	29.97	-491.23	6.20
14	-352.53	-355.26	2.73	-343.46	9.07
15	-341.00	-343.55	2.55	-332.63	8.37
16	-354.00	-354.03	0.03	-342.32	11.68
17	-402.83	-416.50	13.67	-400.11	2.72
18	-440.46	-463.36	22.90	-443.46	3.00
19	-468.63	-487.66	19.03	-465.94	2.69
20	-537.93	-557.57	19.64	-530.61	7.32
21	-533.73	-551.29	17.56	-524.80	8.93
22	-550.93	-555.42	4.49	-528.62	22.31
23	-564.33	-589.34	25.01	-560.00	4.33
24	-558.03	-557.97	0.06	-530.98	27.05
25	-678.93	-703.92	24.99	-666.00	12.93
26	-679.83	-714.93	35.10	-676.18	3.65

ME 67.99
 MAE 26.21
 CMAE 10.86
 Slope 1.081
 Int. 16.02

ADF Scalar-ZORA: B3LY/DZP//OP2

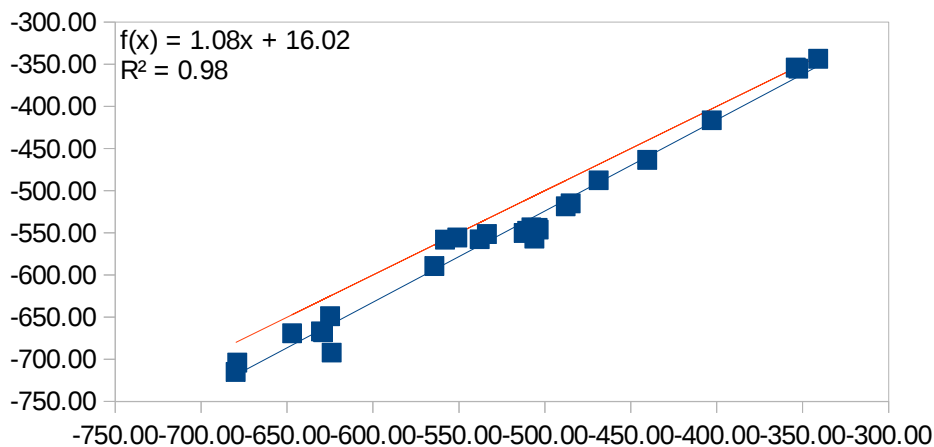


Table S29 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at RS [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-682.79	53.76	-626.84	2.19
2	-624.03	-707.43	83.40	-648.09	24.06
3	-630.13	-681.89	51.76	-626.07	4.06
4	-624.93	-670.99	46.06	-616.67	8.26
5	-647.03	-685.34	38.31	-629.04	17.99
6	-506.13	-580.00	73.87	-538.22	32.09
7	-503.63	-564.91	61.28	-525.21	21.58
8	-512.33	-565.03	52.70	-525.32	12.99
9	-510.23	-560.38	50.15	-521.31	11.08
10	-487.83	-532.16	44.33	-496.98	9.15
11	-504.23	-566.13	61.90	-526.26	22.03
12	-507.83	-557.26	49.43	-518.62	10.79
13	-485.03	-529.66	44.63	-494.82	9.79
14	-352.53	-339.45	13.08	-330.83	21.70
15	-341.00	-327.56	13.44	-320.58	20.42
16	-354.00	-339.26	14.74	-330.66	23.34
17	-402.83	-437.22	34.39	-415.12	12.29
18	-440.46	-472.58	32.12	-445.61	5.15
19	-468.63	-495.77	27.14	-465.60	3.03
20	-537.93	-579.50	41.57	-537.79	0.14
21	-533.73	-572.56	38.83	-531.81	1.92
22	-550.93	-573.28	22.35	-532.43	18.50
23	-564.33	-607.07	42.74	-561.56	2.77
24	-558.03	-582.48	24.45	-540.36	17.67
25	-678.93	-721.66	42.73	-660.36	18.57
26	-679.83	-732.18	52.35	-669.43	10.40

ME	83.40
MAE	42.75
CMAE	13.15
Slope	1.160
Int.	44.27

ADF Scalar-ZORA: B3LY/TZ2P//OP2

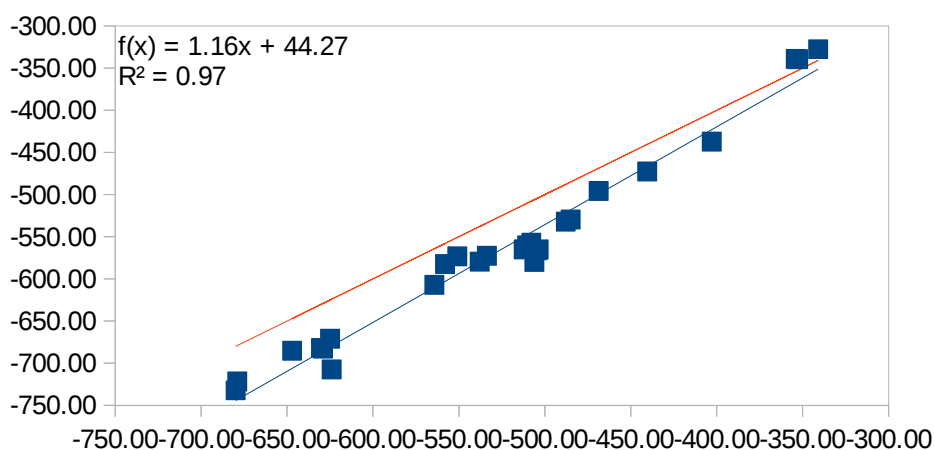


Table S30 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-701.28	72.3	-635.54	6.51
2	-624.03	-726.12	102.1	-661.24	37.21
3	-630.13	-700.43	70.3	-634.66	4.53
4	-624.93	-683.14	58.2	-616.77	8.16
5	-647.03	-702.56	55.5	-636.86	10.17
6	-506.13	-590.01	83.9	-520.42	14.29
7	-503.63	-586.11	82.5	-516.39	12.76
8	-512.33	-587.68	75.3	-518.01	5.68
9	-510.23	-582.67	72.4	-512.83	2.60
10	-487.83	-554.21	66.4	-483.39	4.44
11	-504.23	-576.77	72.5	-506.73	2.50
12	-507.83	-578.20	70.4	-508.21	0.38
13	-485.03	-550.76	65.7	-479.82	5.21
14	-352.53	-439.08	86.6	-364.28	11.75
15	-341.00	-425.37	84.4	-350.09	9.09
16	-354.00	-438.22	84.2	-363.39	9.39
17	-402.83	-445.91	43.1	-371.34	31.49
18	-440.46	-516.71	76.3	-444.59	4.13
19	-468.63	-549.63	81.0	-478.65	10.02
20	-537.93	-593.37	55.4	-523.90	14.03
21	-533.73	-588.30	54.6	-518.65	15.08
22	-550.93	-592.22	41.3	-522.71	28.22
23	-564.33	-627.63	63.3	-559.34	4.99
24	-558.03	-594.37	36.3	-524.93	33.10
25	-678.93	-744.51	65.6	-680.26	1.33
26	-679.83	-755.83	76.0	-691.98	12.15

