

# Reaction between Indazole and Pd-Bound Isocyanides – a Theoretical Mechanistic Study

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## Supplementary Material

### Computational Details

#### *Energy Decomposition Analysis (EDA)*

The corresponding bonding energies of the interactions between the fragments shown in Figure 2 were calculated by considering their decomposition into strain and interaction energy contributions according to the Ziegler-Rauk works as implemented in the ADF package [S1–S3].

According to this scheme, the total energy  $\Delta E$  may be written as:

$$\Delta E = \Delta E_{\text{int}} + \Delta E_{\text{strain}} \quad (1)$$

$$\Delta E_{\text{int}} = \Delta E_{\text{elec}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}} \quad (2)$$

where  $\Delta E_{\text{elec}}$ ,  $\Delta E_{\text{Pauli}}$ , and  $\Delta E_{\text{orb}}$  represent contributions due to the quasi-classical electrostatic interaction, the Pauli repulsion, and the orbital interaction, respectively.  $\Delta E_{\text{disp}}$  represents the contribution due to dispersion corrections. Moreover, the last term  $\Delta E_{\text{strain}}$  provides information about the energy required to distort structure of free fragments to the geometry they assume in the final complex. Finally,  $\Delta E_{\text{int}}$  and  $-\Delta E$  are defined as the bonding (BE) and dissociation (DE) energies, respectively.

Fragment approach does not implement the solvent effects. In this context, as a better approximation to describe also the solvent effect, the single fragments SCFs were run accounting for the solvent before to run the final SCF without inclusion of solvent. This allowed to combine the fragments with the appropriate orbitals energies due to the effect of the solvent.

#### *Voronoi Deformation Density (VDD) analysis*

The charge distribution has been determined by analysis of the electron density deformation using the Voronoi Deformation Density (VDD) approach [S4]. VDD atomic charges were calculated as:

$$\Delta Q_A = - \int_V (\rho(r) - \sum_i \rho_i(r)) dr \quad (3)$$

where V corresponds to the Voronoi cell of atom A into the molecule,  $\rho(r)$  is the electron density of the molecule, and  $\sum_i \rho_i(r)$  is the promolecule, used as reference, obtained as superposition of non-interacting atomic densities. Thus, VDD charges represent the electron density flowed from/towards an atom. Positive and negative values correspond to loss or gain of electrons, respectively.

#### *Crystal orbital overlap population (COOP)*

Crystal orbital overlap population (COOP) [S5] was calculated as implemented in the ADF package.

### **Bond Analysis**

#### *Bond analysis of TS6 and TS14*

Bonding schemes for **TS6** and **TS14** are reported in Figures S1 and S2. Transition states present an intermediate behavior between **1** and Z-**P1**, Z-**P2** where in the Pd bearing fragments are already involved almost all the orbitals occurring in the products, while the CN bearing fragment still show the orbitals involved in the Pd–C bonding in **1**.

#### *VDD charges analysis*

VDD charges ( $\Delta Q$ ) analysis for the fragment schemes in Figure 2 allowed to get further information about the electron density flow during the bond formation between the fragments.

Results are given in Table S1. Also in this case we start by discussing the model systems characterized by the Pd–C interaction.

We will consider the  $\Delta Q$  values for Pd, Cl,  $C_{CN}$ ,  $N_{CN}$  and the  $N_{Ind}$  (the latter is referred to the amino or imino nitrogen, for **TS14/Z-P1** and **TS6/Z-P2**, respectively). For all these systems, the trend for Pd and Cl is the same. The Pd–C bond formation causes an electron density depletion on Pd and an increasing of the electron density of one of the Cl atoms while the second Cl shows a small positive  $\Delta Q$  value. For all the systems, the Cl atoms with negative  $\Delta Q$  are in trans to the interacting fragments. Accounting for the bonding schemes discussed (Figures 5, S1, S2) this is in line with the composition of the **Pd52a** orbital, for which the electron density arising from the  $C_{CN}$  carbon to Pd in the  $\sigma$  interaction is localized into the more electronegative halogen atom. Concerning  $C_{CN}$ , despite its donating role in the  $\sigma$  interaction, its  $\Delta Q$  value remains almost unchanged ranging from low negative values for **1**, **TS6** and **TS14**, to low positive values for **Z-P1** and **Z-P2**. In a qualitative way, this implies an almost similar contributions of the two Pd←C and Pd→C, donation and back-donation pathways. The effect of Pd–C interaction results very small for the  $N_{CN}$  and is quite similar to  $N_{Ind}$ , considering both TSs and products.

Relevant  $\Delta Q$  charges for  $\sigma'$  interactions in the TSs, are also reported in Figure S3. Interestingly,  $C_{CN}$  and  $N_{CN}$  show an opposite trend, with respect to  $\sigma$  interactions, by changing their  $\Delta Q$  charge signs. This trend seems counter-intuitive with respect to an expected negative  $\Delta Q$  charge on the  $C_{CN}$  ensued after the donation from the  $N_{Ind}$ . This could be explained accounting for a withdrawing effect of the  $N_{CN}$  atom which tends to polarize the increased electron density on the  $C_{CN}$  and further affects the  $\Delta Q$  sign change for Pd and Cl, even if smaller in magnitude with respect to  $\sigma$ , with a cascade effect which causes a small electron density depletion on the halogens in favor of the Pd atom. Finally, the indazole hydrogens shows a small negative  $\Delta Q$  charge likely attributable to the occurrence of a hydrogen bond between these atoms, if we considering the  $N_{CN}$ – $H_{Ind}$  distances (see Figure S3), which are in the range for the occurrence of such interaction.

### EDA analysis

More information about the energetic of the interactions so far discussed were provided by EDA analysis. The relevant energies contributions to the interactions, corresponding to the fragments schemes in Figure 2, are given in Table S2. Interestingly, accounting for the Pd–C interactions, it is possible to observe that the formation of both transition states leads to higher bonding energies (BE), around 20 kcal/mol, with respect to **1**. This is due either to the greater contribution provided by the attractive terms, ( $\Delta E_{\text{Elec}}$  and  $\Delta E_{\text{Orb}}$ ), with respect to the repulsive  $\Delta E_{\text{Pauli}}$  ones (increasing of  $\Delta E_{\text{Orb}}$  and  $\Delta E_{\text{Pauli}}$  are in accord with the bonding schemes in Figures S1 and S2), as well as, also to the non-negligible role due to the dispersion corrections. Nonetheless, the  $\Delta E_{\text{Int}}$  values reconciles the expected behavior, *i.e.*, a lower stability of the TSs with respect to compound **1**, due to the high destabilizing  $\Delta E_{\text{prep}}$  term, arising from the high distortion of the C≡N bond during the transition state formation. To note that we found that **TS6** resulted slightly more stable with respect to **TS14**, thus rendering **Z-P2** kinetically favorite. Nonetheless, the Pd–C bond of **TS14** resulted more stable mainly due to the contribution of the  $\Delta E_{\text{disp}}$  term. Concerning **TS6** and **TS14**, the same stability trend was observed for the  $\sigma'$  interaction still mainly ruled by the dispersions corrections term.

Moving from the TSs to the products, as could be expected, the Pd–C bond resulted more stabilized, in **Z-P1** and **Z-P2** (Table S2). The  $\Delta E_{\text{Elec}}$  and the  $\Delta E_{\text{Pauli}}$  terms continue to increase according to the formation of the CNCyInd moiety, while the  $\Delta E_{\text{orb}}$  terms remain almost unchanged. These latter results indicate that the change in the orbital interactions is already attained in the TS. The BE and the  $\Delta E_{\text{Int}}$  of **Z-P1** resulted slightly more stable than **Z-P2**, and an inspection of Table S2 still indicates that  $\Delta E_{\text{disp}}$  term is the discriminant contribution to the different stability of the two products.

Finally, due to the lack of symmetry in these systems, it was not possible to quantify the contribution of the  $\sigma$  and  $\pi$  interactions to the  $\Delta E_{\text{Orb}}$  term. In this respect, we tried to estimate these

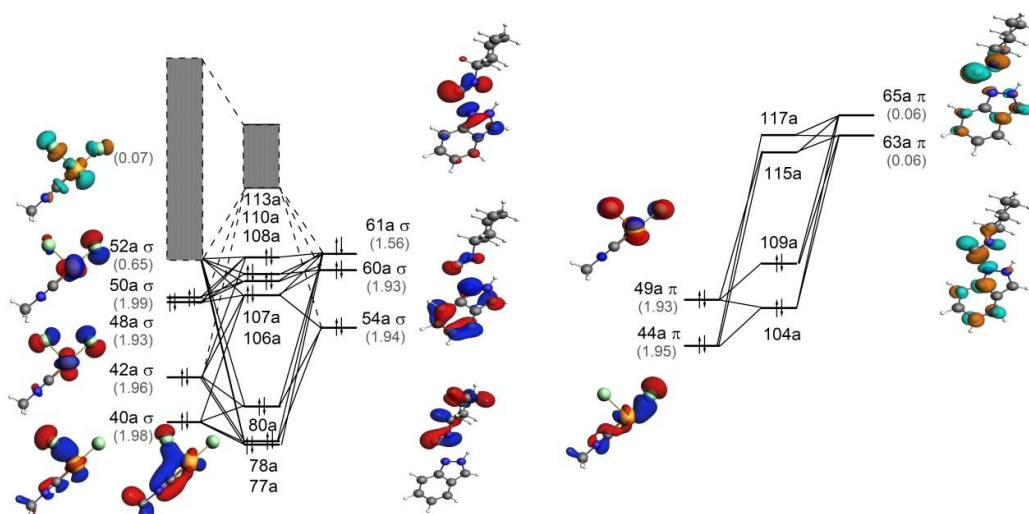
contributions by inspection of the Pd–C bond in homologous *cis*-PdCl<sub>2</sub>(CNMe)<sub>2</sub> and *cis*-PdCl<sub>2</sub>(CNMe)(CNPh) symmetric systems, in C<sub>s</sub> symmetry, at least for what concerns the compound **1**. For both symmetric models, bonding mechanisms, and relevant orbital populations, along with EDA analysis resulted very similar to **1**, then allowing a comparison between these systems (bonding schemes, VDD, and EDA analyses are given in Figures S4, S5 and Table S3). To note that the  $\pi$  interactions were recognized in both A' and A'' irreducible representations (irreps) and they correspond to the Pd44a-L31a and Pd(45,49)a-L32a ones given in Figure 5, respectively. Interactions in the A' irreps were not determined due to the occurrence of the  $\sigma$  interactions in this irrep. However, only the  $\Delta E_{\text{Orb}}$  terms corresponding only to a  $\pi$  interaction were estimated around to 14–15 kcal/mol from a total  $\Delta E_{\text{Orb}}$  of 75–77 kcal/mol (thus, *ca.* 20 %), to which we should consider the unknown contribution arising from A'  $\pi$ . We cannot make an estimation for the products, due to the lack of any likely model showing symmetry; nonetheless, accounting for the corresponding COOPs (Figure 2), small  $\pi$  overlaps, and the bonding schemes (Figure 5) where only the analogous A'  $\pi$  interaction is given, this should indicate a minor contribution to the Pd–C bond, with respect to **1**.

#### *Bond analysis of the real molecular systems*

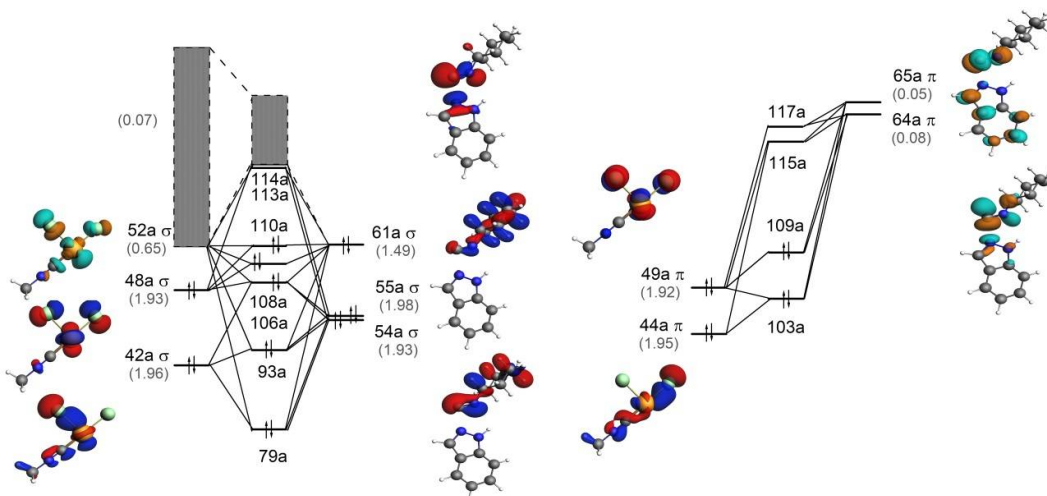
The model systems so far investigated were chosen as simplified paradigm of the *cis*-[PdCl<sub>2</sub>{C(Ind)vN(H)Cy}(CNCy)] (**RP**) complex obtained by reaction of the *cis*-[PdCl<sub>2</sub>(CNCy)<sub>2</sub>] (**R1**) with indazole (see Figure S6). Results for **R1** and **RP** were in very close agreement with what obtained for the corresponding model systems **1** and **Z-P1** so far discussed, which further supports the reliability of the proposed reaction mechanisms also for the real system. Relevant FMO overlaps, COOPs, bonding schemes, VDD and EDA analyses are given in Tables S4, S6 and Figures S7, S8).

## References

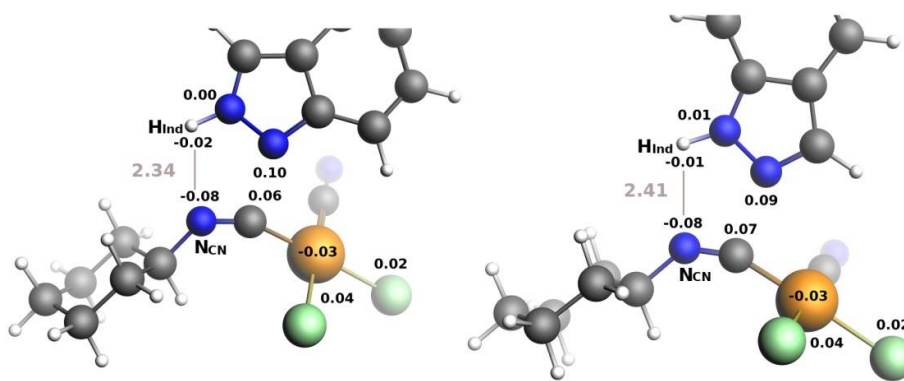
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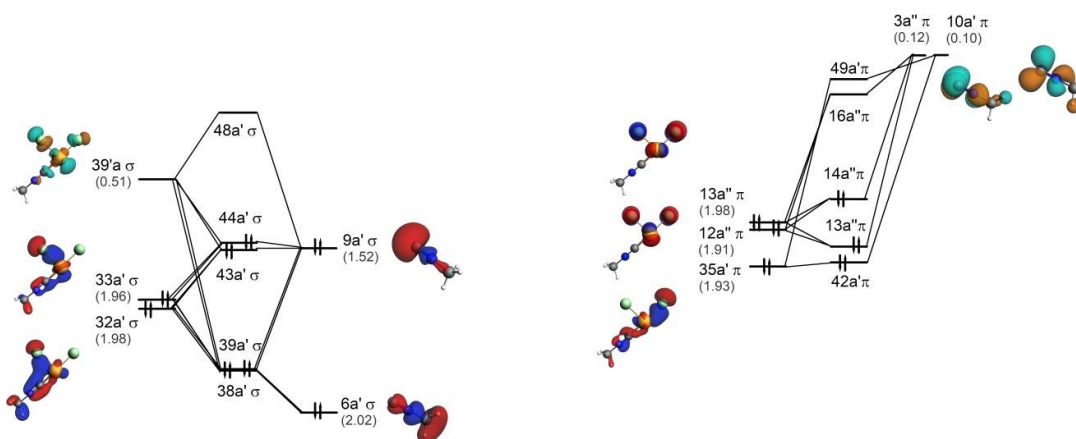
**Figure S1.** Bonding scheme for TS14. Left scheme: Pd←C ( $\sigma$  type). Right scheme: Pd→C ( $\pi$  type). Corresponding orbitals populations are given in parentheses. Isosurfaces values:  $0.05 e^{1/2}/\text{\AA}^{3/2}$ . Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.



**Figure S2.** Bonding scheme for TS6. Left scheme: Pd←C ( $\sigma$  type). Right scheme: Pd→C ( $\pi$  type). Corresponding orbitals populations are given in parentheses. Isosurfaces values:  $0.05 e^{1/2}/\text{\AA}^{3/2}$ . Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.

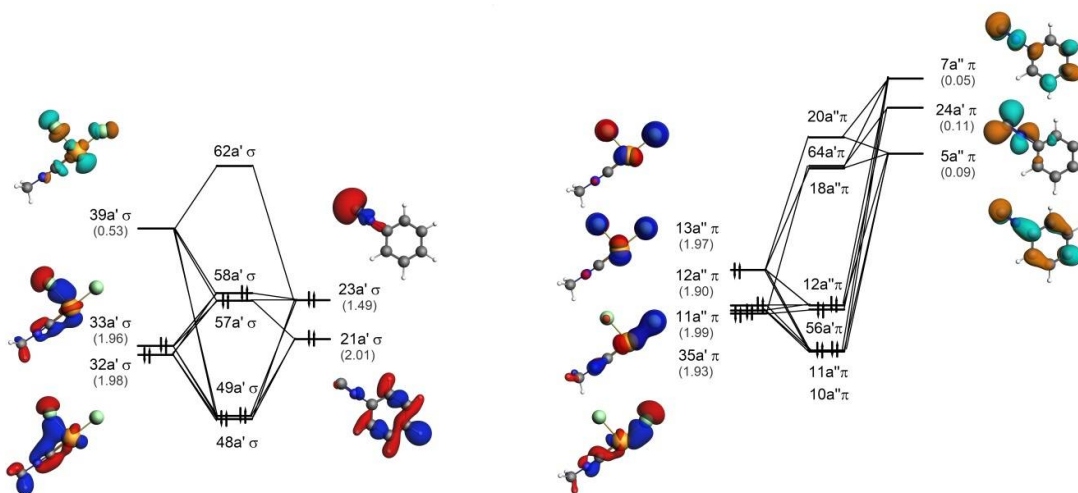


**Figure S3.** VDD charges ( $\Delta Q$ ), in electrons, of selected regions of **TS14** (left) and **TS6** (right) accounting for the  $\sigma'$  interaction (see fragment scheme in Figure 2).  $H_{\text{Ind}}-N_{\text{CN}}$  distances, in Angstrom, are given in gray.

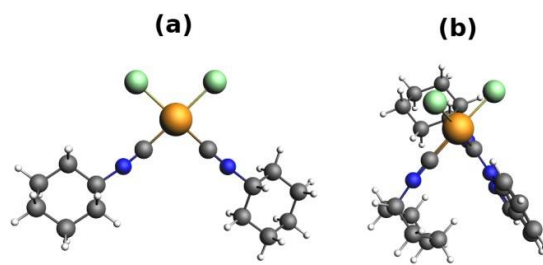


**Figure S4.** Bonding scheme for the symmetric *cis*-PdCl<sub>2</sub>(CNMe)<sub>2</sub> model in C<sub>s</sub> symmetry. Left scheme: Pd←C ( $\sigma$  type). Right scheme: Pd→C ( $\pi$  type). Corresponding orbitals populations are given in parentheses. Isosurfaces values:  $0.05 e^{1/2}/\text{\AA}^{3/2}$ . Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.

