Supporting Information for

Towards a quantitative understanding of palladium metal scavenger performance: an electronic structure calculation approach

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Table of Contents

Computational Method Evaluation:

Based on Binding Enthalpies (ΔH) and Energies (ΔE):

All data sets are presented here with three different metal systems **6**, **7** and **8** (see main text for numbering). We have calculated the binding enthalpies for scavenger ligand **9** according to Reaction (**1**) in Scheme 1 and presented in Table S1.

Table S1. Binding enthalpies (ΔH, in kcal/mol) with different functionals and basis sets.

Metal	M06-L	B97-D	B2PLYP	Av
		BS3		
6	-79.9	-74.2	-73.2	-75.8
7	-107.1	-109.0	-	-
8	-20.6	-18.5	-	-
		BS2		
6	-79.4	-73.9	-71.9	-75.1
7	-107.4	-108.9	-103.4	-106.5
8	-20.9	-18.6	-	-
		BS1		
6	-74.4	-70.0	-66.4	-70.3
7	-101.8	-105.3	-98.8	-101.9
8	-16.8	-13.4	-	-

Note: Frequency calculations could not be performed due to large memory requirement with the larger system size with B2PLYP functional for **7** and **8**.

Table S2. Binding energies (ΔE, in kcal/mol) with different functionals and basis sets.

Metal	M06-L	B97-D	B2PLYP	Av
		BS3		
6	-82.4	-77.9	-76.6	-79.0
7	-110.8	-113.2	-108.4	-110.8
8	-23.0	-20.8	-22.5	-22.1
		BS2		
6	-82.7	-77.6	-75.3	-78.5
7	-111.2	-113.1	-107.7	-110.7
8	-23.4	-20.9	-21.7	-22.0
		BS1		
6	-77.6	-73.7	-69.8	-73.7
7	-106.1	-109.5	-102.8	-106.1
8	-18.9	-15.8	-15.3	-16.7

Table S1 shows that ΔHs calculated for **6**, **7** and **8** with three different functionals and basis sets differ significantly. For **6** with BS3, ΔH is overestimated with M06-L by 6.0 kcal/mol compared to B2PLYP, whereas, B97-D produces a ΔH value which is closer to the B2PLYP

result. Similar results are found for BS1 and BS2 as well. With **6**, B97-D therefore appears to be the more accurate functional producing ΔH values in closer agreement with the more accurate B2PLYP method. Moving on to **7**, M06-L and B97-D turn out to be equally good with an uncertainty limit of approximately 2.0 kcal/mol. More precisely, M06-L is slightly better than B97-D for **7**. For **8** we could not calculate frequencies using the B2PLYP functional and therefore ΔH data at the same level could not be produced. Both M06-L and B97-D functionals produce ΔH around 2 kcal/mol uncertainty limits at three different basis set levels. Therefore, we can take both M06-L and B97-D, as both of them are equally effective in terms of binding enthalpies for Pd-metal system. It is important to note here that B2PLYP computational time is significantly larger compare to M06-L and B97-D.

In terms of basis sets used for main group elements, we need to choose one which is economic as well as capable of producing reliable results. With the results presented in Table S1, BS2 is able to produce reasonably good ΔH values at lower computational cost compared to the largest basis BS3. BS1 always produces ΔH values outside the >2.0 kcal/mol uncertainty limit and therefore should be discarded. To minimise computational cost and for the sake of accuracy, BS2 can be used as a good basis set for all calculations with palladium metal-ligand systems.

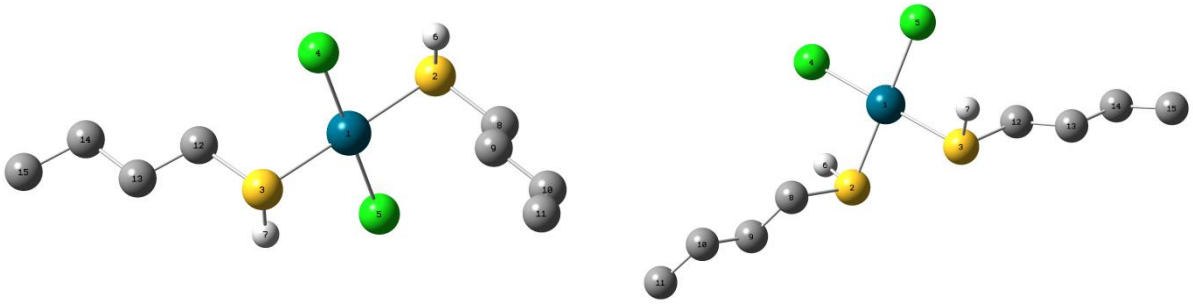
Due to the limitations of computer memory during frequency calculation for larger systems, we could not produce ΔH values with B2PLYP functional. Therefore, we decided to examine the binding energies (ΔE, kcal/mol) for all species with different functionals and basis set combinations described above. Table S2 presents binding energies using three different functional and basis sets. From the calculated binding energies presented in Table S2, it can be concluded that B97-D is better than M06-L for **6** and **8**. For **7**, B97-D and M06-L produces values within the theoretical error limit (~ 2.0 kca/mol). Therefore, B97-D in conjunction with BS2 can be chosen as a good level of theory for current systems considering accuracy and computational cost together. Table S3 summarises the performance of B97-D functional with different basis sets.