ME 102.09
 MAE 69.06
 CMAE 11.51
 Slope 0.967
 Int. -86.98

ADF SO-ZORA: B3LY/DZP//OP2

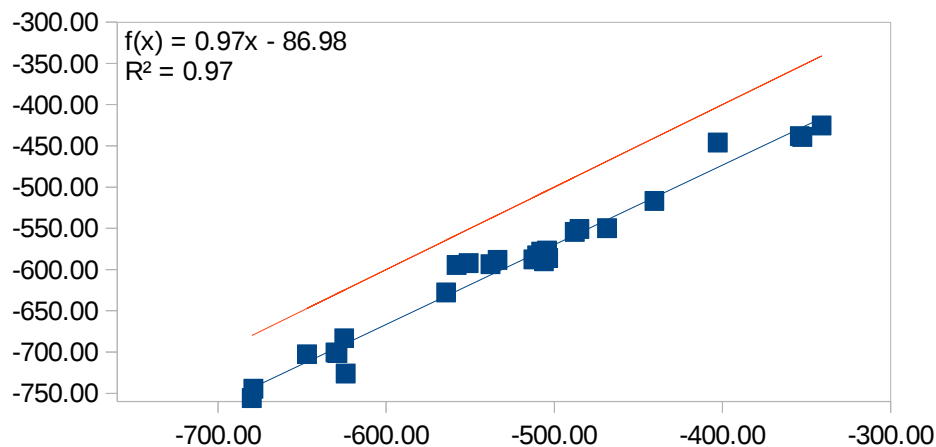


Table S31 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-668.43	39.40	-632.01	2.98
2	-624.03	-692.74	68.71	-654.28	30.25
3	-630.13	-667.43	37.30	-631.10	0.97
4	-624.93	-649.52	24.59	-614.69	10.24
5	-647.03	-669.74	22.71	-633.21	13.82
6	-506.13	-557.57	51.44	-530.47	24.34
7	-503.63	-549.07	45.44	-522.68	19.05
8	-512.33	-551.57	39.24	-524.97	12.64
9	-510.23	-549.09	38.86	-522.70	12.47
10	-487.83	-519.83	32.00	-495.90	8.07
11	-504.23	-544.74	40.51	-518.71	14.48
12	-507.83	-544.69	36.86	-518.67	10.84
13	-485.03	-516.43	31.40	-492.79	7.76
14	-352.53	-351.74	0.79	-341.93	10.60
15	-341.00	-339.88	1.12	-331.07	9.93
16	-354.00	-351.14	2.86	-341.38	12.62
17	-402.83	-416.36	13.53	-401.12	1.71
18	-440.46	-461.89	21.43	-442.83	2.37
19	-468.63	-487.08	18.45	-465.91	2.72
20	-537.93	-558.38	20.44	-531.21	6.72
21	-533.73	-551.96	18.23	-525.33	8.40
22	-550.93	-556.17	5.24	-529.18	21.75
23	-564.33	-590.89	26.56	-560.99	3.34
24	-558.03	-557.63	0.40	-530.52	27.51
25	-678.93	-705.40	26.47	-665.88	13.05
26	-679.83	-716.45	36.62	-676.00	3.83

ME	68.71
MAE	26.95
CMAE	11.25
Slope	1.092
Int.	21.56

ADF SO-ZORA: B3LY/DZP/OP2
no spinorbit contributions

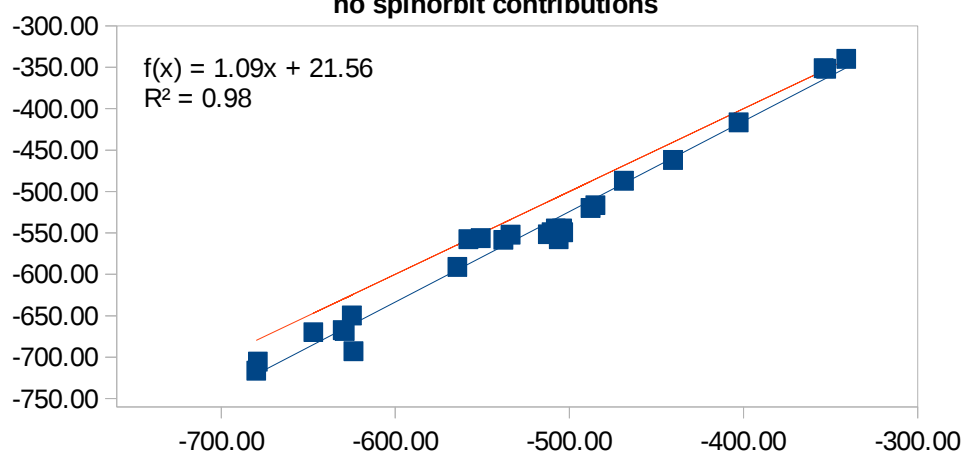


Table S32 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-729.99	101.0	-629.42	0.39
2	-624.03	-721.15	97.1	-621.08	2.95
3	-630.13	-729.68	99.5	-629.13	1.00
4	-624.93	-719.36	94.4	-619.40	5.53
5	-647.03	-733.54	86.5	-632.77	14.26
6	-506.13	-632.96	126.8	-537.89	31.76
7	-503.63	-617.09	113.5	-522.92	19.29
8	-512.33	-604.19	91.9	-510.75	1.58
9	-510.23	-607.20	97.0	-513.58	3.35
10	-487.83	-583.73	95.9	-491.44	3.61
11	-504.23	-620.38	116.2	-526.02	21.79
12	-507.83	-604.19	96.4	-510.75	2.92
13	-485.03	-579.69	94.7	-487.63	2.60
14	-352.53	-422.55	70.0	-339.39	13.14
15	-341.00	-410.38	69.4	-327.90	13.10
16	-354.00	-423.10	69.1	-339.91	14.09
17	-402.83	-486.16	83.3	-399.40	3.43
18	-440.46	-540.83	100.4	-450.97	10.51
19	-468.63	-569.72	101.1	-478.23	9.60
20	-537.93	-635.06	97.1	-539.87	1.94
21	-533.73	-628.56	94.8	-533.74	0.01
22	-550.93	-628.07	77.1	-533.27	17.66
23	-564.33	-662.50	98.2	-565.75	1.42
24	-558.03	-634.63	76.6	-539.46	18.57
25	-678.93	-775.03	96.1	-671.92	7.01
26	-679.83	-786.26	106.4	-682.51	2.68