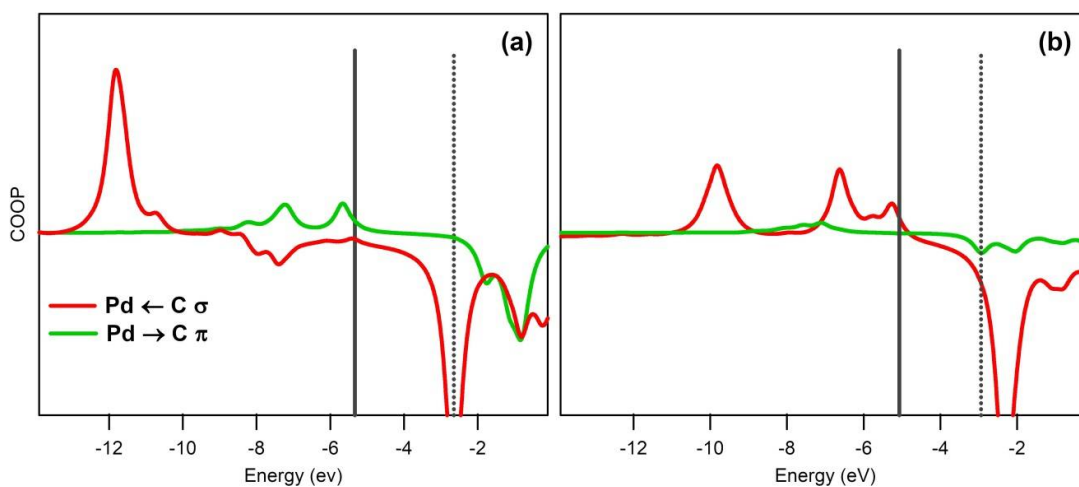




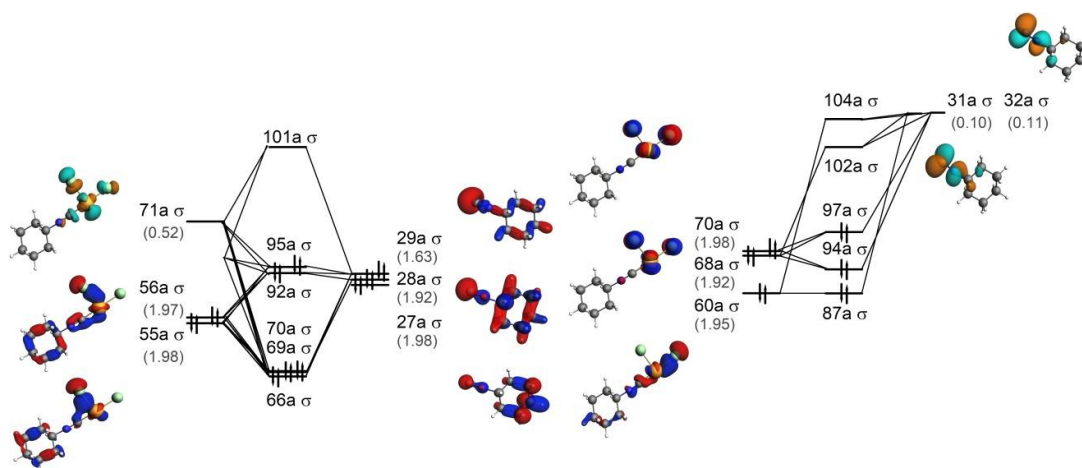
**Figure S5.** Bonding scheme for the symmetric *cis*-PdCl<sub>2</sub>(CNMe)(CNPh) model in C<sub>s</sub> symmetry. Left scheme: Pd←C (σ type). Right scheme: Pd→C (π type). Corresponding orbitals populations are given in parentheses. Isosurfaces values: 0.05 e<sup>1/2</sup>/Å<sup>3/2</sup>. Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.



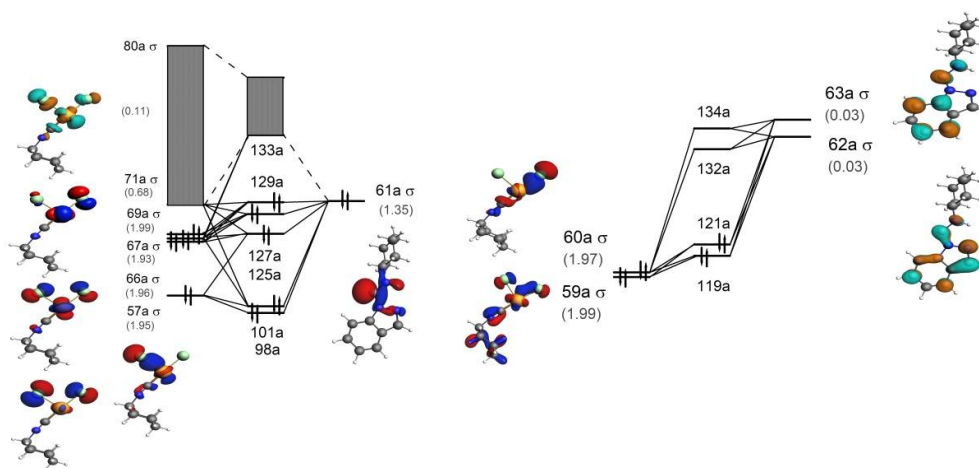
**Figure S6.** Optimized structures of *cis*-[PdCl<sub>2</sub>(CNCy)<sub>2</sub>] (**R1**) (a) and *cis*-[PdCl<sub>2</sub>(CNCy)<sub>2</sub>] (**RP**) (b).



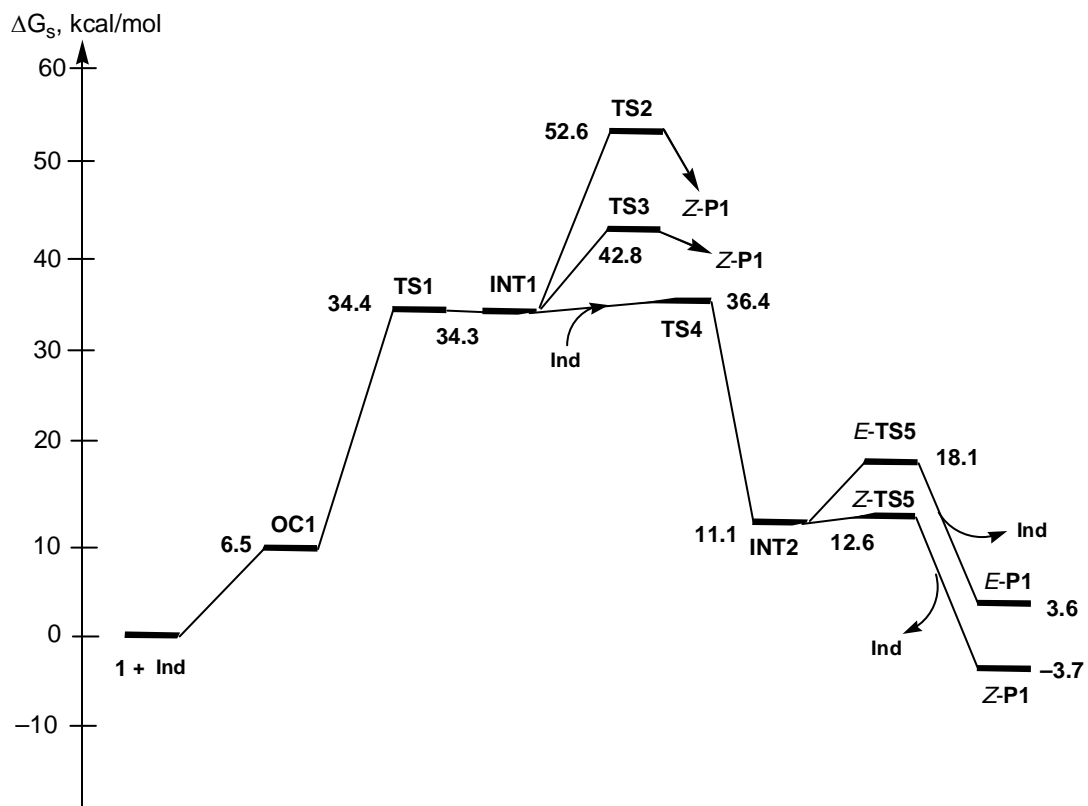
**Figure S7.** COOPs for **R1** (a) and **RP** (b) for the main bonding interactions. [Coordinates in arbitrary units. COOPs:  $x = -13.9, -0.1$ ;  $y = -0.10, 0.12$ ; PDOSs:  $x = -13.9, -0.1$ ;  $y = -0.0, 2.0$ ].



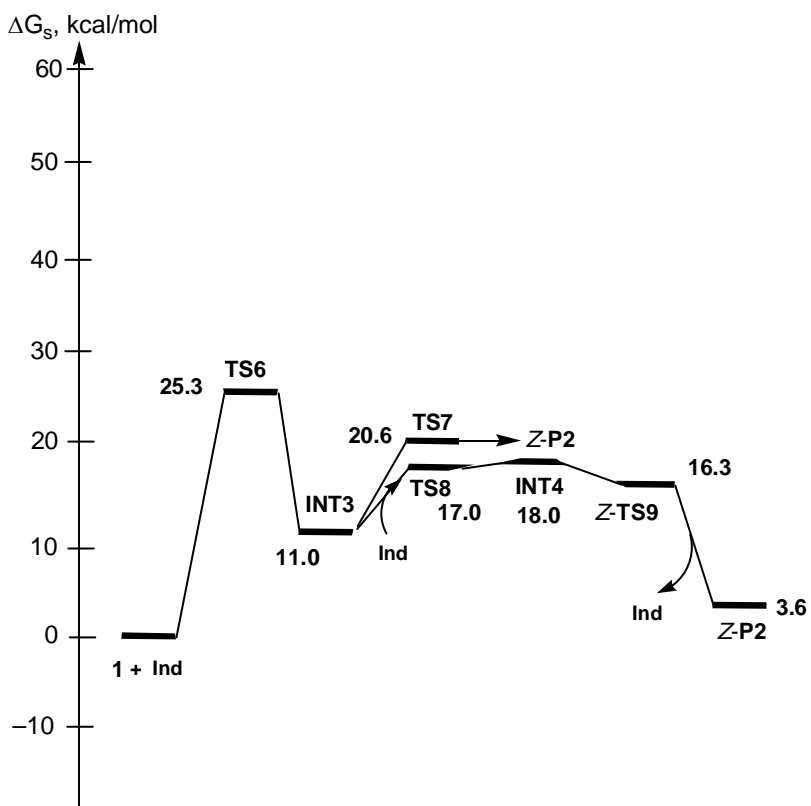
**Figure S8.** Bonding scheme for **R1**. Left scheme: Pd←C ( $\sigma$  type). Right scheme: Pd→C ( $\pi$  type). Corresponding orbitals populations are given in parentheses. Isosurfaces values:  $0.05 e^{1/2}/\text{\AA}^{3/2}$ . Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.



**Figure S9.** Bonding scheme for **RP**. Left scheme: Pd←C ( $\sigma$  type). Right scheme: Pd→C ( $\pi$  type). Corresponding orbitals populations are given in parentheses. Isosurfaces values:  $0.05 e^{1/2}/\text{\AA}^{3/2}$ . Gray bands indicate the overall participation of the virtual orbitals with populations other than 0.00, and are mainly due to the polarization of the fragment bearing the Pd atom.



**Figure S10.** Energy profile for Mechanism I.



**Figure S11.** Energy profile for Mechanism II.

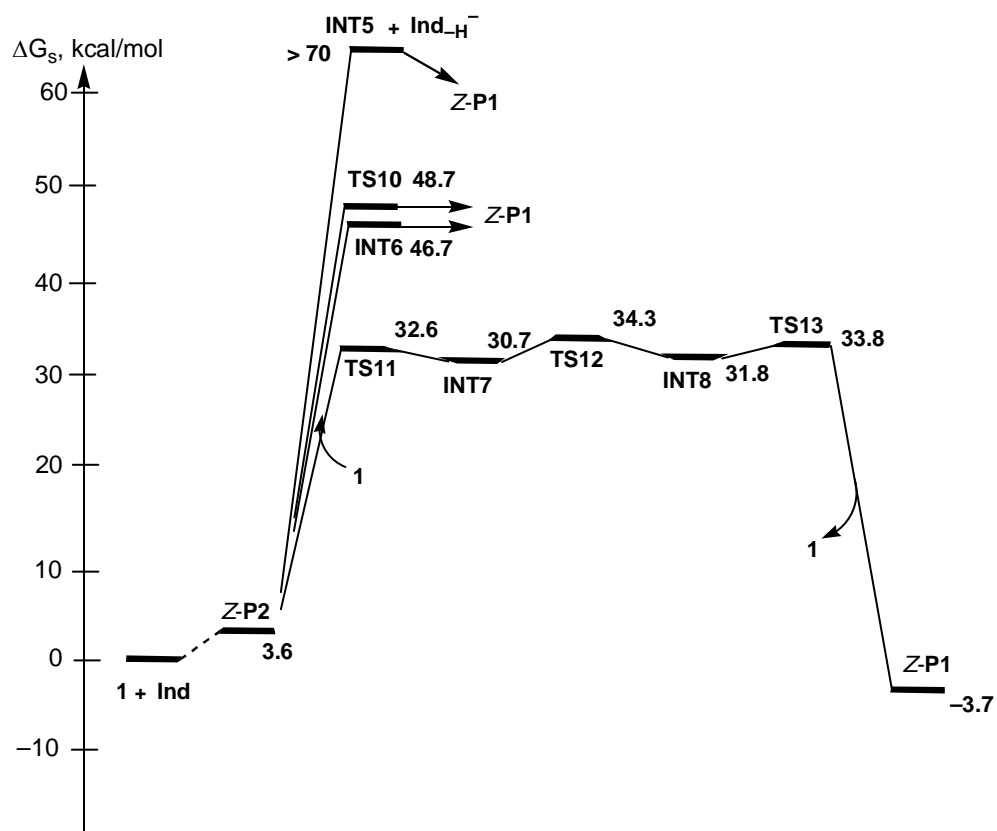


Figure S12. Energy profile for the P2 into P1 isomerization.

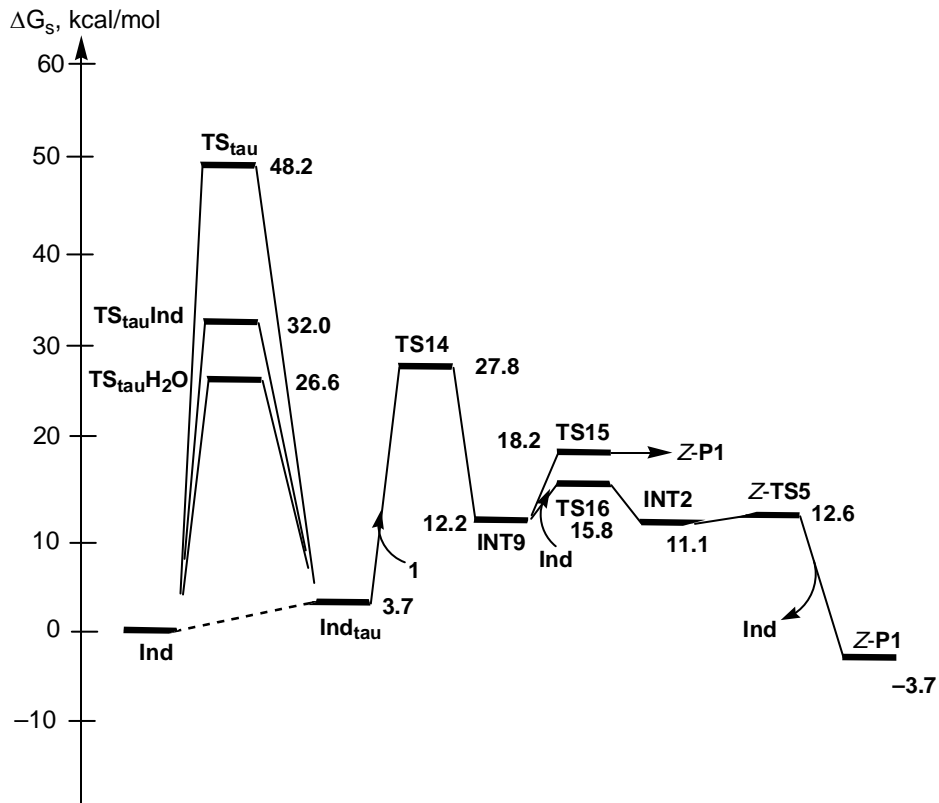
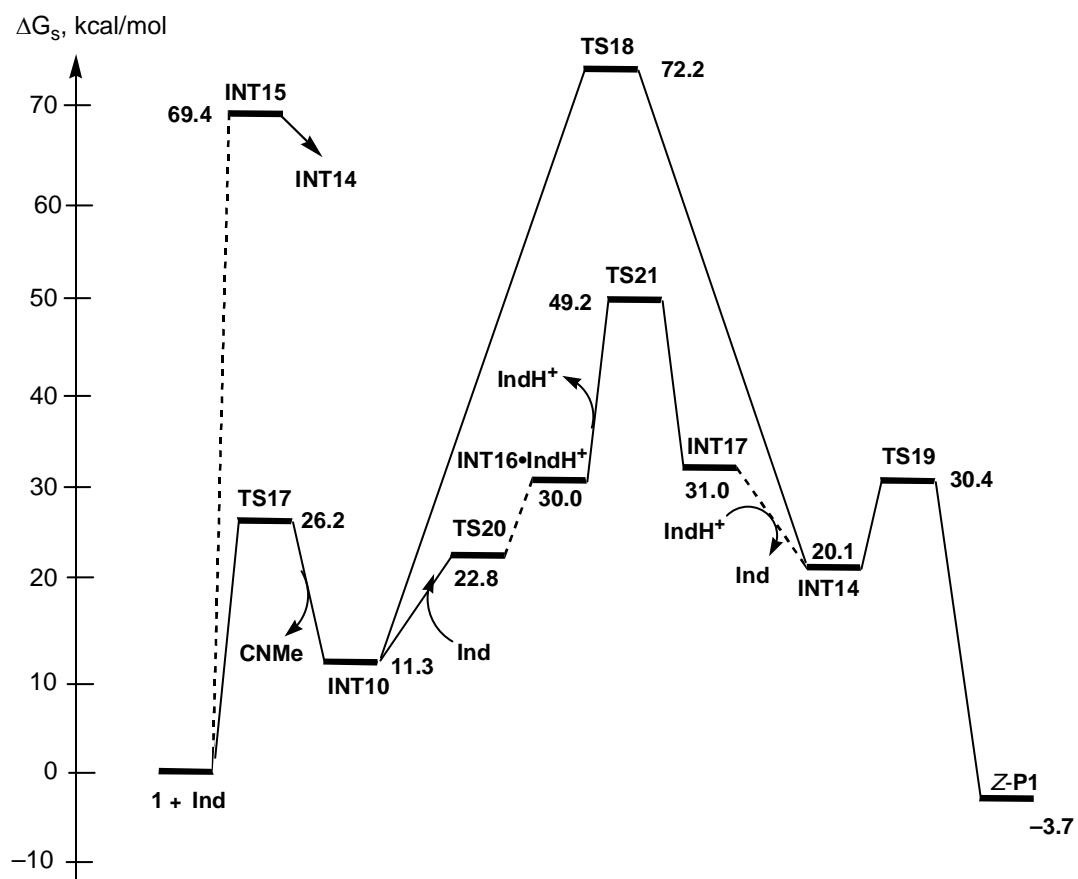


Figure S13. Energy profile for Mechanism III.