ME	126.83
MAE	94.25
CMAE	8.62
Slope	1.060
Int.	-62.80

ADF SO-ZORA: B3LY/TZ2P//OP2

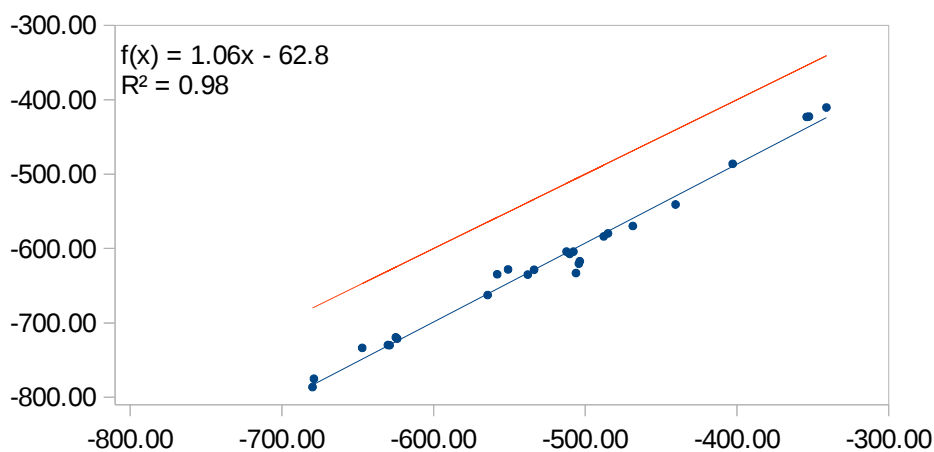


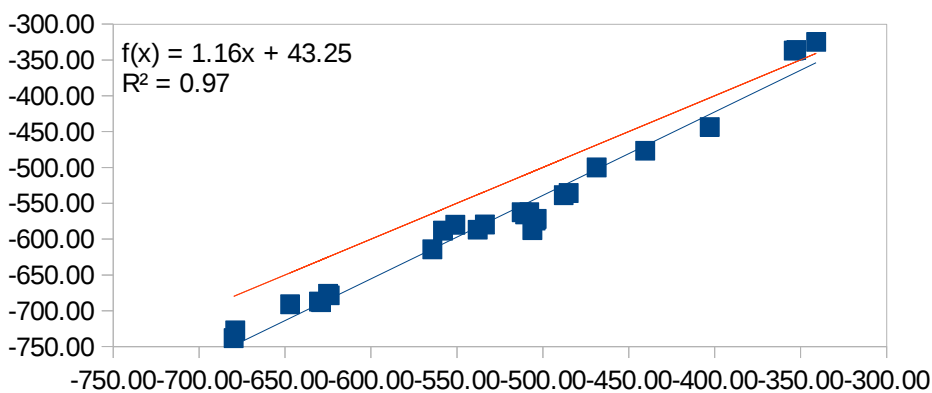
Table S33 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$i(^{113}\text{Cd})_{\text{fit}}$ corrected by fi	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-687.87	58.84	-628.11	7.94
2	-624.03	-678.36	54.33	-619.94	11.59
3	-630.13	-687.11	56.98	-627.46	9.73
4	-624.93	-676.36	51.43	-618.22	14.31
5	-647.03	-690.73	43.70	-630.57	23.33
6	-506.13	-587.26	81.13	-541.68	23.44
7	-503.63	-571.70	68.07	-528.31	11.78
8	-512.33	-562.49	50.16	-520.40	5.30
9	-510.23	-565.52	55.29	-523.00	0.45
10	-487.83	-538.76	50.93	-500.01	2.39
11	-504.23	-573.85	69.62	-530.15	13.13
12	-507.83	-562.49	54.66	-520.40	0.80
13	-485.03	-535.75	50.72	-497.42	2.34
14	-352.53	-336.32	16.21	-326.09	51.27
15	-341.00	-324.85	16.15	-316.23	50.18
16	-354.00	-336.91	17.09	-326.60	52.20
17	-402.83	-443.58	40.75	-418.24	3.99
18	-440.46	-476.63	36.17	-446.63	11.55
19	-468.63	-499.86	31.23	-466.59	18.59
20	-537.93	-586.87	48.94	-541.34	8.72
21	-533.73	-579.42	45.69	-534.94	11.30
22	-550.93	-579.93	29.00	-535.38	28.03
23	-564.33	-614.26	49.93	-564.87	10.21
24	-558.03	-588.17	30.14	-542.45	27.64
25	-678.93	-727.15	48.22	-661.86	22.10
26	-679.83	-737.90	58.07	-671.09	13.22

ME	81.13
MAE	46.67
CMAE	16.75
Slope	1.164
Int.	43.25

ADF SO-ZORA:B3LY/TZ2P//OP2

no spinorbit contributions



OP3 geometry [ADF relativistic scalar ZORA; B3LYP/TZ2P]

Table S34 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-617.67	11.36	-616.78	12.25
2	-624.03	-638.91	14.88	-638.93	14.90
3	-630.13	-620.40	9.73	-619.63	10.50
4	-624.93	-623.06	1.87	-622.40	2.53
5	-647.03	-638.91	8.12	-638.93	8.10
6	-506.13	-540.59	34.46	-536.42	30.29
7	-503.63	-516.08	12.45	-510.87	7.24
8	-512.33	-512.92	0.59	-507.57	4.76
9	-510.23	-516.02	5.79	-510.81	0.58
10	-487.83	-484.76	3.07	-478.21	9.62
11	-504.23	-534.04	29.81	-529.59	25.36
12	-507.83	-510.25	2.42	-504.79	3.04
13	-485.03	-469.49	15.54	-462.30	22.73
14	-352.53	-359.87	7.34	-348.00	4.53
15	-341.00	-344.86	3.86	-332.35	8.65
16	-354.00	-353.95	0.05	-341.83	12.17
17	-402.83	-406.36	3.53	-396.47	6.36
18	-440.46	-449.47	9.01	-441.42	0.96
19	-468.63	-480.05	11.42	-473.30	4.67
20	-537.93	-561.12	23.19	-557.82	19.89
21	-533.73	-545.47	11.74	-541.51	7.78
22	-550.93	-564.85	13.92	-561.72	10.79
23	-564.33	-577.87	13.54	-575.28	10.95
24	-558.03	-556.27	1.76	-552.76	5.27
25	-678.93	-661.83	17.10	-662.83	16.10
26	-679.83	-670.30	9.53	-671.65	8.18

ME	34.46
MAE	10.62
CMAE	10.32
Slope	0.959
Int.	-26.09

G09: B3LYP/Sadlej(Cd);6-31G(d)//OP3

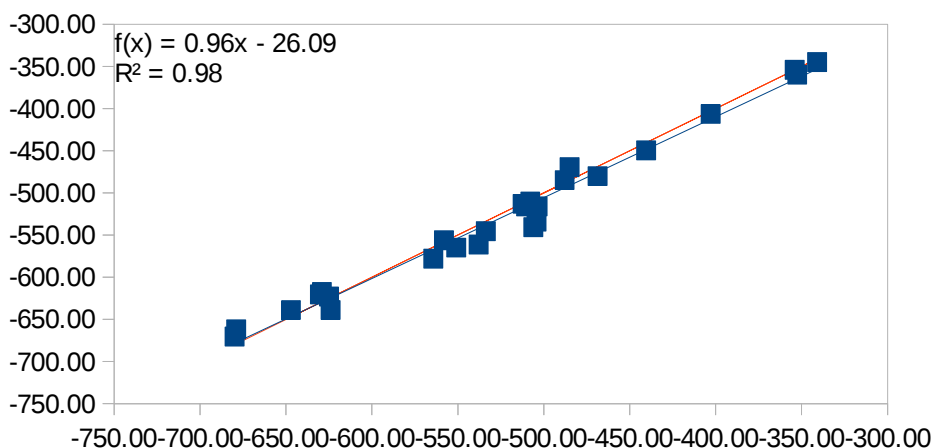


Table S35 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-614.33	14.70	-619.04	9.99
2	-624.03	-610.93	13.10	-615.45	8.58
3	-630.13	-617.06	13.07	-621.92	8.21
4	-624.93	-619.69	5.24	-624.69	0.24
5	-647.03	-635.51	11.52	-641.41	5.62
6	-506.13	-536.82	30.69	-537.19	31.06
7	-503.63	-512.43	8.80	-511.42	7.79
8	-512.33	-509.73	2.60	-508.58	3.75
9	-510.23	-512.99	2.76	-512.01	1.78
10	-487.83	-481.91	5.92	-479.19	8.64
11	-504.23	-530.35	26.12	-530.34	26.11
12	-507.83	-507.19	0.64	-505.89	1.94
13	-485.03	-466.63	18.40	-463.05	21.98
14	-352.53	-357.02	4.49	-347.31	5.22
15	-341.00	-341.32	0.32	-330.72	10.28
16	-354.00	-351.44	2.56	-341.41	12.59
17	-402.83	-402.37	0.46	-395.19	7.64
18	-440.46	-446.06	5.60	-441.33	0.87
19	-468.63	-476.42	7.79	-473.40	4.77
20	-537.93	-557.26	19.33	-558.77	20.84
21	-533.73	-541.64	7.91	-542.27	8.54
22	-550.93	-560.90	9.97	-562.62	11.69
23	-564.33	-574.02	9.69	-576.47	12.14
24	-558.03	-551.88	6.15	-553.09	4.94
25	-678.93	-657.75	21.18	-664.89	14.04
26	-679.83	-666.41	13.42	-674.04	5.79

ME	30.69
MAE	10.09
CMAE	9.81
Slope	0.947
Int.	-28.15

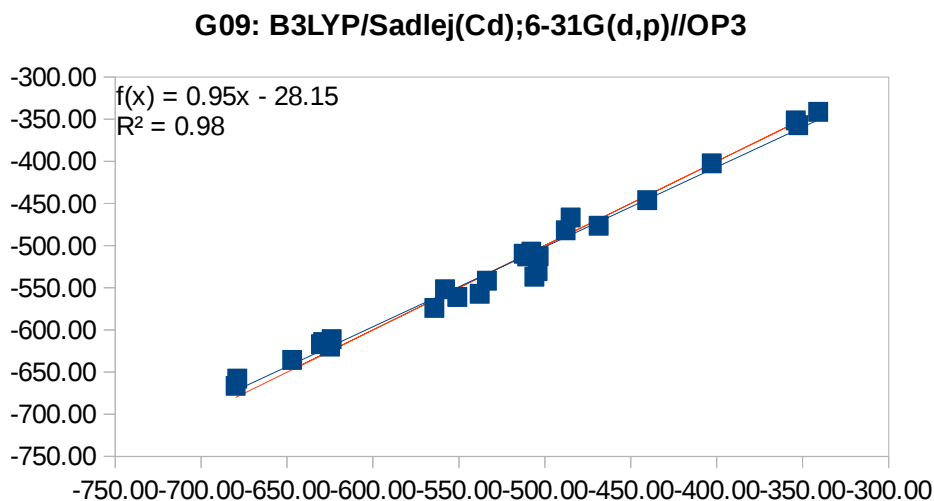


Table S36 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-577.41	51.62	-614.35	14.68
2	-624.03	-580.92	43.11	-618.12	5.91
3	-630.13	-578.95	51.18	-616.01	14.12
4	-624.93	-582.11	42.82	-619.41	5.52
5	-647.03	-602.05	44.98	-640.85	6.18
6	-506.13	-506.38	0.25	-537.96	31.83
7	-503.63	-483.40	20.23	-513.26	9.63
8	-512.33	-478.43	33.90	-507.90	4.43
9	-510.23	-476.75	33.48	-506.10	4.13
10	-487.83	-450.23	37.60	-477.59	10.24
11	-504.23	-501.07	3.16	-532.26	28.03
12	-507.83	-478.81	29.02	-508.31	0.48
13	-485.03	-440.46	44.57	-467.08	17.95
14	-352.53	-332.81	19.72	-351.31	1.22
15	-341.00	-316.47	24.53	-333.74	7.26
16	-354.00	-326.49	27.51	-344.51	9.49
17	-402.83	-369.79	33.04	-391.08	11.75
18	-440.46	-415.12	25.34	-439.83	0.63
19	-468.63	-445.73	22.90	-472.74	4.11
20	-537.93	-526.71	11.22	-559.83	21.90
21	-533.73	-508.34	25.39	-540.08	6.35
22	-550.93	-527.10	23.83	-560.25	9.32
23	-564.33	-541.09	23.24	-575.29	10.96
24	-558.03	-520.04	37.99	-552.66	5.37
25	-678.93	-634.09	44.84	-675.30	3.63
26	-679.83	-640.89	38.94	-682.61	2.78