**Figure S14.** Energy profile for Mechanisms based on the coordinated indazole.

**Table S1.** VDD charges ( $\Delta Q$ ), in electrons, for the systems investigated.

	<b>1</b> (Pd–C)	<b>TS14</b> (Pd–C)	<b>TS6</b> (Pd–C)	<b>TS14</b> (PdC–N)	<b>TS6</b> (PdC–N)	<b>Z-P1</b> (Pd–C)	<b>Z-P2</b> (Pd–C)
$\Delta Q$							
Pd	0.12	0.11	0.11	-0.03	-0.03	0.10	0.10
Cl	0.04; -0.10	0.02;-0.13	0.02;-0.13	0.02;0.04	0.02;0.04	0.01; -0.15	0.02;-0.14
C <sub>CN</sub>	-0.01	-0.01	-0.01	0.06	0.07	0.02	0.01
N <sub>CN</sub>	0.02	0.03	0.03	-0.08	-0.08	0.01	0.01
N <sub>Ind</sub>	–	0.03	0.01	0.10	0.09	0.02	0.03

**Table S2.** EDA analysis. Contributions to the bonding energy (BE) and the interaction energy ( $\Delta E_{\text{int}}$ ) (kcal/mol) for the systems investigated according to the fragmentation scheme of Figure 2.

	<b>1</b> (Pd–C)	<b>TS14</b> (Pd–C)	<b>TS6</b> (Pd–C)	<b>TS14</b> (PdC–N)	<b>TS6</b> (PdC–N)	<b>ZP-1</b> (Pd–C)	<b>Z-P2</b> (Pd–C)
<b>EDA</b>							
$\Delta E_{\text{Pauli}}$	176.38	196.74	194.81	86.96	82.56	221.08	217.60
$\Delta E_{\text{Elec}}$	-154.43	-176.27	-176.56	-44.99	-42.88	-206.26	-204.15
$\Delta E_{\text{Orb}}$	-72.77	-80.17	-78.70	-45.64	-43.00	-80.84	-78.85
$\Delta E_{\text{disp}}$	-4.95	-13.84	-10.16	-11.76	-7.99	-15.57	-13.40
BSSE	-4.71	-6.87	-6.28	-5.88	-5.47	-6.16	-5.99
<b>BE</b>	<b>-60.48</b>	<b>-80.41</b>	<b>-77.33</b>	<b>-21.31</b>	<b>-16.78</b>	<b>-87.75</b>	<b>-84.79</b>
$\Delta E_{\text{prep}}$	3.66	32.39	33.06	17.24	15.99	7.38	6.40
$\Delta E_{\text{int}}^a$	<b>-56.82</b>	<b>-48.27</b>	<b>-44.27</b>	<b>-4.1</b>	<b>-0.79</b>	<b>-80.37</b>	<b>-78.39</b>

$$^a \Delta E_{\text{int}} = \text{BE} + \Delta E_{\text{prep}}$$

**Table S3.** VDD charges ( $\Delta Q$ ) (in electrons, e) and EDA analysis (kcal/mol) for the symmetric *cis*-PdCl<sub>2</sub>(CNMe)<sub>2</sub> and *cis*-PdCl<sub>2</sub>(CNMe)(CNPh). (Symmetry C<sub>s</sub>)

	<i>cis</i> -PdCl <sub>2</sub> (CNMe) <sub>2</sub> (Pd–C)	<i>cis</i> -PdCl <sub>2</sub> (CNMe) <sub>2</sub> (Pd–C)
$\Delta Q$		
<b>Pd</b>	0.13	0.13
<b>Cl</b>	0.04;-0.09	0.04;-0.09
<b>C<sub>CN</sub></b>	0.01	-0.04
<b>N<sub>CN</sub></b>	0.01	0.02
<b>EDA</b>		
$\Delta E_{\text{Pauli}}$	181.38	183.07
$\Delta E_{\text{Elec}}$	-156.82	-156.00
$\Delta E_{\text{Orb}}$	-74.09	-77.24
$\Delta E^{A'}_{\text{Orb}}$	-59.83	-61.67
$\Delta E^{A''}_{\text{Orb}}$	-14.27	-15.57
$\Delta E_{\text{disp}}$	-4.20	-4.75
BSSE	-5.41	-4.02
<b>BE</b>	<b>-59.85</b>	<b>-58.94</b>
$\Delta E_{\text{prep}}$	1.61	1.67
$\Delta E_{\text{int}}^a$	<b>-58.24</b>	<b>-57.27</b>

<sup>a</sup>  $\Delta E_{\text{int}} = \text{BE} + \Delta E_{\text{prep}}$

**Table S4.** Overlap  $\langle L|\text{Pd} \rangle$  (L = CyNC; Pd = *cis*-PdCl<sub>2</sub>) and relevant orbitals populations for the real systems investigated. Virtual orbitals are indicated with an asterisk.

	<b>Reactant</b> (Pd–C)	<b>Product</b> (Pd–C)
<b>FMO overlap, S</b>		
	<b>Pd←C</b>	<b>Pd←C</b>
	0.05 $\langle 28a 55a \rangle$	<b>0.15</b> $\langle 61a 57a \rangle$
	0.06 $\langle 28a 56a \rangle$	0.06 $\langle 61a 66a \rangle$
	0.03 $\langle 28a 67a \rangle$	0.05 $\langle 61a 67a \rangle$
	<b>0.15</b> $\langle 28a 71a \rangle$	<b>0.30</b> $\langle 61a 71^*a \rangle$
	0.09	<b>0.16</b>

	<28a 73*a>	<b>&lt;61a 73*a&gt;</b>
	0.09 <29a 55a>	
	0.09 <29a 56a>	
	0.06 <29a 67a>	
	<b>0.29</b> <b>&lt;29a 71a&gt;</b>	
	<b>0.15</b> <b>&lt;29a 73*a&gt;</b>	
	<b>Pd→C</b>	<b>Pd→C</b>
	<b>0.13</b> <b>&lt;31*a 60a&gt;</b>	0.04 <62*a 60a>
	0.10 <60a 32*a>	0.01 <62*a 59a>
	0.09 <68a 31*a>	0.02 <63*a 59a>
	<b>0.12</b> <b>&lt;68a 32*a&gt;</b>	0.07 <63*a 60a>
	0.01 <70a 31*a>	
	0.02 <70a 32*a>	
<b>FMO population, e<sup>-</sup></b>		
<b>L</b>	28a(1.92) 29a(1.63) 31*a(0.10) 32*a(0.11)	61a(1.35) 62*a(0.03) 63*a(0.03)
<b>Pd</b>	55a(1.98) 56a(1.97) 60a(1.95) 67a(1.95) 68a(1.92) 70a(1.985) 71*a(0.52) 73*a(0.02)	57a(1.95) 59a(1.99) 60a(1.97) 66a(1.96) 67a(1.93) 71*a(0.68) 73*a(0.03)



**Table S5.** VDD charges ( $\Delta Q$ ) (in electrons, e) and EDA analysis (kcal/mol) for **R1**, and **RP**.

	<b>R1</b> (Pd-C)	<b>RP</b> (Pd-C)
$\Delta Q$		
<b>Pd</b>	<b>0.12</b>	<b>0.10</b>
<b>Cl</b>	<b>0.04; -0.10</b>	<b>0.01;-0.15</b>
<b>C<sub>CN</sub></b>	<b>-0.01</b>	<b>0.01</b>
<b>N<sub>CN</sub></b>	<b>0.02</b>	<b>0.01</b>
<b>N<sub>Ind</sub></b>	<b>-</b>	<b>0.03</b>
<b>EDA</b>		
$\Delta E_{\text{Pauli}}$	176.40	224.96
$\Delta E_{\text{Elec}}$	-154.55	-206.76
$\Delta E_{\text{Orb}}$	-72.77	-80.53
$\Delta E_{\text{disp}}$	-4.95	-21.69
<b>BSSE</b>	-4.72	-5.65
<b>BE</b>	<b>-60.59</b>	<b>-89.67</b>
$\Delta E_{\text{prep}}$	3.65	6.04
$\Delta E_{\text{int}}^a$	<b>-56.94</b>	<b>-83.63</b>

<sup>a</sup>  $\Delta E_{\text{int}} = \text{BE} + \Delta E_{\text{prep}}$

**Table S6.** Overlap  $\langle L|Pd \rangle$  ( $L = \text{CyNC}; \text{CyNC}$ );  $Pd = \text{cis-PdCl}_2$ ) and relevant orbitals population of the systems investigated. Virtual orbitals are indicated with an asterisk.

	<b>1</b> (Pd-C)	<b>TS14</b> (Pd-C)	<b>TS6</b> (Pd-C)	<b>TS14</b> (PdC-N)	<b>TS6</b> (PdC-N)	<b>Z-P1</b> (Pd-C)	<b>Z-P2</b> (Pd-C)
<b>FMO overlap, S</b>							
	<b>Pd←C</b>	<b>Pd←C</b>	<b>Pd←C</b>	<b>PdC←N</b>	<b>PdC←N</b>	<b>Pd←C</b>	<b>Pd←C</b>
	0.01 $\langle 27a 40^*a \rangle$	0.03 $\langle 54a 40a \rangle$	0.07 $\langle 54a 42a \rangle$	0.16 $\langle 29a 82^*a \rangle$	0.17 $\langle 29a 82^*a \rangle$	0.03 $\langle 61a 40a \rangle$	0.03 $\langle 61a 40a \rangle$
	0.02 $\langle 28a 40a \rangle$	0.06 $\langle 54a 42a \rangle$	0.03 $\langle 54a 48a \rangle$	0.04 $\langle 31a 82^*a \rangle$		0.15 $\langle 61a 42a \rangle$	0.16 $\langle 61a 42a \rangle$
	0.05 $\langle 29a 40a \rangle$	0.03 $\langle 54a 48a \rangle$	0.14 $\langle 54a 52^*a \rangle$			0.04 $\langle 61a 43a \rangle$	0.06 $\langle 61a 48a \rangle$
	0.08 $\langle 28a 42a \rangle$	0.01 $\langle 54a 50a \rangle$	0.07 $\langle 54a 54^*a \rangle$			0.06 $\langle 61a 48a \rangle$	0.10 $\langle 61a 50a \rangle$
	0.12 $\langle 29a 42a \rangle$	0.13 $\langle 54a 52^*a \rangle$	0.03 $\langle 55a 42a \rangle$			0.10 $\langle 61a 50a \rangle$	0.29 $\langle 61a 52^*a \rangle$
	0.09 $\langle 27a 52^*a \rangle$	0.01 $\langle 60a 40a \rangle$	0.01 $\langle 55a 48a \rangle$			0.31 $\langle 61a 52^*a \rangle$	
	0.16 $\langle 28a 52^*a \rangle$	0.05 $\langle 60a 42a \rangle$	0.07 $\langle 55a 52^*a \rangle$				
	0.28 $\langle 29a 52^*a \rangle$	0.03 $\langle 60a 48a \rangle$	0.11 $\langle 61a 42a \rangle$				
		0.02 $\langle 60a 50a \rangle$	0.05 $\langle 61a 48a \rangle$				
		0.08 $\langle 60a 52^*a \rangle$	0.23 $\langle 61a 52^*a \rangle$				
		0.03 $\langle 61a 4a \rangle$					
		0.10 $\langle 61a 42a \rangle$					
		0.04 $\langle 61a 48a \rangle$					
		0.06 $\langle 61a 50a \rangle$					
		0.20 $\langle 61a 52^*a \rangle$					
	<b>Pd→C</b>	<b>Pd→C</b>	<b>Pd→C</b>			<b>Pd→C</b>	<b>Pd→C</b>
	0.08 $\langle 31^* 40a \rangle$	0.08 $\langle 63^*a 44a \rangle$	0.07 $\langle 64^*a 44a \rangle$			0.05 $\langle 62^*a 44a \rangle$	0.05 $\langle 62^*a 44a \rangle$
	0.15 $\langle 31^* 44a \rangle$	0.05 $\langle 63^*a 49a \rangle$	0.09 $\langle 64^*a 49a \rangle$			0.08 $\langle 63^*a 44a \rangle$	0.08 $\langle 63^*a 44a \rangle$
	0.02 $\langle 31^* 45a \rangle$	0.09 $\langle 65^*a 44a \rangle$	0.10 $\langle 65^*a 44a \rangle$				

	0.06 (31* 49a)	0.08 (65*a 49)	0.04 (65*a 49a)				
	0.04 (32* 40a)						
	0.08 (32* 44a)						
	0.05 (32* 45a)						
	0.13 (32* 49a)						
<b>FMO population, <math>e^-</math></b>							
<b>L</b>	27a(1.98) 28a(1.91) 29a(1.65) 31a*(0.10) 32a*(0.11)	54a(1.94) 60a(1.93) 61a(1.56) 63*a(0.06) 65*a(0.06)	54a(1.93) 55a(1.98) 61a(1.49) 64*a(0.08) 65*a(0.05)	29a(1.80) 31a(1.97)	29a(1.77)	61a(1.33) 62*a(0.03) 63*a(0.03)	61a(1.34) 62*a(0.04) 63*a(0.03)
<b>Pd</b>	40a(1.98) 42a(1.96) 45a(1.98) 44a(1.93) 49a(1.92) 52*a(0.52)	40a(1.98) 42a(1.96) 48a(1.93) 44a(1.95) 49a(1.93) 50a(1.99) 52*a(0.65)	42a(1.96) 44a(1.95) 48a(1.93) 49a(1.92) 52*a(0.65)	82*a(0.24)	82*a(0.23)	40a(1.98) 42a(1.95) 43a(1.99) 44a(1.95) 48a(1.93) 50a(2.00) 52*a(0.69)	40a(1.98) 42a(1.95) 44a(1.95) 48a(1.93) 50a(2.00) 52*a(0.67)

**Table S7.** Calculated total energies, enthalpies, Gibbs free energies (in Hartree) and entropies (in cal/mol•K).

	E (6-311+G**)	E (6-31G*)	H (6-31G*)	S	G (6-31G*)	G (6-311+G**)
<b>1</b>	-1509.428795	-1509.252574	-1509.011549	140.63	-1509.078366	-1509.254587
Ind	-379.905874	-379.810212	-379.684660	78.52	-379.721965	-379.817627
Ind (SMD in H <sub>2</sub> O)	-379.902738	-379.807110	-379.681698	78.71	-379.719096	-379.814724
<b>Ind<sub>tau</sub></b>	-379.900199	-379.804309	-379.678784	78.00	-379.715845	-379.811735
<b>IndH<sup>+</sup></b>	-380.331363	-380.237197	-380.098182	79.93	-380.136159	-380.230325
<b>IndH<sup>+</sup></b> (SMD in H <sub>2</sub> O)	-380.343148	-380.248944	-380.110251	80.41	-380.148457	-380.242661
<b>Ind<sub>H</sub><sup>-</sup></b>	-379.399851	-379.296741	-379.185594	77.51	-379.222423	-379.325533
<b>Ind<sub>H</sub><sup>-</sup></b> (SMD in H <sub>2</sub> O)	-379.416663	-379.313596	-379.202186	77.45	-379.238986	-379.342053
<b>TS<sub>Tau</sub></b>	-379.823338	-379.724887	-379.605299	77.91	-379.642317	-379.740768
<b>TS<sub>Tau</sub>H<sub>2</sub>O</b>	-609.241821	-609.037722	-608.835631	111.35	-608.888538	-609.092637
<b>TS<sub>Tau</sub>Ind</b>	-759.779347	-759.586322	-759.335888	116.47	-759.391228	-759.584253
<b>Z-P1</b>	-1889.366612	-1889.098386	-1888.728581	171.02	-1888.809839	-1889.078065
<b>E-P1</b>	-1889.358560	-1889.090801	-1888.720227	165.29	-1888.798761	-1889.066520
<b>Z-P2</b>	-1889.354721	-1889.085915	-1888.716190	171.59	-1888.797718	-1889.066524
<b>INT1</b>	-1889.305906	-1889.037134	-1888.668817	168.32	-1888.748792	-1889.017564
<b>INT2</b>	-2269.268985	-2268.905033	-2268.409410	208.00	-2268.508237	-2268.872189
<b>INT3</b>	-1889.342007	-1889.073125	-1888.703793	172.73	-1888.785863	-1889.054745
<b>INT4</b>	-2269.257956	-2268.894098	-2268.398076	208.91	-2268.497338	-2268.861196
<b>INT6</b>	-2269.213562	-2268.848651	-2268.352585	206.30	-2268.450603	-2268.815514
<b>INT7</b>	-3398.769387	-3398.324951	-3397.712011	255.51	-3397.833413	-3398.277849
<b>INT8</b>	-3398.767887	-3398.323593	-3397.711196	253.91	-3397.831835	-3398.276129
<b>INT9</b>	-1889.340908	-1889.071969	-1888.702792	170.38	-1888.783746	-1889.052685
<b>INT10</b>	-1756.579037	-1756.344026	-1756.027844	155.88	-1756.101906	-1756.336917
<b>INT14</b>	-1756.570028	-1756.336450	-1756.019199	147.59	-1756.089324	-1756.322902
<b>INT15</b>	-1756.480042	-1756.242803	-1755.932820	156.31	-1756.007088	-1756.244327
<b>INT16</b>	-1756.101665	-1755.865746	-1755.563594	155.08	-1755.637278	-1755.873197
<b>INT16•IndH<sup>+</sup></b>	-2136.476642	-2136.145114	-2135.702383	191.22	-2135.793237	-2136.124765
<b>INT17</b>	-1756.104486	-1755.870249	-1755.566984	148.12	-1755.637358	-1755.871595
<b>TS1</b>	-1889.304196	-1889.034983	-1888.667918	168.99	-1888.748210	-1889.017423
<b>TS2</b>	-1889.270374	-1888.999997	-1888.636620	171.44	-1888.718077	-1888.988454
<b>TS3</b>	-1965.754930	-1965.451128	-1965.060296	179.03	-1965.145358	-1965.449160
<b>TS4</b>	-2269.226357	-2268.862667	-2268.371470	203.39	-2268.468106	-2268.831796
<b>Z-TS5</b>	-2269.262278	-2268.898565	-2268.406978	208.38	-2268.505986	-2268.869699
<b>E-TS5</b>	-2269.256691	-2268.892988	-2268.400934	202.71	-2268.497248	-2268.860951
<b>TS6</b>	-1889.314610	-1889.044517	-1888.677635	177.10	-1888.761779	-1889.031872
<b>TS7</b>	-1889.323083	-1889.052784	-1888.688336	169.94	-1888.769077	-1889.039376

<b>TS8</b>	-2269.255848	-2268.891048	-2268.399311	207.59	-2268.497943	-2268.862743
<b>Z-TS9</b>	-2269.256534	-2268.892315	-2268.400682	208.21	-2268.499610	-2268.863829
<b>TS10</b>	-1889.280055	-1889.011697	-1888.645511	170.10	-1888.726332	-1888.994690
<b>TS11</b>	-3398.763054	-3398.318186	-3397.707022	259.00	-3397.830081	-3398.274949
<b>TS12</b>	-3398.760199	-3398.314939	-3397.706997	252.28	-3397.826862	-3398.272122
<b>TS13</b>	-3398.763609	-3398.318855	-3397.707353	254.34	-3397.828200	-3398.272954
<b>TS14</b>	-1889.311570	-1889.041513	-1888.674658	175.01	-1888.757810	-1889.027867
<b>TS15</b>	-1889.326268	-1889.055976	-1888.691467	171.26	-1888.772839	-1889.043131
<b>TS16</b>	-2269.258400	-2268.893782	-2268.402344	205.56	-2268.500010	-2268.864628
<b>TS17</b>	-1889.311200	-1889.040599	-1888.673845	181.20	-1888.759941	-1889.030542
<b>TS18</b>	-1756.479658	-1756.243854	-1755.932292	150.98	-1756.004028	-1756.239832
<b>TS19</b>	-1889.309769	-1889.041176	-1888.673078	172.86	-1888.755210	-1889.023803
<b>TS20</b>	-2136.486694	-2136.154909	-2135.715395	187.24	-2135.804360	-2136.136145
<b>TS21</b>	-1756.072507	-1755.837382	-1755.536812	148.77	-1755.607496	-1755.842621

**Table S8.** Cartesian atomic coordinates (in Å) of the calculated equilibrium structures (either element symbols or nuclear charges are given in the first column).