ME	51.62
MAE	30.55
CMAE	9.54
Slope	0.930
Int.	-6.12

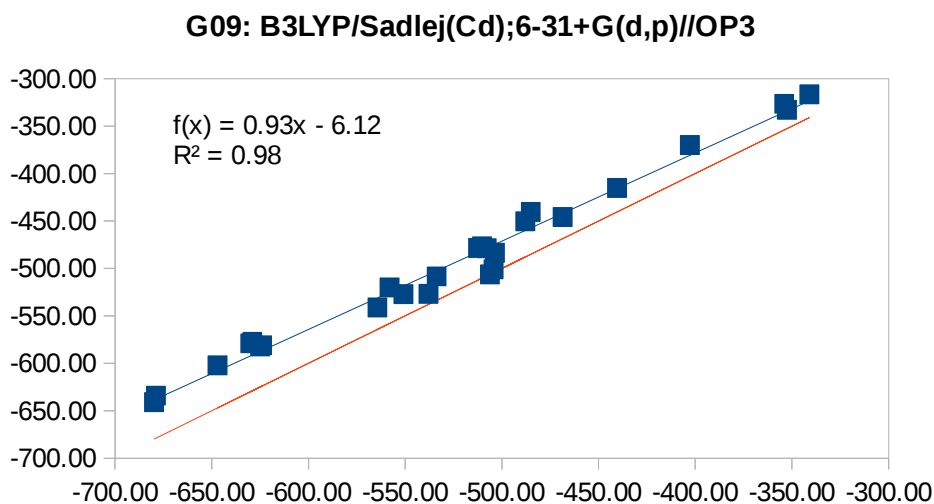


Table S37 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-2 [B3LYP/DZP] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-678.59	49.56	-616.31	12.72
2	-624.03	-677.31	53.28	-615.03	9.00
3	-630.13	-680.18	50.05	-617.90	12.23
4	-624.93	-684.23	59.30	-621.94	2.99
5	-647.03	-702.13	55.10	-639.80	7.23
6	-506.13	-602.91	96.78	-540.78	34.65
7	-503.63	-578.04	74.41	-515.96	12.33
8	-512.33	-581.30	68.97	-519.22	6.89
9	-510.23	-586.45	76.22	-524.36	14.13
10	-487.83	-552.66	64.83	-490.63	2.80
11	-504.23	-596.59	92.36	-534.48	30.25
12	-507.83	-581.82	73.99	-519.73	11.90
13	-485.03	-538.22	53.19	-476.22	8.81
14	-352.53	-399.13	46.60	-337.41	15.12
15	-341.00	-383.12	42.12	-321.43	19.57
16	-354.00	-395.51	41.51	-333.80	20.20
17	-402.83	-451.46	48.63	-389.63	13.20
18	-440.46	-509.36	68.90	-447.42	6.96
19	-468.63	-529.69	61.06	-467.71	0.92
20	-537.93	-616.60	78.67	-554.45	16.52
21	-533.73	-602.43	68.70	-540.30	6.57
22	-550.93	-622.83	71.90	-560.66	9.73
23	-564.33	-640.26	75.93	-578.06	13.73
24	-558.03	-607.55	49.52	-545.41	12.62
25	-678.93	-721.43	42.50	-659.07	19.86
26	-679.83	-730.27	50.44	-667.89	11.94

ME	96.78
MAE	62.10
CMAE	12.80
Slope	1.002
Int.	-61.05

ADF: B3LYP/DZP//OP3

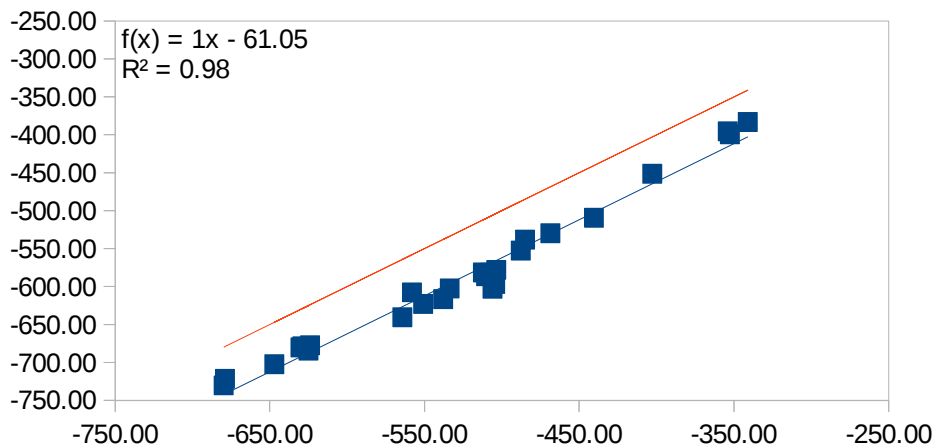


Table S38 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at NR-2 [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-667.78	38.75	-614.83	15.35
2	-624.03	-664.18	40.15	-611.37	13.82
3	-630.13	-669.38	39.25	-616.37	14.92
4	-624.93	-671.81	46.88	-618.71	7.38
5	-647.03	-688.72	41.69	-634.97	13.22
6	-506.13	-600.28	94.15	-549.93	42.64
7	-503.63	-571.11	67.48	-521.88	17.09
8	-512.33	-572.66	60.33	-523.37	9.88
9	-510.23	-576.24	66.01	-526.81	15.43
10	-487.83	-536.72	48.89	-488.81	0.17
11	-504.23	-589.01	84.78	-539.09	33.71
12	-507.83	-573.02	65.19	-523.72	14.73
13	-485.03	-525.16	40.13	-477.70	8.49
14	-352.53	-379.07	26.54	-337.23	16.46
15	-341.00	-359.91	18.91	-318.80	23.35
16	-354.00	-374.86	20.86	-333.18	21.98
17	-402.83	-433.76	30.93	-389.81	14.17
18	-440.46	-486.56	46.1	-440.58	1.03
19	-468.63	-511.65	43.02	-464.71	5.08
20	-537.93	-599.23	61.3	-548.92	9.83
21	-533.73	-588.37	54.64	-538.48	3.59
22	-550.93	-608.14	57.21	-557.48	5.40
23	-564.33	-624.47	60.14	-573.19	7.70
24	-558.03	-600.32	42.29	-549.97	9.22
25	-678.93	-718.86	39.93	-663.95	16.14
26	-679.83	-724.34	44.51	-669.22	11.77