Ind

N	-2.056986	2.122101	1.865767
N	-3.270752	2.338159	1.297698
C	-3.017634	2.710090	0.051586
H	-2.017189	1.827020	2.831908
H	-3.842366	2.941813	-0.613343
C	-1.023291	2.347943	1.007086
C	-1.622278	2.742452	-0.215922
C	0.365091	2.250566	1.164986
C	-0.805239	3.049725	-1.317262
C	1.141451	2.559758	0.062183
C	0.566113	2.954951	-1.165662
H	-1.243457	3.354849	-2.266249
H	1.219699	3.187788	-2.004390
H	2.225461	2.496957	0.142367
H	0.811438	1.946386	2.109576

IndH<sup>+</sup>

H	1.416073	1.382989	-0.436302
N	3.002557	0.247789	0.213629
N	2.415174	1.218439	-0.519217
C	3.307219	1.842842	-1.282290
H	2.452035	-0.321640	0.847709
H	3.001065	2.650279	-1.933366
C	4.328599	0.231808	-0.077132
C	4.557090	1.252776	-1.042202
C	5.357249	-0.581364	0.413140
C	5.859073	1.472012	-1.537460
C	6.617218	-0.338704	-0.093558
C	6.868989	0.671967	-1.054747
H	6.047346	2.248208	-2.274523
H	7.885571	0.811757	-1.413535
H	7.448924	-0.945471	0.257403
H	5.169320	-1.357191	1.149722

Ind<sub>H</sub><sup>-</sup>

N	-2.031023	2.100406	1.933949
N	-3.225696	2.331612	1.314910
C	-3.014206	2.712484	0.042571
H	-3.853726	2.941937	-0.611980
C	-1.059913	2.346923	1.014049
C	-1.633904	2.749496	-0.238210
C	0.340491	2.255392	1.151880
C	-0.800297	3.053786	-1.331333
C	1.138000	2.559696	0.062863
C	0.572348	2.957239	-1.173875
H	-1.222021	3.361566	-2.290730
H	1.232933	3.189224	-2.010187
H	2.223298	2.494229	0.151759
H	0.780967	1.949549	2.102756

**Ind<sub>tau</sub>**

H	1.311987	-0.075062	0.578048
N	0.296865	1.661149	0.294026
N	1.414428	0.917956	0.407113
C	2.577477	1.584511	0.280510
H	3.531409	1.078955	0.354570
C	0.786416	2.903491	0.076877
C	2.221405	2.916479	0.057401
C	0.055011	4.096154	-0.117869
C	2.919696	4.125905	-0.156933
C	0.763027	5.257319	-0.324088
C	2.184529	5.274050	-0.343767
H	4.008342	4.147476	-0.173606
H	2.695937	6.220553	-0.511231
H	0.226185	6.192377	-0.477340
H	-1.033395	4.083465	-0.103140

**TS<sub>tau</sub>**

7	0.222782	-2.182678	-0.221302
7	-1.241083	-2.082361	-0.249732
6	-1.569841	-0.782786	-0.178613
1	-0.628644	-2.614234	0.627280
1	-2.616149	-0.496510	-0.152448
6	0.661070	-0.895597	-0.137727
6	-0.424458	0.024149	-0.173339
6	1.996489	-0.446149	-0.075912
6	-0.178319	1.416009	-0.171648
6	2.207502	0.914058	-0.064850
6	1.130015	1.838162	-0.113666
1	-0.999943	2.128858	-0.207503
1	1.353259	2.903537	-0.103440
1	3.225227	1.298225	-0.020723
1	2.820324	-1.156134	-0.048477

**TS<sub>tau</sub>H<sub>2</sub>O**

N	-3.162286	-1.953875	-0.279540
N	-4.358060	-1.639842	-0.874711
C	-4.346747	-0.379403	-1.308040
H	-3.429372	-3.350553	0.718501
H	-5.215115	0.041433	-1.804548
C	-2.389533	-0.834750	-0.349449
C	-3.101752	0.210635	-1.008733
C	-1.077583	-0.627757	0.119632
C	-2.497005	1.467856	-1.202065
C	-0.509742	0.615243	-0.079052
C	-1.211524	1.656846	-0.733958
H	-3.031035	2.274445	-1.704235
H	-0.723076	2.620824	-0.867799
H	0.501999	0.804233	0.277710
H	-0.533806	-1.425820	0.624322
O	-3.819421	-4.285183	0.869594
H	-3.308450	-4.776262	0.167378

H	-4.886215	-4.100967	0.356777
O	-2.407666	-4.597907	-1.359972
O	-5.861695	-3.646127	-0.274672
H	-2.438375	-3.619253	-1.287905
H	-2.878984	-4.789285	-2.184509
H	-6.047786	-4.212532	-1.042187
H	-5.394404	-2.762094	-0.649499

**TS<sub>tau</sub>ind**

N	-4.147404	-0.412601	0.669107
N	-5.089081	0.270983	1.395439
C	-4.671177	1.526115	1.571178
H	-4.781401	-1.606278	-0.844299
H	-5.283595	2.233041	2.125954
C	-3.126727	0.453569	0.396057
C	-3.413177	1.732360	0.958265
C	-1.933283	0.232894	-0.317125
C	-2.499866	2.790691	0.800409
C	-1.050337	1.289363	-0.457486
C	-1.330495	2.560731	0.095969
H	-2.705970	3.775171	1.222255
H	-0.610970	3.367721	-0.037027
H	-0.119223	1.144103	-1.005134
H	-1.711295	-0.746438	-0.745742
N	-3.984761	-3.061346	0.241656
N	-4.598290	-2.625398	-0.869884
C	-4.825207	-3.616138	-1.722441
H	-3.815842	-2.282912	0.913368
H	-5.314502	-3.432666	-2.668916
C	-3.794501	-4.396487	0.132380
C	-4.324438	-4.791971	-1.132173
C	-3.209620	-5.314965	1.015975
C	-4.263350	-6.144237	-1.524543
C	-3.170258	-6.628989	0.599229
C	-3.688429	-7.041917	-0.653420
H	-4.661848	-6.460840	-2.485469
H	-3.626391	-8.092945	-0.925579
H	-2.726013	-7.375781	1.253796
H	-2.811392	-5.000945	1.976849

**1**

N	-3.378362	-1.739081	0.656574
C	-2.504915	-1.324906	1.309477
Pd	-1.126464	-0.596719	2.466154
Cl	0.507706	0.310434	3.922079
Cl	-2.912743	-0.054737	3.926241
C	0.337978	-1.036057	1.271948
N	1.233559	-1.296758	0.573347
C	2.344111	-1.594638	-0.244281
C	-4.702253	-3.723735	0.208458
C	-5.975111	-4.216861	-0.469637
C	-4.556058	-2.216016	-0.001409



C	-7.202505	-3.461539	0.027142
C	-5.772464	-1.447117	0.518550
C	-7.037097	-1.958146	-0.160505
H	3.223365	-1.751430	0.386080
H	2.526220	-0.758598	-0.925121
H	2.137888	-2.500250	-0.820994
H	-4.417702	-2.007008	-1.072527
H	-5.631552	-0.373107	0.347895
H	-5.835849	-1.595684	1.606538
H	-4.747011	-3.919284	1.289693
H	-3.816772	-4.241646	-0.179856
H	-5.878691	-4.084534	-1.558831
H	-6.084474	-5.294693	-0.296938
H	-7.905235	-1.417821	0.236540
H	-6.991206	-1.724795	-1.236002
H	-8.102000	-3.813813	-0.493427
H	-7.354191	-3.678919	1.095931

**E-P1**

C	-2.271533	-3.277356	-2.511786
C	-1.354652	-3.615243	-3.681486
C	-0.044061	-2.842595	-3.590161
C	0.654649	-3.086914	-2.257336
C	-0.273257	-2.742865	-1.096574
C	-1.583626	-3.521899	-1.173132
N	0.372283	-3.056991	0.193649
C	0.822221	-2.287939	1.153805
N	0.984463	-0.940638	0.904665
N	1.399308	-0.483882	-0.346347
C	1.663559	0.790764	-0.187217
C	1.431862	1.240156	1.147567
C	0.992339	0.093868	1.837060
C	1.548988	2.463619	1.820338
C	1.215282	2.502135	3.164065
C	0.755804	1.351179	3.831232
C	0.624973	0.130674	3.182920
Pd	1.389472	-3.117240	2.903381
C	2.944984	-1.970476	2.971099
N	3.857253	-1.242652	3.006168
C	4.900582	-0.296909	3.072654
Cl	2.147188	-4.083640	4.976204
Cl	-0.498009	-4.566067	2.787317
H	0.302020	-4.037945	0.464896
H	4.622198	0.494766	3.775430
H	5.062126	0.134734	2.080269
H	5.817917	-0.783771	3.414490
H	2.026700	1.361317	-1.036047
H	1.886435	3.355927	1.297318
H	1.293424	3.438162	3.713051
H	0.485255	1.418147	4.882952
H	0.257483	-0.752100	3.702336

H	-0.482305	-1.667765	-1.099728
H	-2.234471	-3.239163	-0.335718
H	-1.368725	-4.596764	-1.057717
H	0.940841	-4.147647	-2.176279
H	1.573150	-2.494175	-2.173597
H	-0.246835	-1.765066	-3.698056
H	0.626848	-3.115011	-4.414847
H	-3.198135	-3.863049	-2.560390
H	-2.569818	-2.219075	-2.576473
H	-1.858254	-3.405050	-4.634084
H	-1.139918	-4.695730	-3.673709

**Z-P1**

6	0.047477	2.420191	-0.611326
6	1.063841	3.476071	-0.191631
6	1.663588	3.151786	1.171729
6	2.280100	1.758042	1.194977
6	1.255710	0.713056	0.770762
6	0.662518	1.025595	-0.600834
7	1.881691	-0.612919	0.778142
6	1.314401	-1.719569	1.190498
7	2.080989	-2.853133	1.101740
7	3.355466	-2.765858	0.543345
6	3.852210	-3.975082	0.591486
6	2.951823	-4.913610	1.178714
6	1.805352	-4.163068	1.507928
6	3.010382	-6.283888	1.456750
6	1.913983	-6.871592	2.064845
6	0.780726	-6.109234	2.396002
6	0.701738	-4.748368	2.128511
46	-0.564607	-1.737191	1.880650
6	-1.259856	-2.295562	0.166907
7	-1.700772	-2.633066	-0.860991
6	-2.289413	-3.037591	-2.077098
17	-2.844872	-1.739750	2.681410
17	0.369613	-1.026409	3.959758
1	2.842136	-0.679098	0.433206
1	-1.710200	-3.858279	-2.509196
1	-2.302487	-2.194115	-2.773474
1	-3.313624	-3.371350	-1.889071
1	4.850036	-4.154594	0.204475
1	3.895573	-6.863018	1.202735
1	1.927310	-7.934096	2.297438
1	-0.062612	-6.592956	2.884464
1	-0.180541	-4.174395	2.406273
1	0.447620	0.673653	1.515644
1	-0.085554	0.261711	-0.857140
1	1.460589	0.961469	-1.358272
1	3.135941	1.719504	0.500543
1	2.665437	1.514133	2.193428
1	0.876888	3.207396	1.939883

1	2.420918	3.895509	1.450266
1	-0.355541	2.642547	-1.607685
1	-0.808005	2.440612	0.081992
1	0.597175	4.469584	-0.176348
1	1.869901	3.521932	-0.941803

**Z-P2**

46	0.038331	-3.263237	1.430813
1	-2.854442	-0.720965	1.105548
17	1.383477	-5.257474	1.554094
17	-0.526267	-3.278389	3.745654
6	0.467810	-3.205241	-0.452298
7	0.738275	-3.202529	-1.588499
6	1.091286	-3.258964	-2.953050
1	1.881786	-4.001798	-3.090046
1	1.448179	-2.278295	-3.279684
1	0.215649	-3.543752	-3.543487
7	-1.290780	0.768903	1.377655
7	-0.521950	-0.361274	1.480554
6	0.797333	-0.114613	1.747972
1	1.493954	-0.936017	1.870467
6	-0.409776	1.757608	1.586972
6	0.921840	1.258720	1.826235
6	-0.662721	3.151275	1.589395
6	1.992884	2.153841	2.072663
6	0.398181	3.987056	1.829267
6	1.716667	3.495895	2.070873
1	2.997422	1.780348	2.259235
1	2.513687	4.212531	2.257461
1	0.236989	5.063599	1.837771
1	-1.665690	3.530681	1.407795
7	-2.377056	-1.627444	1.130789
6	-1.089512	-1.618309	1.329238
6	-4.490390	-2.720196	1.700735
6	-5.354825	-3.955701	1.472072
6	-3.184909	-2.834166	0.924040
6	-5.602609	-4.200317	-0.011620
6	-3.428144	-3.059895	-0.565630
6	-4.289961	-4.298853	-0.780049
1	-2.588184	-3.666108	1.326111
1	-2.463809	-3.153280	-1.084993
1	-3.932512	-2.173308	-0.982129
1	-5.029206	-1.820803	1.359307
1	-4.275981	-2.580957	2.768098
1	-4.849825	-4.831679	1.907316
1	-6.303584	-3.846043	2.012377
1	-4.476432	-4.440464	-1.852170
1	-3.733409	-5.186624	-0.440901
1	-6.196013	-5.112850	-0.152587
1	-6.201951	-3.371955	-0.422165

**INT1**

N	-0.242653	0.402705	0.704443
C	0.869972	0.401394	1.269389
Pd	2.209928	-0.946201	1.935268
N	1.415333	1.875630	1.540206
Cl	3.813110	-2.614840	2.686976
Cl	2.396440	0.340432	3.966546
C	2.105818	-1.955809	0.292618
N	2.102812	-2.605915	-0.678843
C	2.139118	-3.446901	-1.810616
C	-2.303462	-0.860129	1.014867
C	-3.056854	-2.126650	0.623901
C	-0.920905	-0.838425	0.367200
C	-3.152928	-2.278670	-0.890444
C	-1.033456	-0.950702	-1.151605
C	-1.773651	-2.225470	-1.538398
H	1.601728	-4.374153	-1.591071
H	3.179204	-3.681421	-2.054757
H	1.669502	-2.944748	-2.661780
N	0.366054	2.886168	1.565564
H	-0.350417	-1.707727	0.744202
H	-0.030145	-0.919954	-1.600079
H	-1.574126	-0.068937	-1.529547
H	-2.859116	0.031374	0.685361
H	-2.201290	-0.785596	2.105296
H	-2.534792	-3.001212	1.044091
H	-4.057212	-2.119807	1.075736
H	-1.854281	-2.297220	-2.631286
H	-1.183892	-3.097901	-1.211112
H	-3.662001	-3.216402	-1.149628
H	-3.772708	-1.464345	-1.298160
C	0.683922	3.741314	0.648303
H	1.803054	1.796439	2.509305
H	0.029169	4.592977	0.482439
C	2.405901	2.288093	0.557693
C	1.922744	3.452954	-0.036517
C	3.606583	1.698039	0.213576
C	2.655881	4.080636	-1.040948
C	4.334723	2.338047	-0.793052
C	3.867134	3.503067	-1.411392
H	2.297161	4.992334	-1.512260
H	4.467596	3.968305	-2.189749
H	5.290708	1.918324	-1.098087
H	3.968383	0.795015	0.702479

**INT2**

46	2.289624	-0.865069	-0.650017
1	-0.835610	-0.037329	-2.119602
17	4.310076	-1.644286	-1.813766
17	1.109006	-0.377704	-2.735536
6	3.144831	-1.163080	1.035284
7	3.694682	-1.346916	2.052225

6	4.381758	-1.596607	3.257140
1	3.887215	-1.069383	4.078321
1	5.414345	-1.246509	3.169497
1	4.380771	-2.670991	3.463389
7	-0.308773	-1.192269	0.616822
7	-0.189314	-2.433587	0.035346
6	-1.248057	-3.119038	0.404350
1	-1.367285	-4.139482	0.056627
6	-1.460240	-1.111826	1.390259
6	-2.106387	-2.361110	1.252505
6	-1.982071	-0.098730	2.202646
6	-3.331733	-2.594294	1.892779
6	-3.187561	-0.361370	2.837339
6	-3.865874	-1.584144	2.673713
1	-3.843083	-3.548512	1.779217
1	-4.817034	-1.736486	3.180221
1	-3.625264	0.406133	3.473946
1	-1.467622	0.850531	2.324260
7	-2.148423	1.001217	-0.875513
7	-1.835028	0.094466	-1.830014
6	-2.923781	-0.471511	-2.331095
1	-1.386075	1.258440	-0.211502
1	-2.842976	-1.187758	-3.138355
6	-3.496458	0.964604	-0.694550
6	-4.033528	0.046217	-1.637491
6	-4.304759	1.660182	0.213192
6	-5.422779	-0.179962	-1.685690
6	-5.660006	1.408429	0.146572
6	-6.215172	0.502982	-0.790107
1	-5.846637	-0.875677	-2.405522
1	-7.291565	0.348122	-0.796307
1	-6.326400	1.922263	0.836355
1	-3.880553	2.355960	0.932598
7	0.304032	1.014806	0.535034
6	0.634763	-0.198960	0.295601
6	0.608192	3.261546	-0.382673
6	1.578102	4.425368	-0.549623
6	1.276972	2.082019	0.317301
6	2.174591	4.850312	0.787642
6	1.870966	2.510325	1.659226
6	2.840960	3.672974	1.490085
1	2.102182	1.713222	-0.321535
1	2.367617	1.647141	2.126210
1	1.046618	2.801988	2.331122
1	-0.259987	3.581304	0.219907
1	0.215512	2.939232	-1.358233
1	2.389990	4.120696	-1.228393
1	1.072032	5.270461	-1.034695
1	3.237128	3.978856	2.467618
1	3.705220	3.337675	0.895216