ME	94.15
MAE	49.23
CMAE	13.56
Slope	1.040
Int.	-28.36

ADF: B3LYP/TZ2P//OP3

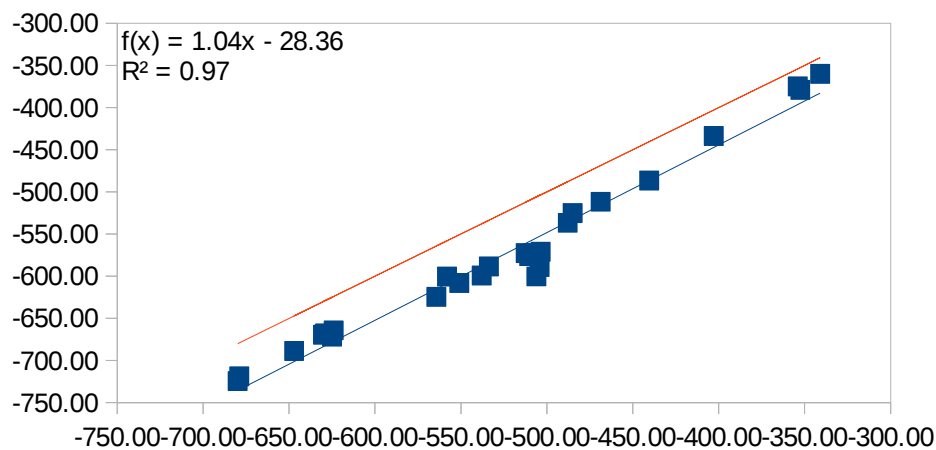


Table S39 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SR [B3LYP/DZP] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-614.07	14.96	-614.82	14.21
2	-624.03	-638.22	14.19	-637.34	13.31
3	-630.13	-612.98	17.15	-613.80	16.33
4	-624.93	-594.93	30.00	-596.96	27.97
5	-647.03	-615.75	31.28	-616.38	30.65
6	-506.13	-502.92	3.21	-511.14	5.01
7	-503.63	-492.36	11.27	-501.29	2.34
8	-512.33	-496.41	15.92	-505.06	7.27
9	-510.23	-493.88	16.35	-502.70	7.53
10	-487.83	-464.57	23.26	-475.37	12.46
11	-504.23	-490.35	13.88	-499.41	4.82
12	-507.83	-489.53	18.30	-498.65	9.18
13	-485.03	-461.20	23.83	-472.22	12.81
14	-352.53	-301.46	51.07	-323.22	29.31
15	-341.00	-289.72	51.28	-312.27	28.73
16	-354.00	-300.48	53.52	-322.30	31.70
17	-402.83	-402.40	0.43	-417.37	14.54
18	-440.46	-456.79	16.33	-468.11	27.65
19	-468.63	-485.12	16.49	-494.53	25.90
20	-537.93	-577.33	39.40	-580.55	42.62
21	-533.73	-569.19	35.46	-572.95	39.22
22	-550.93	-592.67	41.74	-594.85	43.92
23	-564.33	-609.87	45.54	-610.90	46.57
24	-558.03	-583.39	25.36	-586.20	28.17
25	-678.93	-650.12	28.81	-648.44	30.49
26	-679.83	-661.13	18.70	-658.71	21.12

ME	53.52
MAE	25.30
CMAE	22.07
Slope	1.072
Int.	45.05

ADF Scalar ZORA: B3LYP/DZP//OP3

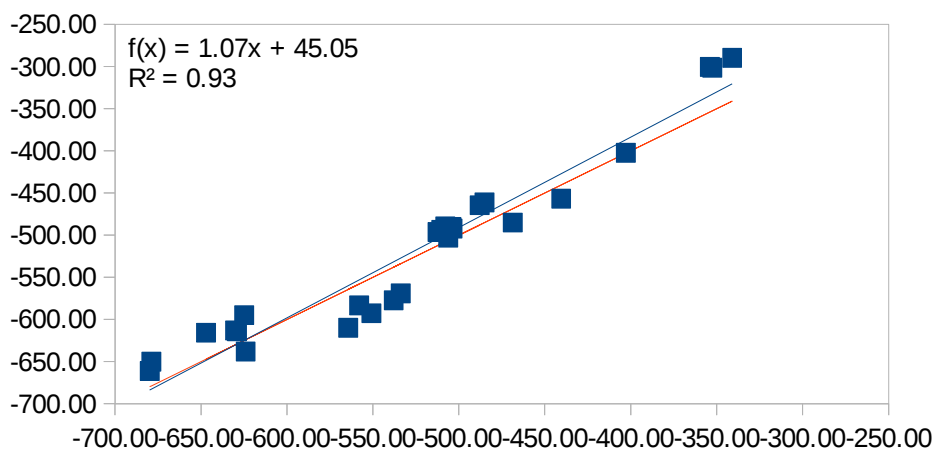


Table S40 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SR [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-652.69	23.66	-608.53	20.50
2	-624.03	-652.61	28.58	-608.46	15.57
3	-630.13	-655.15	25.02	-610.67	19.46
4	-624.93	-658.99	34.06	-614.02	10.91
5	-647.03	-676.85	29.82	-629.57	17.46
6	-506.13	-590.42	84.29	-554.31	48.18
7	-503.63	-562.84	59.21	-530.30	26.67
8	-512.33	-554.97	42.64	-523.44	11.11
9	-510.23	-557.93	47.70	-526.02	15.79
10	-487.83	-523.42	35.59	-495.97	8.14
11	-504.23	-582.07	77.84	-547.04	42.81
12	-507.83	-554.28	46.45	-522.84	15.01
13	-485.03	-509.04	24.01	-483.45	1.58
14	-352.53	-321.17	31.36	-319.86	32.67
15	-341.00	-304.74	36.26	-305.56	35.44
16	-354.00	-318.11	35.89	-317.20	36.80
17	-402.83	-421.85	19.02	-407.53	4.70
18	-440.46	-464.44	23.98	-444.62	4.16
19	-468.63	-490.90	22.27	-467.66	0.97
20	-537.93	-594.90	56.97	-558.21	20.28
21	-533.73	-578.69	44.96	-544.10	10.37
22	-550.93	-602.17	51.24	-564.54	13.61
23	-564.33	-619.37	55.04	-579.52	15.19
24	-558.03	-592.89	34.86	-556.46	1.57
25	-678.93	-704.47	25.54	-653.62	25.31
26	-679.83	-714.16	34.33	-662.06	17.77