1	2.893756	5.667478	0.643316
1	1.373988	5.249640	1.431533

**INT3**

46	1.301352	-2.929109	0.458917
1	-1.406326	0.653800	-0.338063
17	2.912994	-4.679397	1.005644
17	1.558188	-1.810021	2.558214
6	1.004515	-3.810928	-1.227638
7	0.795149	-4.380414	-2.227812
6	0.551496	-5.089722	-3.421221
1	0.206032	-4.398610	-4.195672
1	-0.215454	-5.849730	-3.243559
1	1.472900	-5.577392	-3.751923
7	-0.413364	0.871404	-0.305173
7	0.437621	-0.173032	-0.118459
6	1.694885	0.274384	-0.054641
1	2.506612	-0.425792	0.098177
6	0.299343	2.021192	-0.353687
6	1.670941	1.667879	-0.203455
6	-0.113507	3.349460	-0.515524
6	2.662272	2.669228	-0.222295
6	0.884037	4.304098	-0.526396
6	2.254077	3.973538	-0.384111
1	3.711368	2.409030	-0.107289
1	2.991661	4.772163	-0.400249
1	0.607360	5.349369	-0.646400
1	-1.162378	3.610951	-0.623587
7	-1.327284	-1.587935	-0.182408
6	-0.074191	-1.526070	-0.001465
6	-3.024850	-2.852398	1.035004
6	-3.784945	-4.172775	1.093774
6	-2.012167	-2.866567	-0.108862
6	-4.457756	-4.493818	-0.236257
6	-2.703938	-3.152181	-1.440352
6	-3.451362	-4.478727	-1.381963
1	-1.287161	-3.678224	0.090511
1	-1.961081	-3.152267	-2.251246
1	-3.406241	-2.331228	-1.656577
1	-3.725581	-2.017189	0.876437
1	-2.503612	-2.657180	1.981977
1	-3.080998	-4.980427	1.349353
1	-4.525504	-4.142081	1.903708
1	-3.951152	-4.673224	-2.340279
1	-2.724015	-5.295040	-1.238736
1	-4.963780	-5.466819	-0.183959
1	-5.241578	-3.745509	-0.436960

**INT4**

46	-2.583320	-0.644890	-0.493049
1	1.875428	1.960514	-0.653091
17	-4.707632	-1.615886	-1.254195

17	-2.104627	0.412038	-2.593988
6	-2.837876	-1.506564	1.205768
7	-2.961604	-2.083649	2.216996
6	-3.135374	-2.807458	3.413480
1	-4.160647	-3.184370	3.468055
1	-2.940174	-2.156271	4.270439
1	-2.437666	-3.651023	3.433943
7	0.335707	2.268989	0.298884
7	-0.819602	1.542669	0.299682
6	-1.926447	2.298954	0.498912
1	-2.908940	1.842193	0.518760
6	-0.074455	3.536080	0.510196
6	-1.497138	3.612946	0.650936
6	0.721828	4.700493	0.589369
6	-2.127544	4.856895	0.881338
6	0.079228	5.895602	0.812885
6	-1.333648	5.976483	0.957576
1	-3.208384	4.922129	0.988437
1	-1.788370	6.949929	1.129492
1	0.663976	6.811456	0.881614
1	1.804152	4.643865	0.483601
7	0.288547	-0.481646	0.314700
6	-0.816066	0.123969	0.124720
6	1.210765	-2.279911	-1.082006
6	1.335431	-3.792087	-1.231397
6	0.362614	-1.927817	0.140122
6	1.897916	-4.434426	0.031951
6	0.938467	-2.557750	1.406498
6	1.064369	-4.068495	1.255346
1	-0.648203	-2.341544	-0.028529
1	0.308080	-2.296715	2.268991
1	1.931098	-2.115540	1.601654
1	2.213269	-1.834371	-0.970329
1	0.761958	-1.830573	-1.978000
1	0.340490	-4.214937	-1.440684
1	1.961667	-4.032953	-2.100170
1	1.496309	-4.505719	2.165584
1	0.055888	-4.501720	1.151298
1	1.950443	-5.525058	-0.083181
1	2.933916	-4.088419	0.184028
1	1.984928	0.121899	0.600457
7	2.908869	0.534166	0.313340
7	2.806387	1.493133	-0.630708
6	3.959706	1.695685	-1.249948
1	4.055670	2.464832	-2.004345
6	4.171874	0.034535	0.260305
6	4.887792	0.779608	-0.720148
6	4.773036	-1.000305	0.989707
6	6.244399	0.495137	-0.968873
6	6.100800	-1.258955	0.714904

6	6.830897	-0.521929	-0.249072
1	6.802403	1.061751	-1.710439
1	7.875638	-0.770674	-0.420003
1	6.605694	-2.055133	1.257789
1	4.220932	-1.562945	1.738331

**INT6**

46	-0.024764	-1.046230	1.572489
1	-0.377590	-0.946176	-2.316311
17	0.645005	-1.404764	3.842624
17	-2.038484	-2.320505	1.810312
6	1.642375	-0.091586	1.320170
7	2.669054	0.438353	1.160672
6	3.896945	1.101304	0.958258
1	4.072941	1.797572	1.783320
1	3.859716	1.659858	0.015577
1	4.706066	0.364681	0.925242
7	-2.630574	-0.548550	-1.659589
7	-1.867436	-0.222546	-0.540091
6	-2.475291	0.712535	0.195279
1	-1.917958	1.195012	1.006228
6	-3.821525	0.128156	-1.518784
6	-3.723137	0.975800	-0.386327
6	-4.967285	0.075456	-2.310410
6	-4.789049	1.830952	-0.045923
6	-6.005792	0.914168	-1.941992
6	-5.919793	1.784472	-0.831327
1	-4.711922	2.494001	0.811803
1	-6.767799	2.422507	-0.595309
1	-6.919630	0.906549	-2.532197
1	-5.038679	-0.585609	-3.169810
7	0.005258	-1.195551	-1.400778
6	-0.587849	-0.759433	-0.319958
6	1.077771	-3.263262	-2.161349
6	2.392592	-4.035294	-2.208156
6	1.272007	-1.936905	-1.432257
6	3.511709	-3.205108	-2.826165
6	2.366476	-1.093664	-2.075675
6	3.675613	-1.873869	-2.101177
1	1.526651	-2.139667	-0.383297
1	2.472244	-0.145518	-1.532462
1	2.063404	-0.836798	-3.103954
1	0.726758	-3.059916	-3.186191
1	0.295695	-3.848483	-1.660239
1	2.673868	-4.321943	-1.183239
1	2.249975	-4.971355	-2.762578
1	4.459926	-1.266595	-2.569964
1	4.001295	-2.060360	-1.065093
1	4.454104	-3.767262	-2.810147
1	3.281499	-3.013350	-3.886184
7	0.073480	2.013623	-0.274437



7	-0.219039	2.348632	1.021612
6	0.666415	3.239256	1.479614
1	0.584213	3.629882	2.490533
6	1.188074	2.715116	-0.613792
6	1.618006	3.535276	0.478333
6	1.906571	2.714566	-1.827515
6	2.753755	4.353769	0.346269
6	3.028333	3.519319	-1.929131
6	3.449522	4.335722	-0.851208
1	3.085257	4.989788	1.168244
1	4.331857	4.962715	-0.975223
1	3.597415	3.536415	-2.858558
1	1.578166	2.098360	-2.666379
1	-2.613041	-1.536345	-1.910640

**INT7**

N	-0.649509	-1.087914	-1.183854
N	0.694276	-1.249732	-0.807858
C	1.007320	-2.561692	-0.773149
H	2.028884	-2.859984	-0.567263
C	-1.147898	-2.354316	-1.337825
C	-0.120947	-3.303613	-1.101889
C	-2.449202	-2.743827	-1.673640
C	-0.380861	-4.685674	-1.223881
C	-2.677470	-4.102322	-1.775430
C	-1.660454	-5.064465	-1.554086
H	0.409213	-5.413181	-1.059138
H	-1.904669	-6.119186	-1.652403
H	-3.673550	-4.447605	-2.044561
H	-3.229307	-2.012030	-1.864705
Pd	-2.490653	-0.482518	1.027019
Cl	-3.569093	-1.044143	3.143482
Cl	-0.321890	-0.287905	2.029405
C	-4.250869	-0.561893	0.229932
N	-5.351608	-0.561223	-0.168028
C	-6.686673	-0.488434	-0.614698
H	-7.361476	-0.528231	0.245017
H	-6.900777	-1.327127	-1.283296
H	-6.838452	0.453699	-1.152772
N	-1.458128	1.068236	-1.391764
C	-1.538874	0.031457	-0.674919
C	-3.534641	2.145242	-2.042716
C	-4.350435	3.431470	-2.016770
C	-2.246525	2.287177	-1.224946
C	-4.628050	3.887422	-0.589274
C	-2.537622	2.741491	0.204570
C	-3.329154	4.043824	0.192450
H	-1.646974	3.078753	-1.705593
H	-1.597243	2.853703	0.761924
H	-3.119766	1.971807	0.732430
H	-4.122402	1.319575	-1.614869

H	-3.285159	1.856383	-3.072207
H	-3.796628	4.221331	-2.548356
H	-5.287763	3.285962	-2.570525
H	-3.531752	4.363042	1.222505
H	-2.722927	4.841395	-0.267373
H	-5.193872	4.828140	-0.591144
H	-5.264268	3.139974	-0.085432
Pd	3.439878	-0.694980	0.063697
Cl	5.599262	-1.261840	0.934030
Cl	3.946157	-1.507404	-2.134385
C	2.999812	-0.103981	1.855413
N	2.798362	0.247182	2.948468
C	2.448055	0.671988	4.245508
H	3.354354	0.848441	4.831083
H	1.841163	-0.100410	4.726189
H	1.866450	1.596216	4.175092
N	1.320824	0.901625	-1.290682
C	1.658609	-0.217768	-0.726755
C	1.787376	2.851336	0.133176
C	2.365516	4.260347	0.154525
C	2.021637	2.204964	-1.230435
C	3.839165	4.258891	-0.234521
C	3.497943	2.169746	-1.602433
C	4.049999	3.592948	-1.589060
H	1.498793	2.802335	-1.991039
H	3.631900	1.693798	-2.581501
H	4.057546	1.561475	-0.875027
H	2.274584	2.231566	0.901216
H	0.713214	2.855599	0.366003
H	1.801692	4.891854	-0.550622
H	2.222926	4.702756	1.148468
H	5.115221	3.570836	-1.849350
H	3.550354	4.186122	-2.372016
H	4.231965	5.283719	-0.247290
H	4.415168	3.712018	0.528769
H	0.379723	0.974978	-1.717065

**INT8**

7	-0.740545	-1.184982	-1.068087
7	0.648954	-1.353742	-0.737543
6	0.889146	-2.651990	-0.564546
1	1.903620	-2.975825	-0.354433
6	-1.284474	-2.464273	-1.078804
6	-0.274267	-3.398002	-0.773788
6	-2.586112	-2.875209	-1.365832
6	-0.545290	-4.776810	-0.730666
6	-2.836824	-4.237563	-1.308712
6	-1.837294	-5.180262	-0.990698
1	0.245200	-5.486311	-0.501216
1	-2.093261	-6.236171	-0.964778
1	-3.841983	-4.589559	-1.530632

1	-3.365357	-2.174681	-1.646753
46	-3.063135	-0.282999	0.544225
17	-4.812549	-0.477961	2.178334
17	-1.306402	-0.724634	2.112186
6	-4.458914	0.026042	-0.765418
7	-5.322189	0.189623	-1.534867
6	-6.384187	0.410169	-2.436936
1	-7.330728	0.396527	-1.889595
1	-6.387990	-0.377444	-3.195833
1	-6.253584	1.382811	-2.920627
7	-1.020385	1.096080	-1.095262
6	-1.504514	-0.040164	-0.697022
6	-2.786575	2.899792	-1.210880
6	-2.980815	4.386134	-0.919343
6	-1.411303	2.469279	-0.715446
6	-2.808979	4.685373	0.565817
6	-1.264724	2.713755	0.785155
6	-1.459903	4.195641	1.079134
1	-0.661425	3.084550	-1.236304
1	-0.284026	2.355958	1.128928
1	-2.022286	2.119179	1.319981
1	-3.558714	2.328099	-0.679241
1	-2.893117	2.683482	-2.282666
1	-2.247279	4.968681	-1.498934
1	-3.972519	4.703077	-1.266234
1	-1.367930	4.373166	2.158014
1	-0.650750	4.769710	0.598082
1	-2.921489	5.761016	0.752284
1	-3.611162	4.184229	1.129994
46	3.287109	-0.854310	0.415333
17	5.223241	-1.256267	1.828353
17	4.150901	-2.160040	-1.422532
6	2.431750	-0.004560	1.931191
7	1.926678	0.470278	2.871585
6	1.331976	0.992706	4.038343
1	2.047265	1.642792	4.550381
1	1.048686	0.168371	4.699377
1	0.436998	1.563400	3.773568
7	1.559626	0.612578	-1.565649
6	1.742936	-0.365041	-0.782190
6	2.455404	2.630625	-0.469329
6	3.282260	3.890827	-0.686939
6	2.488806	1.739173	-1.711812
6	4.714806	3.543982	-1.075343
6	3.925162	1.368505	-2.072658
6	4.747357	2.633630	-2.297513
1	2.080691	2.325635	-2.551261
1	3.935236	0.720681	-2.958288
1	4.369587	0.780808	-1.254486
1	2.864934	2.059505	0.377592

1	1.415368	2.879242	-0.213202
1	2.820767	4.494011	-1.485805
1	3.263031	4.509840	0.219597
1	5.780184	2.360899	-2.548335
1	4.349369	3.178287	-3.169537
1	5.293598	4.458211	-1.261806
1	5.202769	3.030574	-0.231633
1	-0.112277	1.035419	-1.609482

**INT9**

Pd	-0.595858	-1.180713	-1.523449
Cl	-2.407738	-1.984961	-2.963639
Cl	0.727425	-0.307584	-3.326049
C	-1.524466	-1.962168	-0.028603
N	-2.055598	-2.503893	0.862207
C	-2.719755	-3.188669	1.900159
H	-3.754094	-3.385772	1.604412
H	-2.709525	-2.580613	2.809467
H	-2.212123	-4.138916	2.093797
N	1.051358	0.895575	-0.215372
N	2.164449	1.361572	0.413211
C	2.197396	2.683163	0.449832
H	3.026782	3.204377	0.909698
C	0.320179	1.990866	-0.603382
C	1.037096	3.150181	-0.187414
C	-0.909675	2.100363	-1.266891
C	0.530770	4.438913	-0.442599
C	-1.381340	3.377701	-1.497223
C	-0.675833	4.536109	-1.096359
H	1.084557	5.319970	-0.128081
H	-1.099665	5.514065	-1.311554
H	-2.332217	3.493479	-2.012587
H	-1.468509	1.226807	-1.593442
N	1.761184	-1.177629	0.332261
C	0.881692	-0.535079	-0.320378
C	3.082001	-3.138220	-0.269345
C	3.144128	-4.660075	-0.222648
C	1.773513	-2.629123	0.333194
C	2.950946	-5.183998	1.196231
C	1.599588	-3.140687	1.762639
C	1.653271	-4.662578	1.803772
H	0.940274	-3.018665	-0.282095
H	0.651078	-2.766424	2.175165
H	2.402681	-2.718217	2.387950
H	3.922346	-2.708715	0.299682
H	3.176073	-2.772572	-1.300949
H	2.355591	-5.072076	-0.871898
H	4.098763	-5.009637	-0.637506
H	1.538174	-5.017528	2.836780
H	0.798493	-5.068612	1.238168
H	2.964595	-6.281987	1.204993

H	3.797278	-4.856811	1.821834
H	2.796374	0.641432	0.768338

**INT10**

7	-2.085269	-1.549727	0.289035
6	-2.437212	-0.555828	-0.216453
46	-3.125073	1.073859	-0.989225
17	-4.048660	3.067229	-1.857444
17	-5.229752	0.287608	-0.306890
6	-2.337915	-2.548204	2.470744
6	-2.151309	-3.831383	3.271347
6	-1.863750	-2.754100	1.030801
6	-2.863100	-5.007153	2.612626
6	-2.585774	-3.922119	0.355599
6	-2.396619	-5.194253	1.174097
1	-0.778829	-2.935699	1.021220
1	-2.214347	-4.047045	-0.668740
1	-3.654437	-3.670534	0.285381
1	-3.401053	-2.266655	2.444206
1	-1.791841	-1.711908	2.923439
1	-1.075921	-4.054472	3.355180
1	-2.516766	-3.677576	4.294218
1	-2.937575	-6.018093	0.692438
1	-1.331441	-5.475244	1.167777
1	-2.696474	-5.926091	3.188935
1	-3.948872	-4.824453	2.621038
7	-0.263374	0.942234	-2.000029
7	-1.251392	1.765742	-1.554474
6	-0.754302	2.991568	-1.470101
1	-1.383802	3.798395	-1.118498
6	0.870202	1.651686	-2.260224
6	0.591923	2.994447	-1.903094
6	2.114297	1.251764	-2.760488
6	1.592113	3.973175	-2.037582
6	3.075568	2.238186	-2.885665
6	2.822155	3.581511	-2.527618
1	1.395362	5.007194	-1.763747
1	3.614894	4.317167	-2.642857
1	4.057162	1.971089	-3.272195
1	2.312936	0.219419	-3.037348
1	-0.499142	-0.002304	-2.275527

**INT14**

7	-2.746535	-1.278869	0.365078
6	-3.145538	-0.037128	0.385292
46	-4.783264	1.113738	0.399344
17	-6.312424	2.940920	0.476019
17	-6.509162	-0.453509	0.315397
6	-3.064541	-3.469026	-0.666900
6	-3.944460	-4.713596	-0.719803
6	-3.637272	-2.450206	0.310132
6	-4.140773	-5.316857	0.665755

6	-3.818478	-3.044677	1.703234
6	-4.702426	-4.285332	1.636933
1	-4.601799	-2.076253	-0.051493
1	-4.251208	-2.288965	2.371441
1	-2.829076	-3.309934	2.110763
1	-2.050349	-3.749903	-0.334563
1	-2.961590	-3.016590	-1.661634
1	-4.924609	-4.441815	-1.140386
1	-3.504683	-5.447499	-1.407095
1	-4.815578	-4.714457	2.640383
1	-5.710950	-3.986963	1.310738
1	-4.803626	-6.189921	0.609748
1	-3.172903	-5.683900	1.043519
7	-2.227069	0.999412	0.445398
7	-2.979580	2.168054	0.468694
6	-2.160572	3.185672	0.508367
1	-2.545347	4.197877	0.531538
6	-0.871309	1.304165	0.473517
6	-0.811057	2.719489	0.514085
6	0.280614	0.518894	0.466012
6	0.427944	3.369318	0.550111
6	1.495875	1.189573	0.503279
6	1.573571	2.591717	0.544661
1	0.479989	4.455113	0.581605
1	2.550171	3.068976	0.572604
1	2.414370	0.606700	0.500373
1	0.255344	-0.566592	0.433983
1	-1.752989	-1.499886	0.424441

**INT15**

7	-3.747206	-0.993102	0.969376
6	-2.770408	-1.339354	1.491636
46	-1.153199	-1.973091	2.442585
17	0.702238	-2.662152	3.668730
17	-2.618863	-2.845377	4.078789
6	-5.637888	-1.796510	-0.309949
6	-6.952616	-1.372186	-0.952554
6	-4.967413	-0.585426	0.342812
6	-7.874878	-0.695559	0.054809
6	-5.875308	0.087555	1.374156
6	-7.187744	0.494041	0.714998
1	-4.675868	0.140332	-0.430157
1	-5.362515	0.952777	1.810406
1	-6.063815	-0.626578	2.188777
1	-5.820524	-2.552076	0.467895
1	-4.959300	-2.242739	-1.046543
1	-6.743569	-0.679647	-1.782508
1	-7.436521	-2.250781	-1.396245
1	-7.840924	0.953407	1.466776
1	-6.989934	1.269858	-0.040982
1	-8.803028	-0.375020	-0.434578

1	-8.164260	-1.423647	0.828614
7	-0.478821	-0.174348	0.252034
7	0.020100	-1.191772	0.984474
6	1.265581	-1.575734	0.633392
1	1.784090	-2.367824	1.156847
6	0.510721	0.104237	-0.631921
6	1.637560	-0.758359	-0.440969
6	0.519421	1.088166	-1.644323
6	2.777704	-0.634919	-1.264458
6	1.645927	1.187835	-2.429549
6	2.766567	0.334437	-2.242811
1	3.640066	-1.285373	-1.127253
1	3.632592	0.454294	-2.891728
1	1.685520	1.940379	-3.215811
1	-0.337590	1.744025	-1.787603
1	-1.036598	-0.658018	3.179748

**INT16**

7	1.944507	1.936182	-0.295766
7	2.084568	0.596261	-0.431467
6	3.115510	0.096233	0.275375
6	3.734908	1.170382	0.931978
6	2.956779	2.303121	0.529833
6	4.836864	1.338837	1.795394
6	5.137699	2.611648	2.236905
6	4.365180	3.731777	1.835350
6	3.282797	3.595821	0.990470
46	0.734906	-0.459875	-1.540225
17	-0.927858	-1.634183	-2.794857
6	-0.654627	0.734581	-0.972344
7	-1.507857	1.452567	-0.620075
6	-2.531995	2.343821	-0.185623
6	-3.309390	2.885275	-1.386712
6	-4.405080	3.832908	-0.915286
6	-5.334300	3.159028	0.088079
6	-4.551229	2.598171	1.270046
6	-3.456190	1.643281	0.812238
17	2.438272	-1.978596	-2.237356
1	-2.017911	3.176108	0.318972
1	-2.869679	1.273664	1.662042
1	-3.898145	0.765188	0.318631
1	-3.749300	2.033950	-1.926755
1	-2.620035	3.384494	-2.078089
1	-3.943641	4.717843	-0.448919
1	-4.969245	4.199467	-1.782135
1	-5.219647	2.080407	1.969547
1	-4.095283	3.428376	1.832570
1	-6.097651	3.866859	0.436997
1	-5.873433	2.338801	-0.411850
1	3.349632	-0.960424	0.238942
1	5.438575	0.484750	2.106695

1	5.984551	2.765727	2.904646
1	4.637482	4.720071	2.205417
1	2.692367	4.457746	0.680195

**INT16•IndH<sup>+</sup>**

6	-2.498045	-2.444335	3.526560
6	-1.134906	-2.635886	3.489321
6	-0.538273	-2.852772	2.231669
6	-1.345522	-2.889096	1.061202
6	-2.731399	-2.691816	1.100013
6	-3.280913	-2.467118	2.346260
6	0.782157	-3.038671	1.786149
7	0.743014	-3.189006	0.468368
7	-0.526850	-3.144932	0.006883
7	1.925521	1.918685	-0.279409
7	2.087120	0.584175	-0.419099
6	3.140760	0.097141	0.267592
6	3.756114	1.182960	0.906730
6	2.950531	2.301695	0.523454
6	4.876666	1.368459	1.743571
6	5.162303	2.645490	2.179098
6	4.359534	3.752022	1.798501
6	3.262574	3.600403	0.977506
46	0.733330	-0.460145	-1.507720
17	-0.947029	-1.656101	-2.765920
6	-0.640317	0.761023	-0.943486
7	-1.503857	1.448146	-0.562277
6	-2.539614	2.330075	-0.130669
6	-3.247567	2.939175	-1.341768
6	-4.353107	3.879096	-0.878214
6	-5.338977	3.172657	0.044808
6	-4.622640	2.540938	1.233375
6	-3.517479	1.592391	0.784920
17	2.361418	-2.152392	-2.046455
1	-2.039750	3.128128	0.438459
1	-2.976955	1.177094	1.644758
1	-3.943848	0.743764	0.228250
1	-3.669030	2.121784	-1.945068
1	-2.517181	3.462251	-1.970427
1	-3.902679	4.732845	-0.347916
1	-4.868120	4.295669	-1.752681
1	-5.331588	1.999915	1.872831
1	-4.183753	3.333826	1.859048
1	-6.105581	3.876226	0.394262
1	-5.867717	2.388322	-0.519487
1	3.403073	-0.952232	0.219806
1	5.502679	0.525778	2.036209
1	6.022307	2.815586	2.825406
1	4.624702	4.743952	2.162772
1	2.650259	4.451468	0.682100
1	1.509435	-3.210689	-0.221132



1	1.725518	-3.075161	2.314442
1	-0.531843	-2.616523	4.393453
1	-2.991233	-2.269802	4.479896
1	-4.353216	-2.300250	2.425715
1	-3.333314	-2.712678	0.195389
1	-0.685840	-2.930662	-0.991360

**INT17**

7	-2.750883	-1.220605	0.330103
6	-3.219203	-0.049769	0.438690
46	-4.842790	1.134974	0.541553
17	-6.390871	3.085839	0.649465
17	-6.541860	-0.506356	0.518941
6	-2.917135	-3.448514	-0.615481
6	-3.737616	-4.729933	-0.692145
6	-3.614864	-2.387279	0.232149
6	-4.049157	-5.268943	0.699239
6	-3.927633	-2.929854	1.626511
6	-4.745888	-4.213132	1.550678
1	-4.570470	-2.110381	-0.242019
1	-4.462549	-2.158581	2.196775
1	-2.977074	-3.120458	2.152126
1	-1.933298	-3.661495	-0.164863
1	-2.719838	-3.047028	-1.619127
1	-4.683062	-4.524104	-1.219296
1	-3.208617	-5.484401	-1.290668
1	-4.940505	-4.597877	2.561248
1	-5.730489	-3.985641	1.111553
1	-4.665171	-6.176483	0.631732
1	-3.107871	-5.567615	1.190323
7	-2.301572	1.034505	0.519531
7	-3.014791	2.203966	0.595506
6	-2.159973	3.206722	0.614983
1	-2.516940	4.227474	0.673436
6	-0.955351	1.286027	0.482215
6	-0.831243	2.700115	0.547716
6	0.151450	0.437565	0.398107
6	0.446796	3.279959	0.531188
6	1.397618	1.043061	0.382211
6	1.546290	2.444255	0.448190
1	0.564218	4.360885	0.580891
1	2.546634	2.871859	0.432019
1	2.287341	0.419381	0.316557
1	0.028066	-0.640510	0.346092

**TS1**

7	0.309222	-0.419738	1.545837
6	1.472048	-0.411515	1.921216
46	3.017003	-1.549370	2.443578
7	2.091623	1.340189	1.841111
17	4.827183	-3.051597	2.977098
17	3.668589	0.006544	4.148466

6	2.539326	-2.837517	1.081489
7	2.308546	-3.649273	0.274482
6	2.076029	-4.667157	-0.673595
6	-1.836495	-1.436962	2.129064
6	-2.736972	-2.648117	1.908283
6	-0.517206	-1.614347	1.386282
6	-2.966646	-2.913920	0.424444
6	-0.754832	-1.840530	-0.104410
6	-1.644080	-3.059398	-0.319955
1	1.512732	-5.479191	-0.204859
1	3.034892	-5.051260	-1.032788
1	1.505389	-4.263713	-1.515264
7	1.015374	2.250856	1.919033
1	0.011148	-2.491727	1.801396
1	0.208441	-1.950287	-0.621913
1	-1.235270	-0.941875	-0.520978
1	-2.326664	-0.525288	1.754557
1	-1.643385	-1.278424	3.197668
1	-2.271757	-3.533986	2.368971
1	-3.692288	-2.498107	2.427146
1	-1.815006	-3.212739	-1.393701
1	-1.119583	-3.958325	0.043914
1	-3.583482	-3.811826	0.287838
1	-3.534460	-2.076503	-0.010874
6	0.907953	2.776212	0.732249
1	2.670006	1.345426	2.698324
1	0.105825	3.481842	0.536625
6	2.737589	1.483610	0.579655
6	1.942957	2.351364	-0.176930
6	3.868800	0.858124	0.080686
6	2.279918	2.627926	-1.502576
6	4.199449	1.152632	-1.242243
6	3.417768	2.018370	-2.020705
1	1.677039	3.301694	-2.107404
1	3.712227	2.218461	-3.048699
1	5.088135	0.700506	-1.677476
1	4.466889	0.182021	0.690150

**TS2**

N	-1.316827	1.570504	0.446523
C	-0.409807	0.749886	0.048261
Pd	-0.238429	-1.174608	-0.352075
H	-0.208549	2.423282	0.411011
Cl	0.000652	-3.522435	-0.871937
Cl	-1.038534	-1.615848	1.851033
C	0.454940	-0.800999	-2.115407
N	0.892886	-0.603134	-3.179289
C	1.455769	-0.296928	-4.433658
H	0.803920	-0.666043	-5.230322
H	2.436694	-0.773194	-4.519442
H	1.563201	0.788928	-4.522895

C	-3.017333	1.557716	2.176638
C	-4.482909	1.278685	2.484274
C	-2.707795	1.245611	0.713552
C	-5.403774	2.055860	1.550984
C	-3.614530	2.039955	-0.224419
C	-5.080708	1.764156	0.089742
H	-2.843868	0.166319	0.538081
H	-3.381020	1.787790	-1.267181
H	-3.398478	3.112846	-0.098844
H	-2.788658	2.619380	2.364033
H	-2.357245	0.962565	2.820999
H	-4.672726	0.199214	2.374604
H	-4.696150	1.524785	3.532425
H	-5.720469	2.358535	-0.575691
H	-5.303340	0.707619	-0.127160
H	-6.454293	1.818314	1.764033
H	-5.284170	3.135191	1.739985
N	0.768281	1.703465	0.026045
N	1.264530	2.053035	-1.274522
C	2.558975	2.111661	-1.149080
H	3.155886	2.413238	-2.005802
C	1.878920	1.456284	0.887785
C	3.035570	1.753478	0.161891
C	1.890456	1.024622	2.202726
C	4.287310	1.642456	0.771090
C	3.147104	0.905660	2.793998
C	4.322600	1.214070	2.093207
H	5.201051	1.876467	0.229712
H	5.280902	1.109985	2.596646
H	3.216075	0.560988	3.823274
H	0.975272	0.776689	2.736673

**TS3**

7	-1.948070	0.307191	0.311977
6	-0.871412	-0.361494	0.247290
46	-0.565021	-2.337632	0.293346
1	-1.611058	2.006219	0.731706
8	-0.781439	2.562871	0.937419
1	-0.062901	1.677472	0.644790
17	-0.229748	-4.763603	0.284060
17	-1.101437	-2.243950	2.639439
6	-0.141136	-2.329847	-1.585886
7	0.124412	-2.347646	-2.724703
6	0.470725	-2.378970	-4.089818
1	1.219816	-3.157937	-4.258941
1	0.879104	-1.407063	-4.384444
1	-0.418259	-2.594923	-4.689372
1	-0.764473	2.680424	1.908745
6	-4.093052	0.264799	1.466883
6	-5.474006	-0.376431	1.522086
6	-3.236149	-0.378232	0.381148

6	-6.169008	-0.307976	0.167254
6	-3.925544	-0.300744	-0.980706
6	-5.309154	-0.938014	-0.922946
1	-3.074615	-1.440135	0.636518
1	-3.297336	-0.792545	-1.736933
1	-4.009341	0.757748	-1.275840
1	-4.191369	1.341431	1.246378
1	-3.583531	0.179717	2.436139
1	-5.368829	-1.429738	1.825970
1	-6.082153	0.109631	2.296142
1	-5.800040	-0.852969	-1.901365
1	-5.201088	-2.015499	-0.722345
1	-7.149308	-0.800624	0.213125
1	-6.361814	0.746899	-0.088269
7	0.347293	0.510955	0.088374
7	0.512516	0.929704	-1.284794
6	1.789715	0.852986	-1.527034
1	2.157962	1.172072	-2.498509
6	1.612192	0.070909	0.569987
6	2.556788	0.335361	-0.428455
6	1.946112	-0.489791	1.794468
6	3.908858	0.057704	-0.208552
6	3.294552	-0.776388	1.992739
6	4.261268	-0.499990	1.013064
1	4.656152	0.266450	-0.970928
1	5.303578	-0.737156	1.215028
1	3.602977	-1.232606	2.930802
1	1.191418	-0.727593	2.542091

**TS4**

46	2.223820	0.550390	-0.948419
1	-1.207336	-1.320104	-0.543872
17	4.476395	1.074435	-1.777971
17	1.110622	1.769424	-2.681689
6	3.077169	-0.403015	0.495651
7	3.635331	-0.959801	1.361466
6	4.376039	-1.601354	2.374387
1	3.757984	-1.714066	3.270055
1	5.258619	-1.001529	2.615718
1	4.695895	-2.588495	2.026485
7	-0.029336	-1.333937	-0.456585
7	0.472101	-1.874978	-1.703146
6	1.081998	-2.978117	-1.397852
1	1.523343	-3.569603	-2.195137
6	0.389199	-2.217962	0.601480
6	1.093220	-3.270231	0.014933
6	0.176999	-2.107806	1.963631
6	1.627158	-4.282645	0.812400
6	0.714538	-3.126181	2.751389
6	1.429368	-4.191809	2.186460
1	2.177337	-5.112069	0.374046

1	1.833735	-4.962790	2.838874
1	0.576782	-3.089464	3.830000
1	-0.373827	-1.274588	2.394870
7	-3.192166	-0.179672	0.086036
7	-2.643782	-1.233513	-0.559616
6	-3.625394	-1.939111	-1.100534
1	-2.537968	0.492643	0.487167
1	-3.399851	-2.835706	-1.664530
6	-4.543567	-0.177796	-0.049105
6	-4.869336	-1.328354	-0.815446
6	-5.522430	0.707072	0.423491
6	-6.215350	-1.609239	-1.112850
6	-6.833792	0.404141	0.110323
6	-7.179779	-0.739598	-0.646156
1	-6.483021	-2.486706	-1.697683
1	-8.228620	-0.930462	-0.862958
1	-7.625637	1.066207	0.455519
1	-5.260625	1.588265	1.004371
7	-0.448539	0.773951	0.416158
6	0.405996	0.114390	-0.238370
6	-1.334830	3.046070	0.460966
6	-1.060159	4.487621	0.869411
6	-0.137952	2.156958	0.782069
6	-0.700002	4.579443	2.348147
6	0.208272	2.228856	2.268381
6	0.475748	3.669914	2.689148
1	0.733130	2.511904	0.203229
1	1.080421	1.590455	2.473768
1	-0.633603	1.815869	2.849250
1	-2.213413	2.670368	1.014765
1	-1.575420	2.974333	-0.608064
1	-0.227959	4.878827	0.263597
1	-1.930668	5.116409	0.641728
1	0.699380	3.712208	3.763415
1	1.376570	4.031918	2.169750
1	-0.470421	5.617239	2.623499
1	-1.573772	4.283580	2.951730

**E-TS5**

46	-0.234088	-1.438099	-0.333993
1	1.062316	1.142719	-0.175460
17	1.222131	-3.358250	-0.907440
17	-1.271217	-1.362046	-2.485029
6	0.693555	-1.353736	1.361095
7	1.361884	-1.267044	2.318556
6	2.212319	-1.225200	3.442581
1	3.156620	-1.722773	3.200851
1	1.736788	-1.738357	4.283472
1	2.407875	-0.184568	3.718613
7	-2.557879	0.308082	0.061470
7	-3.309599	1.285412	-0.574001

6	-4.558383	0.885695	-0.501089
1	-5.335122	1.499269	-0.945921
6	-3.372015	-0.722412	0.513405
6	-4.692536	-0.360847	0.173765
6	-3.092140	-1.897646	1.216600
6	-5.766723	-1.188352	0.528099
6	-4.169989	-2.704994	1.550388
6	-5.492062	-2.358964	1.213423
1	-6.787341	-0.913136	0.269214
1	-6.305596	-3.022219	1.500604
1	-3.984303	-3.631498	2.090647
1	-2.076854	-2.176432	1.489506
7	-0.430734	1.377911	-0.010603
6	-1.158377	0.321409	-0.006556
6	0.005858	3.548946	1.038669
6	-0.497655	4.980620	1.188123
6	-0.921355	2.754951	0.122780
6	-0.623979	5.666081	-0.168807
6	-0.998623	3.420184	-1.250348
6	-1.495636	4.854941	-1.121306
1	-1.927196	2.749464	0.566312
1	-1.652493	2.830192	-1.903005
1	0.007636	3.407326	-1.701364
1	1.016613	3.566581	0.598333
1	0.088191	3.053838	2.017039
1	-1.482212	4.965357	1.681752
1	0.170059	5.550019	1.848346
1	-1.533826	5.331377	-2.109871
1	-2.531231	4.837918	-0.745016
1	-1.026849	6.680506	-0.047820
1	0.379959	5.781567	-0.608517
1	2.051071	-0.804689	-1.310756
7	2.689420	-0.135261	-0.875624
7	2.186719	0.918282	-0.193119
6	3.159726	1.499553	0.497488
1	2.949658	2.377364	1.095494
6	4.009695	-0.274046	-0.590618
6	4.359058	0.792918	0.280333
6	4.939862	-1.230079	-1.019381
6	5.688844	0.924381	0.726232
6	6.230152	-1.077977	-0.554125
6	6.604686	-0.013539	0.302157
1	5.976493	1.742395	1.382760
1	7.639532	0.057021	0.629387
1	6.987079	-1.798427	-0.856867
1	4.651258	-2.046241	-1.676285

**Z-TS5**

Pd	-2.521855	-0.554603	-0.081043
H	1.836952	-0.261141	-0.387202
Cl	-4.840458	-1.342111	0.135273