ME	84.29
MAE	39.64
CMAE	18.16
Slope	1.148
Int.	46.18

ADF Scalar ZORA: B3LYP/TZ2P//OP3

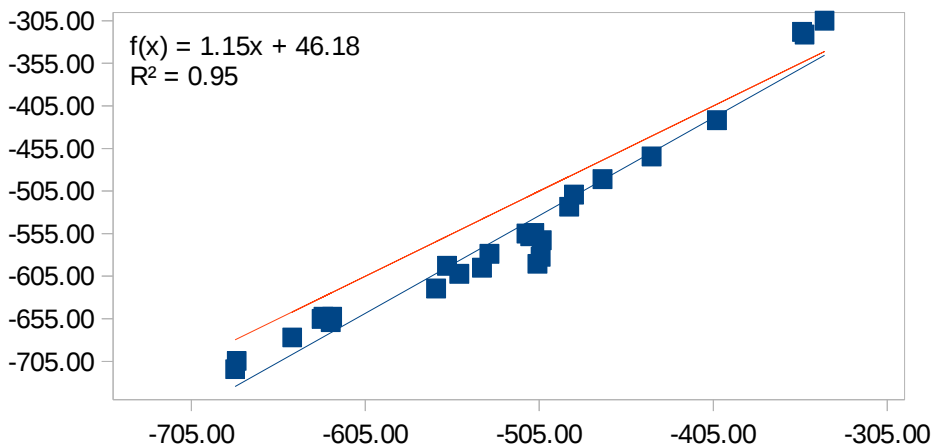


Table S41 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-671.22	42.19	-612.67	16.36
2	-624.03	-678.84	54.81	-620.65	3.38
3	-630.13	-674.48	44.35	-616.09	14.04
4	-624.93	-677.41	52.48	-619.15	5.78
5	-647.03	-694.99	47.96	-637.56	9.47
6	-506.13	-609.74	103.61	-548.31	42.18
7	-503.63	-581.49	77.86	-518.74	15.11
8	-512.33	-575.81	63.48	-512.79	0.46
9	-510.23	-578.63	68.40	-515.74	5.51
10	-487.83	-544.56	56.73	-480.07	7.76
11	-504.23	-601.80	97.57	-540.00	35.77
12	-507.83	-572.92	65.09	-509.76	1.93
13	-485.03	-528.80	43.77	-463.58	21.45
14	-352.53	-423.73	71.20	-353.58	1.05
15	-341.00	-405.13	64.13	-334.11	6.89
16	-354.00	-419.43	65.43	-349.08	4.92
17	-402.83	-430.31	27.48	-360.47	42.36
18	-440.46	-509.83	69.37	-443.72	3.26
19	-468.63	-548.04	79.41	-483.72	15.09
20	-537.93	-609.97	72.04	-548.55	10.62
21	-533.73	-592.86	59.13	-530.64	3.09
22	-550.93	-619.52	68.59	-558.55	7.62
23	-564.33	-638.58	74.25	-578.50	14.17
24	-558.03	-604.09	46.06	-542.40	15.63
25	-678.93	-729.97	51.04	-674.18	4.75
26	-679.83	-738.35	58.52	-682.95	3.12

ME	103.61
MAE	62.50
CMAE	11.99
Slope	0.955
Int.	-85.99

ADF SO-ZORA: B3LYP/DZP//OP3

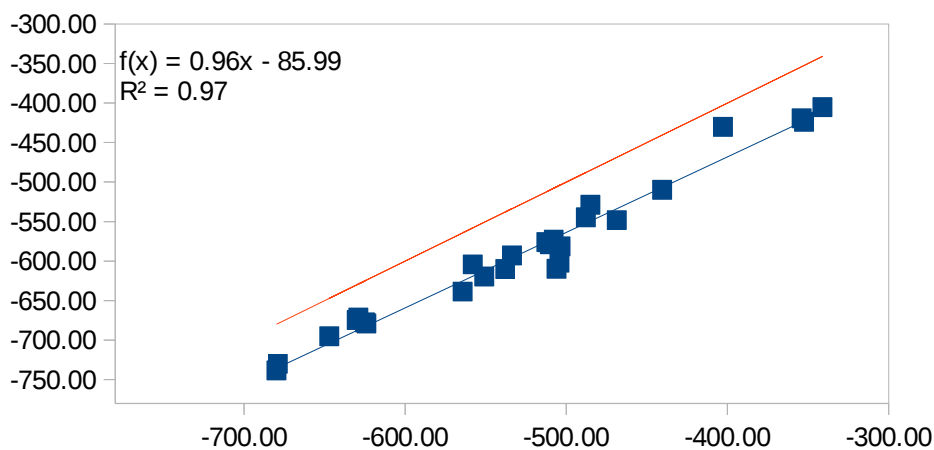


Table S42 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-641.21	12.18	-611.19	17.84
2	-624.03	-646.22	22.19	-615.78	8.25
3	-630.13	-644.40	14.26	-614.11	16.02
4	-624.93	-647.10	22.17	-616.59	8.34
5	-647.03	-664.79	17.76	-632.84	14.19
6	-506.13	-576.49	70.36	-551.76	45.63
7	-503.63	-548.27	44.64	-525.85	22.22
8	-512.33	-542.98	30.65	-520.99	8.66
9	-510.23	-548.60	38.37	-526.15	15.92
10	-487.83	-513.58	25.74	-493.98	6.15
11	-504.23	-568.62	64.39	-544.53	40.30
12	-507.83	-543.09	35.26	-521.09	13.26
13	-485.03	-497.94	12.91	-479.62	5.41
14	-352.53	-336.11	16.42	-331.02	21.51
15	-341.00	-319.63	21.37	-315.89	25.11
16	-354.00	-332.33	21.67	-327.55	26.45
17	-402.83	-403.63	0.80	-393.02	9.81
18	-440.46	-456.40	15.94	-441.48	1.02
19	-468.63	-485.67	17.04	-468.36	0.27
20	-537.93	-579.20	41.27	-554.24	16.31
21	-533.73	-560.32	26.58	-536.90	3.17
22	-550.93	-586.20	35.27	-560.68	9.75
23	-564.33	-605.87	41.54	-578.74	14.41
24	-558.03	-571.03	13.00	-546.74	11.29
25	-678.93	-693.73	14.80	-659.41	19.52
26	-679.83	-702.02	22.19	-667.03	12.80