Cl	-2.342796	-1.176798	-2.394216
C	-2.597352	-0.036005	1.769653
N	-2.664551	0.273975	2.896301
C	-2.809821	0.620710	4.254887
H	-3.777986	0.265950	4.619582
H	-2.756785	1.707662	4.364937
H	-2.009587	0.157761	4.839559
N	-0.367269	1.460123	-0.147713
N	0.831654	1.951463	0.333786
C	0.739233	3.263601	0.286151
H	1.571481	3.868896	0.632122
C	-1.212941	2.499219	-0.505101
C	-0.511415	3.694753	-0.229446
C	-2.491255	2.519758	-1.075617
C	-1.099357	4.941958	-0.488314
C	-3.051394	3.763935	-1.319769
C	-2.371654	4.962951	-1.028230
H	-0.560454	5.863080	-0.274038
H	-2.855414	5.913905	-1.242278
H	-4.045292	3.810744	-1.760318
H	-3.025161	1.607342	-1.333022
N	0.423359	-0.695448	-0.207516
C	-0.603494	0.073750	-0.185045
C	0.941727	-2.848050	-1.268106
C	0.792435	-4.359548	-1.144248
C	0.261747	-2.144341	-0.097737
C	1.344195	-4.862435	0.185271
C	0.828265	-2.630081	1.236170
C	0.691019	-4.143485	1.360529
H	-0.813573	-2.391457	-0.126965
H	0.309305	-2.120003	2.060814
H	1.891219	-2.340643	1.301774
H	2.014036	-2.587512	-1.273416
H	0.513056	-2.482965	-2.210531
H	-0.274951	-4.619924	-1.221233
H	1.292981	-4.857868	-1.984906
H	1.120932	-4.485086	2.311559
H	-0.379030	-4.402387	1.392752
H	1.201507	-5.947507	0.274775
H	2.432594	-4.687871	0.214092
H	2.741075	1.294867	1.117631
N	3.432042	0.736299	0.618427
N	2.960086	-0.009443	-0.404059
C	3.970153	-0.450628	-1.137237
H	3.784288	-1.097911	-1.984889
C	4.783493	0.843400	0.515873
C	5.172606	0.063241	-0.606520
C	5.712653	1.540172	1.298833
C	6.533611	-0.038192	-0.951017
C	7.038255	1.424658	0.929434

C	7.447679	0.645089	-0.177892
H	6.845684	-0.636725	-1.803521
H	8.506671	0.589574	-0.419172
H	7.794659	1.949700	1.509196
H	5.404896	2.137353	2.152968

**TS6**

46	3.289607	-2.433048	1.011825
1	-0.452522	0.249104	0.545314
17	5.564671	-3.181134	1.176790
17	2.769324	-3.052106	3.245644
6	3.688825	-1.929326	-0.819923
7	3.945303	-1.612326	-1.913551
6	4.298107	-1.251760	-3.230756
1	3.600110	-1.714207	-3.934103
1	5.313512	-1.598694	-3.440724
1	4.253241	-0.163986	-3.334670
7	0.398366	0.801439	0.508728
7	1.573011	0.156189	0.617004
6	2.544493	1.052816	0.599804
1	3.576674	0.730025	0.683240
6	0.586816	2.147803	0.421301
6	1.991527	2.352550	0.473787
6	-0.319400	3.208743	0.297071
6	2.507625	3.658419	0.396234
6	0.220899	4.479428	0.225949
6	1.615106	4.704808	0.273800
1	3.580623	3.834514	0.434444
1	1.986229	5.725723	0.213949
1	-0.447904	5.332727	0.132022
1	-1.393012	3.040223	0.261997
7	0.228714	-2.049365	0.825827
6	1.422775	-1.884008	0.859885
6	-1.479895	-3.130409	2.186996
6	-2.387209	-4.349166	2.311298
6	-0.592668	-3.258100	0.953742
6	-3.221437	-4.553233	1.051875
6	-1.424566	-3.432895	-0.312325
6	-2.335304	-4.648805	-0.184669
1	0.076473	-4.124145	1.075119
1	-0.763446	-3.525467	-1.183657
1	-2.028107	-2.523769	-0.462876
1	-2.086975	-2.216532	2.088614
1	-0.857702	-3.007539	3.082162
1	-1.769875	-5.243205	2.490170
1	-3.032218	-4.239686	3.192213
1	-2.943086	-4.751164	-1.092859
1	-1.717651	-5.558371	-0.121706
1	-3.842973	-5.453203	1.146265
1	-3.915610	-3.705473	0.936063

**TS7**



46	0.692094	-3.078788	1.567998
1	-2.172242	-0.309416	1.075296
17	2.368062	-4.816234	1.767818
17	0.737904	-2.534501	3.889094
6	0.553884	-3.530422	-0.301777
7	0.429595	-3.828884	-1.424754
6	0.301444	-4.221517	-2.773240
1	0.203714	-3.334151	-3.405314
1	-0.587251	-4.849846	-2.887706
1	1.187494	-4.788084	-3.072702
7	-1.366663	0.574532	1.396641
7	-0.334133	-0.281173	1.613737
6	0.778445	0.342696	2.021571
1	1.677016	-0.219143	2.242919
6	-0.903266	1.808943	1.679168
6	0.468619	1.706400	2.084440
6	-1.557019	3.051615	1.613605
6	1.189715	2.866787	2.440361
6	-0.820313	4.161269	1.964603
6	0.536099	4.074973	2.375657
1	2.227993	2.797769	2.756460
1	1.061716	4.988449	2.644592
1	-1.292957	5.140924	1.927779
1	-2.595777	3.123706	1.302260
7	-1.912255	-1.674982	0.993974
6	-0.681031	-1.652785	1.354218
6	-3.783220	-3.113334	1.616858
6	-4.585226	-4.347984	1.222824
6	-2.638536	-2.878104	0.633001
6	-5.094131	-4.251940	-0.211063
6	-3.156407	-2.759257	-0.798962
6	-3.949932	-4.000772	-1.186820
1	-1.941446	-3.732263	0.693778
1	-2.313549	-2.595605	-1.485283
1	-3.797876	-1.866239	-0.869484
1	-4.434761	-2.224979	1.617930
1	-3.377163	-3.212591	2.632104
1	-3.947027	-5.239838	1.323718
1	-5.420189	-4.486696	1.921557
1	-4.328524	-3.897568	-2.212065
1	-3.276152	-4.873291	-1.190044
1	-5.637022	-5.165728	-0.485817
1	-5.818615	-3.425136	-0.284860

**TS8**

46	-2.649500	-0.507470	-0.485823
1	1.683205	1.675473	0.021071
17	-4.821236	-1.378745	-1.232631
17	-2.166858	0.587220	-2.561994
6	-2.926840	-1.393707	1.198582
7	-3.075391	-1.982340	2.199766

6	-3.305317	-2.707595	3.386086
1	-4.361292	-2.986357	3.444399
1	-3.042424	-2.092570	4.251770
1	-2.691934	-3.614264	3.386441
7	0.460052	2.219785	0.349657
7	-0.738288	1.570245	0.299289
6	-1.779147	2.418036	0.428988
1	-2.795376	2.043635	0.402176
6	0.158317	3.524833	0.510449
6	-1.257653	3.700827	0.579578
6	1.033288	4.626059	0.606295
6	-1.809626	4.988091	0.759049
6	0.463795	5.868035	0.776661
6	-0.943037	6.051025	0.855229
1	-2.886996	5.127580	0.813654
1	-1.334826	7.056800	0.990228
1	1.109074	6.741169	0.854056
1	2.111957	4.493113	0.551666
7	0.233055	-0.517936	0.321816
6	-0.831950	0.147447	0.124074
6	1.081726	-2.338612	-1.082178
6	1.106619	-3.850643	-1.275013
6	0.212914	-1.962034	0.117418
6	1.559057	-4.570493	-0.009218
6	0.681393	-2.672502	1.385442
6	0.694889	-4.182756	1.185886
1	-0.815958	-2.300800	-0.104069
1	0.035119	-2.388197	2.228545
1	1.698960	-2.329823	1.645357
1	2.106304	-1.963966	-0.923289
1	0.696866	-1.832731	-1.977812
1	0.096087	-4.194781	-1.546162
1	1.756911	-4.109442	-2.120717
1	1.045632	-4.682410	2.098722
1	-0.337716	-4.530187	1.018096
1	1.539908	-5.658004	-0.158936
1	2.608316	-4.305014	0.204127
1	2.267579	-0.368632	0.969633
7	3.075603	0.126002	0.587317
7	2.781697	1.219601	-0.148310
6	3.850028	1.584186	-0.838774
1	3.820204	2.467185	-1.464192
6	4.344793	-0.281990	0.319344
6	4.892137	0.663062	-0.589860
6	5.075511	-1.384043	0.781911
6	6.218109	0.515733	-1.036849
6	6.370567	-1.503951	0.315939
6	6.938888	-0.566709	-0.578377
1	6.653072	1.233769	-1.728145
1	7.964996	-0.710607	-0.909152

1	6.973769	-2.347489	0.645545
1	4.645269	-2.105171	1.472735

**Z-TS9**

46	-2.850829	0.053685	-0.089141
1	1.434577	-0.727781	-0.401541
17	-5.282654	-0.140708	0.078429
17	-2.866217	0.457448	-2.448201
6	-2.761128	-0.271357	1.807782
7	-2.726496	-0.491384	2.956390
6	-2.733621	-0.764557	4.339211
1	-3.640420	-1.319524	4.596431
1	-2.712729	0.175294	4.898618
1	-1.854497	-1.361684	4.599531
7	1.019371	1.765318	0.029737
7	-0.312139	1.518529	-0.157792
6	-1.048410	2.647662	-0.341177
1	-2.113180	2.586628	-0.529843
6	1.111666	3.105987	-0.046089
6	-0.165010	3.715188	-0.280052
6	2.274980	3.902576	0.072507
6	-0.281639	5.120117	-0.396253
6	2.128462	5.263942	-0.046292
6	0.861435	5.871511	-0.276649
1	-1.248766	5.584794	-0.576996
1	0.807951	6.954796	-0.362438
1	3.006206	5.903217	0.031653
1	3.250829	3.447606	0.236904
7	-0.003156	-0.769416	-0.273454
6	-0.837173	0.200230	-0.192992
6	-0.152970	-2.780717	-1.656853
6	-0.563581	-4.247520	-1.695851
6	-0.487945	-2.152509	-0.304878
6	0.059673	-5.031508	-0.547219
6	0.122258	-2.942720	0.852321
6	-0.296716	-4.407003	0.796848
1	-1.585560	-2.152179	-0.189438
1	-0.174417	-2.482743	1.805853
1	1.220955	-2.873816	0.800914
1	0.931430	-2.695321	-1.836160
1	-0.646034	-2.211820	-2.455181
1	-1.660449	-4.315444	-1.629458
1	-0.285972	-4.686132	-2.662949
1	0.172088	-4.960893	1.620725
1	-1.384664	-4.479210	0.952189
1	-0.260687	-6.081051	-0.579363
1	1.156639	-5.037604	-0.663678
1	2.690169	0.901864	0.681391
7	3.254691	0.096018	0.401904
7	2.617374	-0.799738	-0.379572
6	3.492429	-1.689120	-0.830244

1	3.166906	-2.513916	-1.452140
6	4.583562	-0.174673	0.427573
6	4.776397	-1.345386	-0.355873
6	5.644990	0.482857	1.064167
6	6.069320	-1.883714	-0.500576
6	6.899598	-0.068814	0.897230
6	7.112704	-1.237601	0.127788
1	6.234608	-2.781404	-1.092022
1	8.123421	-1.628257	0.034376
1	7.753162	0.409313	1.373526
1	5.484179	1.378683	1.658645

**TS10**

46	-1.034188	1.606970	-0.013840
1	0.322314	-2.015393	0.378004
17	-2.469733	3.510527	-0.452463
17	-0.498891	1.285103	-2.326610
6	-1.474678	1.828598	1.843954
7	-1.763612	1.982319	2.966749
6	-2.170631	2.234737	4.293185
1	-2.985085	2.964562	4.287504
1	-1.329079	2.633582	4.866784
1	-2.517825	1.305521	4.754320
7	1.706597	0.376562	0.110408
7	1.256491	0.128010	1.411312
6	2.024856	-0.812379	2.002281
1	1.790287	-1.165994	2.999060
6	2.774597	-0.456687	-0.086525
6	3.067604	-1.149552	1.127513
6	3.561351	-0.603763	-1.238190
6	4.201012	-1.990965	1.200229
6	4.644932	-1.450332	-1.142182
6	4.961832	-2.132036	0.062625
1	4.453320	-2.512369	2.120484
1	5.834519	-2.781497	0.079256
1	5.282448	-1.601163	-2.010723
1	3.318751	-0.068349	-2.152557
7	-0.277244	-1.228284	0.131017
6	0.142717	0.013931	0.371755
6	-1.425227	-2.690714	-1.462113
6	-2.778074	-3.078673	-2.048577
6	-1.586191	-1.580905	-0.430094
6	-3.767334	-3.475891	-0.959096
6	-2.565947	-1.979523	0.670773
6	-3.915257	-2.368066	0.077522
1	-1.956101	-0.677430	-0.933664
1	-2.675076	-1.148440	1.382297
1	-2.144072	-2.829655	1.232624
1	-0.968897	-3.569023	-0.974209
1	-0.733019	-2.364268	-2.249264
1	-3.180663	-2.223047	-2.612872

1	-2.649472	-3.893348	-2.772818
1	-4.603056	-2.672292	0.877276
1	-4.364236	-1.482179	-0.398173
1	-4.742915	-3.719889	-1.399178
1	-3.411522	-4.393230	-0.462282

**TS11**

N	-0.566861	-0.929349	-1.434155
N	0.665973	-1.208835	-0.863385
C	0.844427	-2.533775	-0.649840
H	1.783760	-2.905081	-0.256420
C	-1.164194	-2.149108	-1.551047
C	-0.309214	-3.184912	-1.072398
C	-2.449718	-2.433168	-2.035517
C	-0.727473	-4.533298	-1.099492
C	-2.837967	-3.757501	-2.037379
C	-1.989033	-4.797958	-1.577313
H	-0.069906	-5.326136	-0.752081
H	-2.349801	-5.823015	-1.611218
H	-3.826049	-4.019565	-2.411926
H	-3.098601	-1.641630	-2.405587
Pd	-2.355174	-0.443130	1.090795
Cl	-3.248053	-1.286797	3.163384
Cl	-0.232047	0.084825	2.045133
C	-4.084811	-0.817896	0.299338
N	-5.142716	-1.034250	-0.145709
C	-6.415373	-1.317624	-0.680771
H	-7.066658	-1.699058	0.110436
H	-6.319018	-2.071145	-1.468998
H	-6.846724	-0.403888	-1.100625
N	-1.674200	1.368688	-1.278755
C	-1.680710	0.371606	-0.576177
C	-3.761707	2.426223	-1.918505
C	-4.593963	3.701729	-1.863712
C	-2.459047	2.599034	-1.136836
C	-4.859774	4.131901	-0.425836
C	-2.731809	3.005250	0.308183
C	-3.556395	4.286633	0.348700
H	-1.868119	3.389716	-1.624745
H	-1.785589	3.125974	0.851967
H	-3.278768	2.190779	0.811078
H	-4.320923	1.590644	-1.465991
H	-3.539650	2.140431	-2.954678
H	-4.056430	4.504885	-2.391685
H	-5.535800	3.551589	-2.407168
H	-3.754139	4.565435	1.391238
H	-2.970458	5.111677	-0.087222
H	-5.431264	5.068800	-0.407019
H	-5.486348	3.373133	0.070188
Pd	3.448530	-0.764770	-0.023871
Cl	5.633343	-1.428838	0.714901

Cl	3.795851	-1.547837	-2.261876
C	3.111842	-0.204338	1.797118
N	2.957949	0.114478	2.908182
C	2.674787	0.507589	4.231282
H	3.609200	0.626962	4.786519
H	2.055520	-0.256613	4.709836
H	2.128521	1.455735	4.215187
N	1.324614	0.929707	-1.243357
C	1.654301	-0.221769	-0.731015
C	1.841527	2.811815	0.256524
C	2.455848	4.203464	0.335494
C	2.033266	2.223225	-1.139289
C	3.922095	4.186562	-0.079841
C	3.500736	2.180733	-1.546008
C	4.089506	3.586519	-1.470833
H	1.499179	2.859903	-1.859416
H	3.603464	1.753386	-2.550987
H	4.058319	1.520334	-0.863437
H	2.322749	2.143497	0.986550
H	0.772995	2.830147	0.509025
H	1.897213	4.883231	-0.327706
H	2.340704	4.600389	1.352146
H	5.148480	3.552391	-1.754623
H	3.589519	4.232576	-2.210688
H	4.341282	5.200556	-0.047447
H	4.497781	3.586496	0.643016
H	0.405719	1.000611	-1.691229

**TS12**

N	0.758573	-0.806620	-1.117440
N	-0.578649	-1.064032	-0.690064
C	-0.824519	-2.382476	-0.803959
H	-1.808060	-2.763359	-0.553518
C	1.272308	-2.027821	-1.502860
C	0.293419	-3.032589	-1.309096
C	2.537690	-2.334838	-2.016992
C	0.563696	-4.382587	-1.618294
C	2.779524	-3.666232	-2.304997
C	1.813666	-4.682010	-2.104603
H	-0.197106	-5.144835	-1.472865
H	2.068607	-5.708955	-2.353212
H	3.750746	-3.939218	-2.711752
H	3.284686	-1.566550	-2.202015
Pd	3.352970	-0.357809	0.217569
Cl	5.401576	-1.110434	1.272456
Cl	4.510116	0.721752	-1.600653
C	2.368966	-1.297576	1.595456
N	1.757577	-1.895775	2.390922
C	1.050268	-2.616975	3.375809
H	1.721588	-3.344321	3.841026
H	0.205972	-3.133526	2.910270

H	0.671657	-1.924505	4.132466
N	1.071593	1.420618	-0.616081
C	1.605666	0.265253	-0.567307
C	2.601131	2.620999	1.034725
C	2.911283	4.029766	1.532046
C	1.568619	2.688093	-0.082644
C	3.410668	4.911068	0.393304
C	2.052098	3.560704	-1.244588
C	2.401091	4.958682	-0.747370
H	0.663464	3.167975	0.332544
H	1.280206	3.603912	-2.025427
H	2.934323	3.076985	-1.688862
H	3.529569	2.168475	0.658687
H	2.233347	1.983166	1.850915
H	2.003171	4.474037	1.971865
H	3.654623	3.978834	2.337366
H	2.785048	5.560983	-1.580899
H	1.482397	5.458817	-0.399069
H	3.623253	5.925105	0.756843
H	4.363351	4.505965	0.016894
Pd	-3.206559	-0.856465	0.546300
Cl	-5.039093	-1.645968	1.889127
Cl	-1.726800	-0.543805	2.408356
C	-4.312802	-1.205393	-1.006073
N	-5.009184	-1.416787	-1.919619
C	-5.915019	-1.641250	-2.978088
H	-6.413167	-2.603853	-2.832763
H	-5.373994	-1.647313	-3.928280
H	-6.662357	-0.842390	-2.985841
N	-1.399072	1.087774	-0.841585
C	-1.638865	-0.117378	-0.471594
C	-3.624868	2.062162	-1.466929
C	-4.415742	3.365186	-1.433667
C	-2.309624	2.240208	-0.717279
C	-4.670184	3.812207	0.001530
C	-2.563237	2.638882	0.735789
C	-3.366475	3.934403	0.781374
H	-1.754408	3.056814	-1.204914
H	-1.612242	2.738334	1.276282
H	-3.119641	1.828562	1.233107
H	-4.213902	1.276700	-0.973180
H	-3.434068	1.732235	-2.497595
H	-3.854512	4.147132	-1.969456
H	-5.362833	3.237266	-1.973325
H	-3.563961	4.207007	1.825452
H	-2.760934	4.750786	0.355424
H	-5.213385	4.765909	0.014449
H	-5.319913	3.074840	0.499036
H	-0.237223	1.365195	-0.946187

TS13

7	-0.673086	-1.238164	-0.808107
7	0.455695	-1.262935	-1.645061
6	0.629348	-2.509949	-2.048939
1	1.486155	-2.754839	-2.663363
6	-1.176035	-2.543153	-0.696813
6	-0.360674	-3.361182	-1.510332
6	-2.245219	-3.075059	0.020531
6	-0.600328	-4.738179	-1.623016
6	-2.462819	-4.441778	-0.102634
6	-1.660388	-5.266369	-0.912139
1	0.043854	-5.360130	-2.239485
1	-1.872709	-6.331503	-0.962016
1	-3.276169	-4.888632	0.464943
1	-2.868945	-2.469774	0.673976
46	-2.900256	0.043236	0.646254
17	-4.828861	0.261190	2.067573
17	-1.369652	-0.031715	2.473241
6	-4.110544	-0.069850	-0.863983
7	-4.830443	-0.160218	-1.778908
6	-5.725020	-0.227486	-2.867549
1	-6.751082	-0.147625	-2.498651
1	-5.596583	-1.180722	-3.387989
1	-5.517554	0.596308	-3.556799
7	-0.813386	0.999066	-1.204048
6	-1.311951	-0.040020	-0.569982
6	-2.560436	2.828953	-1.407846
6	-2.708871	4.346157	-1.320154
6	-1.134123	2.437056	-1.038175
6	-2.342417	4.857697	0.069085
6	-0.765632	2.922970	0.357850
6	-0.931803	4.433503	0.458379
1	-0.460439	2.918567	-1.762175
1	0.263527	2.616072	0.585210
1	-1.414967	2.416941	1.088863
1	-3.264356	2.364237	-0.703178
1	-2.811276	2.458932	-2.411956
1	-2.057841	4.822078	-2.070951
1	-3.737390	4.628875	-1.577376
1	-0.695892	4.766003	1.477753
1	-0.202647	4.926153	-0.206338
1	-2.439775	5.950023	0.110810
1	-3.056205	4.450906	0.802917
46	2.616762	-1.172611	0.569175
17	3.609262	-2.015373	2.585425
17	3.399838	-3.040883	-0.697856
6	2.037938	0.338995	1.636395
7	1.771332	1.236469	2.332708
6	1.348749	2.254552	3.210112
1	1.713222	3.223706	2.853890
1	1.749925	2.059711	4.208803



1	0.253692	2.254114	3.248672
7	2.173519	0.549957	-1.925895
6	1.965320	-0.337246	-1.107063
6	2.739029	2.805444	-1.204693
6	3.801087	3.898235	-1.215681
6	3.255100	1.543128	-1.896674
6	5.103507	3.411930	-0.590990
6	4.549284	1.051845	-1.256087
6	5.604539	2.150175	-1.284958
1	3.454086	1.792237	-2.949931
1	4.900130	0.146033	-1.767780
1	4.345315	0.764267	-0.212479
1	2.477861	2.548082	-0.164904
1	1.815466	3.148898	-1.692369
1	3.988703	4.208020	-2.255708
1	3.422173	4.785455	-0.691154
1	6.527650	1.788296	-0.815121
1	5.860016	2.385687	-2.330697
1	5.864275	4.202253	-0.630829
1	4.933639	3.193325	0.476037
1	-0.026378	0.833104	-1.835622

**TS14**

Pd	-0.224151	-1.523940	-0.131986
Cl	-1.298886	-3.666968	0.007996
Cl	1.083076	-2.137689	-2.019530
C	-1.283151	-0.997893	1.410729
N	-1.959960	-0.665597	2.301516
C	-2.844578	-0.254353	3.319281
H	-3.344767	-1.129743	3.742614
H	-3.591290	0.422802	2.891790
H	-2.286666	0.262955	4.104692
N	-0.769317	1.579161	-0.529236
N	-0.386351	2.783466	-0.075315
C	-1.398587	3.590430	0.264138
H	-1.220683	4.595610	0.623360
C	-2.122784	1.592983	-0.454679
C	-2.572993	2.859161	0.036894
C	-3.034843	0.575275	-0.798106
C	-3.953790	3.107627	0.192646
C	-4.374041	0.845916	-0.623139
C	-4.831030	2.097893	-0.132724
H	-4.309655	4.070367	0.554308
H	-5.901523	2.259004	-0.023294
H	-5.107358	0.082199	-0.874534
H	-2.686097	-0.381600	-1.184876
N	1.696053	0.882369	-0.152704
C	0.709192	0.188363	-0.210607
C	3.925471	1.028580	-1.126957
C	5.403675	0.723396	-0.911132
C	3.104663	0.522652	0.053266

C	5.908251	1.309828	0.402493
C	3.588595	1.128776	1.366159
C	5.067786	0.824586	1.577923
H	3.180541	-0.574527	0.105095
H	2.984132	0.745942	2.198832
H	3.431034	2.218567	1.327399
H	3.772707	2.115492	-1.219052
H	3.560033	0.572997	-2.055418
H	5.549134	-0.368129	-0.903458
H	5.986680	1.106000	-1.758462
H	5.407722	1.281947	2.515928
H	5.199951	-0.262060	1.697209
H	6.964217	1.052347	0.556495
H	5.859196	2.409477	0.351979
H	0.614716	2.963263	-0.031413

**TS15**

Pd	-0.776487	-1.044553	0.459511
Cl	-2.833725	-2.220047	1.005112
Cl	-0.863447	-1.607505	-1.856540
C	-0.673322	-0.532800	2.317721
N	-0.643766	-0.225911	3.445649
C	-0.673435	0.098688	4.817936
H	-1.497060	-0.437083	5.297908
H	-0.820453	1.176040	4.936587
H	0.272179	-0.191822	5.284540
N	0.885155	1.341825	-0.109198
N	2.113502	1.864692	-0.389122
C	2.015305	3.171612	-0.525455
H	2.888895	3.771120	-0.749787
C	-0.044452	2.346450	-0.071948
C	0.664070	3.552008	-0.329327
C	-1.425054	2.326436	0.148948
C	-0.022820	4.777712	-0.356487
C	-2.070831	3.549886	0.112702
C	-1.384571	4.759704	-0.132261
H	0.507451	5.706352	-0.554055
H	-1.946424	5.690630	-0.149638
H	-3.146609	3.576939	0.272090
H	-1.961950	1.396294	0.326563
N	2.112670	-0.485019	-0.145963
C	0.910004	-0.075686	0.033663
C	3.350764	-2.258066	-1.270890
C	3.821888	-3.704427	-1.178923
C	2.502290	-1.883617	-0.059403
C	4.578288	-3.961248	0.119163
C	3.260160	-2.133512	1.243666
C	3.734476	-3.579633	1.330168
H	1.584539	-2.497250	-0.060579
H	2.614048	-1.878185	2.095822
H	4.125450	-1.451759	1.284354

H	4.221371	-1.582736	-1.310089
H	2.774125	-2.088329	-2.189270
H	2.947164	-4.371830	-1.229906
H	4.447033	-3.949700	-2.047364
H	4.297643	-3.733134	2.260086
H	2.857616	-4.243851	1.384911
H	4.884263	-5.013787	0.182889
H	5.506098	-3.366376	0.121785
H	2.705559	0.807623	-0.392912

**TS16**

Pd	-2.279532	-0.858273	-0.503757
H	1.410735	2.114108	-0.024352
Cl	-4.201960	-2.180119	-1.301905
Cl	-2.107297	0.455027	-2.503361
C	-2.278307	-1.943201	1.086207
N	-2.238317	-2.643590	2.023802
C	-2.216403	-3.509832	3.135325
H	-3.196470	-3.980800	3.253458
H	-1.973651	-2.942989	4.039185
H	-1.459495	-4.285411	2.981149
N	-0.885085	1.578355	0.371917
N	0.166913	2.452187	0.268225
C	-0.286513	3.682474	0.409552
H	0.399708	4.519179	0.342979
C	-2.043603	2.296952	0.582900
C	-1.681206	3.666406	0.621118
C	-3.373571	1.894974	0.763944
C	-2.653865	4.659615	0.826592
C	-4.311795	2.892822	0.958726
C	-3.963557	4.260141	0.990777
H	-2.373290	5.710300	0.851206
H	-4.742498	5.003260	1.146009
H	-5.354279	2.609325	1.089304
H	-3.666381	0.847472	0.737759
N	0.509364	-0.237695	0.374800
C	-0.677749	0.180454	0.176572
C	1.781491	-1.628703	-1.178320
C	2.203496	-3.051629	-1.522349
C	0.856839	-1.612986	0.040895
C	2.850973	-3.743518	-0.327762
C	1.510308	-2.303617	1.236489
C	1.925235	-3.727050	0.884086
H	-0.051003	-2.184134	-0.229092
H	0.821108	-2.289510	2.093370
H	2.403590	-1.733877	1.546284
H	2.672801	-1.017078	-0.963675
H	1.269339	-1.152738	-2.025479
H	1.317156	-3.624834	-1.836201
H	2.886364	-3.043325	-2.381965
H	2.405165	-4.207003	1.747531

H	1.023147	-4.319726	0.660058
H	3.129153	-4.774304	-0.583885
H	3.788390	-3.221636	-0.071493
H	2.441320	0.392425	1.193830
N	3.131952	0.998176	0.748547
N	2.629211	1.864745	-0.160335
C	3.615587	2.317145	-0.916568
H	3.420903	3.057640	-1.681736
C	4.463327	0.817603	0.530624
C	4.822813	1.686583	-0.533789
C	5.393695	-0.017531	1.162047
C	6.159623	1.739826	-0.969083
C	6.695253	0.051469	0.703095
C	7.077427	0.919983	-0.345308
H	6.453936	2.404017	-1.778673
H	8.117435	0.935192	-0.662846
H	7.451018	-0.582499	1.162491
H	5.106380	-0.681481	1.973826

**TS17**

7	-2.301450	0.090129	-0.415816
6	-2.661547	1.178273	-0.189753
46	-3.108609	2.992387	0.206267
17	-3.612113	5.235923	0.790139
17	-5.165666	2.187753	1.101778
6	-2.462498	3.791826	-1.863703
7	-2.894796	4.478992	-2.711794
6	-3.474137	5.351356	-3.657579
6	-0.215162	-1.105335	-0.653656
6	0.394337	-2.487359	-0.852990
6	-1.741631	-1.209705	-0.614173
6	-0.070370	-3.461688	0.223021
6	-2.216084	-2.164936	0.481015
6	-1.592100	-3.540125	0.275618
1	-3.758471	6.282402	-3.157758
1	-4.363173	4.882852	-4.088994
1	-2.755423	5.569400	-4.452789
1	-2.109857	-1.561539	-1.589458
1	-3.311221	-2.217673	0.477206
1	-1.914301	-1.752851	1.454974
1	0.125055	-0.674009	0.300389
1	0.091484	-0.413678	-1.449351
1	0.105864	-2.870631	-1.844372
1	1.488323	-2.405679	-0.858101
1	-1.919921	-4.211198	1.079025
1	-1.969520	-3.973335	-0.663973
1	0.356599	-4.456885	0.044679
1	0.309278	-3.128812	1.201631
7	0.098138	2.945429	-0.289844
7	-0.761890	3.252270	0.709211
6	-0.073502	3.215044	1.839413

1	-0.246087	2.995533	-1.243438
1	-0.576342	3.419113	2.777438
6	1.360882	2.743045	0.176398
6	1.287324	2.902414	1.584675
6	2.553105	2.414042	-0.480430
6	2.446795	2.732325	2.361970
6	3.673791	2.250403	0.313365
6	3.624386	2.407333	1.716601
1	2.413051	2.852857	3.443064
1	4.535860	2.269420	2.294719
1	4.622120	1.993537	-0.155119
1	2.593786	2.292431	-1.560724

**TS18**

7	-1.858500	-1.518532	-0.240824
6	-2.374269	-0.386652	-0.379090
46	-2.622469	1.389539	-0.636045
17	-2.617373	3.686071	-1.064491
17	-4.923153	1.273692	-1.183959
6	-2.034404	-3.254608	1.492823
6	-2.752269	-4.538461	1.906100
6	-2.556295	-2.805055	0.136761
6	-4.264602	-4.355086	1.906787
6	-4.059065	-2.594229	0.118554
6	-4.760623	-3.878510	0.546712
1	-2.247365	-3.505850	-0.650176
1	-4.385044	-2.277383	-0.880423
1	-4.311360	-1.781519	0.819365
1	-2.234605	-2.460848	2.226933
1	-0.948018	-3.401915	1.455119
1	-2.479217	-5.347792	1.211998
1	-2.393026	-4.842042	2.896711
1	-5.843796	-3.709652	0.559212
1	-4.575740	-4.659007	-0.207284
1	-4.759804	-5.294057	2.183064
1	-4.541859	-3.617199	2.675276
7	0.193980	0.431249	-0.363438
7	-0.602771	1.512670	-0.147489
6	0.044952	2.548195	0.411337
1	-0.820799	-1.464600	-0.336534
1	-0.462396	3.479300	0.625244
6	1.420939	0.820359	0.067841
6	1.381000	2.156001	0.574867
6	2.628610	0.089856	0.067521
6	2.548791	2.765634	1.077876
6	3.753553	0.708477	0.569765
6	3.717329	2.035311	1.071285
1	2.524895	3.784949	1.460275
1	4.633898	2.479312	1.455941
1	4.699857	0.169225	0.580500
1	2.665999	-0.926764	-0.321623

**TS19**

7	-0.244653	-1.281194	-0.219043
6	0.395992	-0.151454	-0.067107
46	0.035281	1.759660	-0.359949
17	-0.018756	4.152454	-0.476686
17	-1.183085	1.538563	-2.394096
6	-1.587357	-2.146018	-2.093824
6	-3.005974	-2.307586	-2.627617
6	-1.607293	-1.417026	-0.755581
6	-3.902878	-3.016889	-1.619748
6	-2.485868	-2.130723	0.265936
6	-3.901322	-2.292294	-0.278585
1	-1.970373	-0.393656	-0.908765
1	-2.486778	-1.572783	1.212497
1	-2.057615	-3.124325	0.479958
1	-1.123815	-3.136928	-1.955985
1	-0.961842	-1.587566	-2.801174
1	-3.418204	-1.310319	-2.847492
1	-2.985114	-2.851054	-3.580566
1	-4.522092	-2.824205	0.453684
1	-4.352115	-1.295412	-0.405713
1	-4.926642	-3.095972	-2.007723
1	-3.544084	-4.048662	-1.474871
7	1.620621	-0.125507	0.566051
7	1.966732	1.192300	0.845562
6	3.129824	1.164897	1.442626
1	3.593358	2.089776	1.764813
6	2.614303	-0.998423	0.995224
6	3.607373	-0.175291	1.573776
6	2.763409	-2.382366	0.906125
6	4.769806	-0.745047	2.105245
6	3.926731	-2.922230	1.438405
6	4.914523	-2.120901	2.034841
1	5.537000	-0.117284	2.552711
1	5.808386	-2.591710	2.437104
1	4.076752	-3.998343	1.384349
1	2.030706	-3.026546	0.427935
1	0.157535	-2.141910	0.151253
6	-1.443877	1.682380	1.597632
7	-2.618768	1.717787	1.518502
6	-4.013074	1.783429	1.311704
1	-4.500349	0.921117	1.777245
1	-4.219462	1.784208	0.235566
1	-4.409401	2.702162	1.753729

**TS20**

6	4.381750	2.348850	-2.314032
6	3.301998	2.966432	-1.720151
6	2.105032	2.233142	-1.607566
6	2.044789	0.903351	-2.105553
6	3.138612	0.278034	-2.717555

6	4.297183	1.023193	-2.805169
6	0.841049	2.471366	-1.032204
7	0.094415	1.385817	-1.177688
7	0.796242	0.440376	-1.839167
7	-2.258846	0.895263	-0.063451
7	-2.504769	-0.380232	0.320121
6	-3.694672	-0.507616	0.910054
6	-4.304536	0.761638	0.932567
6	-3.352968	1.614794	0.298534
6	-5.523403	1.288259	1.401914
6	-5.761459	2.636829	1.230435
6	-4.811624	3.477044	0.599091
6	-3.609369	2.988156	0.128707
46	-1.101984	-1.789150	-0.133645
17	0.665748	-3.239233	-0.806132
6	0.192972	-1.013789	1.072355
7	1.041205	-0.580118	1.750945
6	2.209950	-0.136202	2.445214
6	3.116013	-1.330541	2.748508
6	4.392546	-0.855256	3.432872
6	5.119213	0.193134	2.598388
6	4.207637	1.373615	2.286014
6	2.925508	0.919745	1.600285
17	-2.644778	-2.773627	-1.634296
1	1.866709	0.315994	3.387004
1	2.249463	1.764932	1.419845
1	3.156923	0.474214	0.619768
1	3.356820	-1.830169	1.798468
1	2.575786	-2.057148	3.367105
1	4.140352	-0.428734	4.416512
1	5.042417	-1.717334	3.627245
1	4.720268	2.105203	1.647781
1	3.953777	1.898492	3.220406
1	6.021027	0.536654	3.120825
1	5.458373	-0.263510	1.655373
1	-4.039663	-1.474599	1.254438
1	-6.258812	0.645974	1.884283
1	-6.696181	3.068448	1.583967
1	-5.040930	4.535233	0.481360
1	-2.883881	3.637477	-0.360277
1	-0.935589	1.182870	-0.760589
1	0.437099	3.339741	-0.526858
1	3.367349	3.984378	-1.342453
1	5.322843	2.885223	-2.412024
1	5.176540	0.577373	-3.265305
1	3.074954	-0.740281	-3.091847
1	0.398839	-0.490068	-1.959122

**TS21**

7	-2.852589	-1.838985	-0.163104
6	-3.425784	-0.776350	-0.080002

46	-4.857158	0.533014	-0.020519
17	-6.456260	2.327666	0.056528
17	-6.508916	-1.158901	-0.252788
6	-2.523040	-4.020917	-1.214382
6	-3.080576	-5.432661	-1.357732
6	-3.429857	-3.176838	-0.328303
6	-3.286500	-6.088662	0.002813
6	-3.613079	-3.817403	1.044508
6	-4.170568	-5.229028	0.899721
1	-4.418235	-3.072189	-0.801566
1	-4.277144	-3.191990	1.655057
1	-2.637008	-3.845377	1.553831
1	-1.520944	-4.054380	-0.758562
1	-2.409497	-3.540831	-2.194923
1	-4.044786	-5.388462	-1.888726
1	-2.411031	-6.037468	-1.983705
1	-4.282247	-5.688826	1.890487
1	-5.182934	-5.171750	0.469062
1	-3.721700	-7.090141	-0.116653
1	-2.307368	-6.230485	0.488620
7	-2.172755	0.796090	0.155161
7	-3.205685	1.695977	0.166445
6	-2.760829	2.949681	0.216895
1	-3.450754	3.784685	0.234901
6	-1.021094	1.515260	0.193226
6	-1.350983	2.907400	0.240599
6	0.318579	1.084946	0.197734
6	-0.322577	3.867338	0.300304
6	1.302292	2.052103	0.251062
6	0.987536	3.431718	0.303357
1	-0.559408	4.929923	0.341236
1	1.797830	4.158079	0.346033
1	2.348770	1.749656	0.253989
1	0.560751	0.024288	0.159115