ME	70.36
MAE	26.88
CMAE	15.14
Slope	1.089
Int.	24.37

ADF SO-ZORA: B3LYP/DZP//OP3

No spinorbit contributions

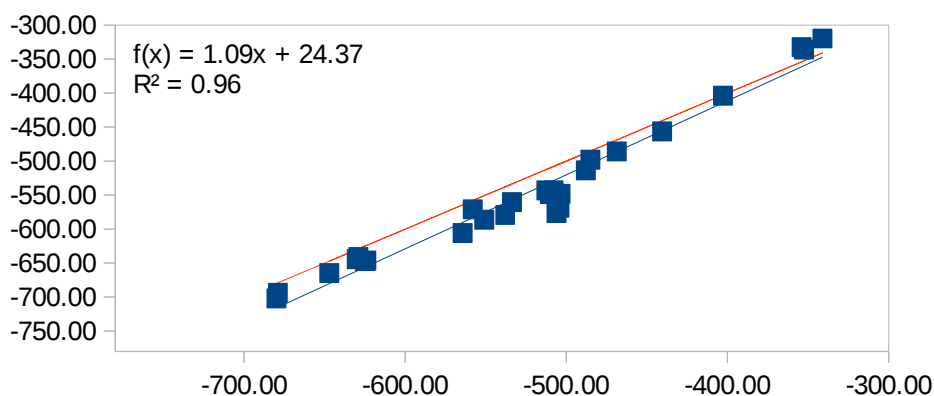


Table S43 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/TZ2P] level. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-696.75	67.72	-607.76	21.27
2	-624.03	-698.44	74.41	-609.37	14.66
3	-630.13	-699.45	69.32	-610.33	19.80
4	-624.93	-703.85	78.92	-614.53	10.40
5	-647.03	-722.44	75.41	-632.25	14.78
6	-506.13	-638.20	132.07	-551.94	45.81
7	-503.63	-612.68	109.05	-527.62	23.99
8	-512.33	-601.31	88.98	-516.78	4.45
9	-510.23	-601.59	91.36	-517.04	6.81
10	-487.83	-571.49	83.66	-488.35	0.52
11	-504.23	-631.82	127.59	-545.86	41.63
12	-507.83	-597.85	90.02	-513.48	5.65
13	-485.03	-555.91	70.88	-473.50	11.53
14	-352.53	-405.46	52.93	-330.08	22.45
15	-341.00	-388.31	47.31	-313.72	27.28
16	-354.00	-399.30	45.30	-324.20	29.80
17	-402.83	-468.24	65.41	-389.92	12.91
18	-440.46	-531.06	90.60	-449.81	9.35
19	-468.63	-563.27	94.64	-480.51	11.88
20	-537.93	-644.39	106.46	-557.85	19.92
21	-533.73	-630.25	96.52	-544.37	10.64
22	-550.93	-654.47	103.54	-567.45	16.52
23	-564.33	-670.52	106.19	-582.76	18.43
24	-558.03	-643.42	85.39	-556.92	1.11
25	-678.93	-752.04	73.11	-660.47	18.46
26	-679.83	-757.95	78.12	-666.10	13.73

ME	132.07
MAE	84.80
CMAE	16.68
Slope	1.049
Int.	-59.21

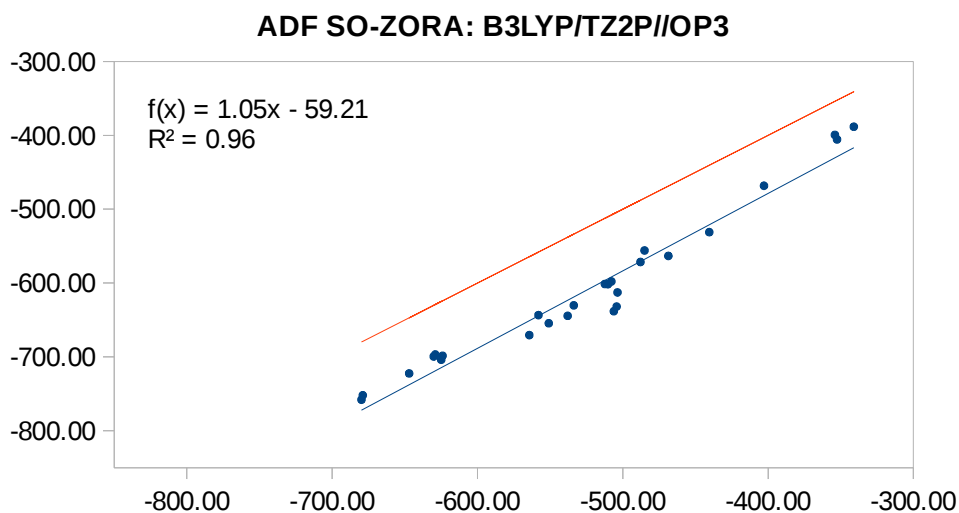


Table S44 Calculated $\delta(^{113}\text{Cd})$, statistical data and graphical correlation obtained at SO [B3LYP/TZ2P] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd .

MODEL	Exptl. $\delta(^{113}\text{Cd})$	Calcd $\delta(^{113}\text{Cd})$	ABS diff $\delta(^{113}\text{Cd})$	$\delta(^{113}\text{Cd})_{\text{fit}}$ corrected by fit	ABS diff $\delta(^{113}\text{Cd})_{\text{fit}}$
1	-629.03	-657.66	28.63	-613.31	28.38
2	-624.03	-658.16	34.13	-613.74	22.96
3	-630.13	-660.21	30.07	-615.51	27.31
4	-624.93	-664.25	39.32	-619.01	18.65
5	-647.03	-682.21	35.18	-634.58	25.39
6	-506.13	-596.82	90.69	-560.58	42.50
7	-503.63	-569.82	66.19	-537.19	21.92
8	-512.33	-560.21	47.88	-528.86	5.00
9	-510.23	-563.07	52.84	-531.34	9.55
10	-487.83	-529.84	42.01	-502.54	3.54
11	-504.23	-589.09	84.86	-553.89	37.80
12	-507.83	-559.37	51.54	-528.14	8.79
13	-485.03	-515.09	30.06	-489.76	6.27
14	-352.53	-318.31	34.22	-319.24	42.00
15	-341.00	-303.48	37.52	-306.39	43.15
16	-354.00	-312.08	41.92	-313.84	48.80
17	-402.83	-415.34	12.51	-403.32	9.35
18	-440.46	-468.21	27.75	-449.14	1.78
19	-468.63	-494.43	25.80	-471.86	7.53
20	-537.93	-563.04	25.11	-531.31	18.18
21	-533.73	-547.90	14.17	-518.19	26.92
22	-550.93	-571.12	20.19	-538.31	24.27
23	-564.33	-625.99	61.66	-585.86	9.24
24	-558.03	-598.83	40.80	-562.33	7.68
25	-678.93	-709.03	30.10	-657.82	34.36
26	-679.83	-701.01	21.18	-650.87	42.13

ME	90.69
MAE	39.47
CMAE	22.06
Slope	1.154
Int.	50.10