Table S3. Binding enthalpies (ΔH, in kcal/mol) at B97-D level with different basis sets.

	B97-D			
	BS1	**BS2**	**BS3**	**Av**
6	-70.0	-73.9	-74.2	-72.7
7	-105.3	-108.9	-109.0	-107.7
8	-13.4	-18.6	-18.5	-16.8

Based on Structural Parameters (interatomic distances are in Å and bond angles are in degrees)

6/9 complexes



cis-**6/9** *trans*-**6/9**

(Hydrogens on C-atoms are not shown for clarity; hydrogens on S-atoms are shown for thiols)

Figure S1. Geometry for *cis* and *trans* complexes of **6** with **9**.

Table S4. Optimised geometrical parameters for **6/9** *cis* and *trans* complexes with three different functionals.

Trans				***Cis***			
Parameters	**M06-L**	**B97-D**	**B2PLYP**	**Parameters**	**M06-L**	**B97-D**	**B2PLYP**
Pd(1)-Cl(4)	2.349	2.366	2.336	Pd(1)-Cl(4)	2.338	2.350	2.320
Pd(1)-Cl(5)	2.353	2.367	2.337	Pd(1)-Cl(5)	2.338	2.350	2.320
Pd(1)-S(2)	2.369	2.362	2.353	Pd(1)-S(2)	2.384	2.377	2.374
Pd(1)-S(3)	2.361	2.353	2.348	Pd(1)-S(3)	2.384	2.377	2.374
Cl(4)-Pd(1)-Cl(5)	178.9	179.7	179.9	Cl(4)-Pd(1)-Cl(5)	92.7	91.8	91.8
S(2)-Pd(1)-S(3)	179.2	179.5	178.8	S(2)-Pd(1)-S(3)	94.8	92.8	92.4
Cl(4)-Pd(1)-S(3)	89.7	89.2	89.2	Cl(4)-Pd(1)-S(3)	178.9	179.3	179.6
Cl(5)-Pd(1)-S(2)	90.3	89.8	89.8	Cl(5)-Pd(1)-S(2)	178.9	179.3	179.6

7/9 complex

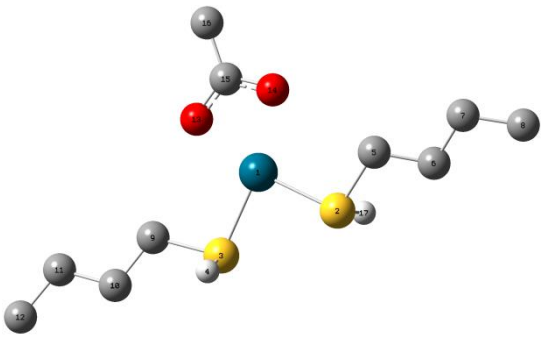


Figure S2. Geometry for complex of **7** with **9**.

(Hydrogens on C-atoms are not shown for clarity; hydrogens on S-atoms are shown for thiols)

Table S5. Optimised geometrical parameters for **7**/**9** complex with three different functionals.

Parameters	M06-L	B97-D	B2PLYP
Pd(1)−O(13)	2.098	2.108	2.080
Pd(1)−O(14)	2.097	2.108	2.080
Pd(1)−S(2)	2.349	2.340	2.342
Pd(1)−S(3)	2.348	2.337	2.341
O(13)−Pd(1)−O(14)	65.5	62.5	63.2
O(13)−Pd(1)−S(2)	165.1	164.9	165.8
O(14)−Pd(1)−S(3)	165.0	164.7	165.8
S(2)−Pd(1)−S(3)	92.2	92.7	91.5
O(13)−C(15)−O(14)	116.6	116.3	116.4

8/9 complex

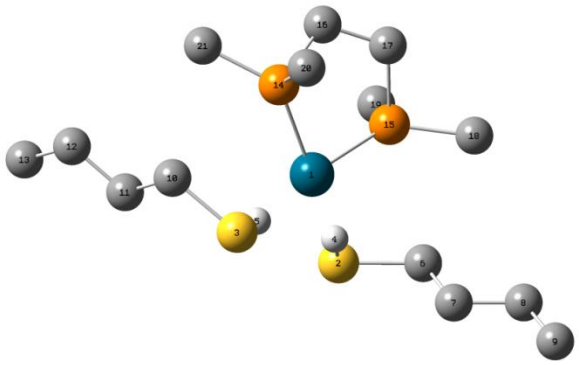


Figure S3. Geometry for complex of **8** with **9**.

(Hydrogens on C-atoms are not shown for clarity; hydrogens on S-atoms are shown for thiols)

Table S6. Optimised geometrical parameters for **8**/**9** complex with three different functionals.

Parameter	M06-L	B97-D	B2PLYP
Pd(1)−P(14)	2.297	2.306	2.319
Pd(1)−P(15)	2.308	2.306	2.319
Pd(1)−S(2)	2.670	2.543	2.522
Pd(1)−S(3)	2.588	2.556	2.522
S(2)−C(6)	1.828	1.855	1.838
S(3)−C(10)	1.830	1.854	1.838
P(14)−Pd(1)−P(15)	91.4	91.7	90.4
P(14)−Pd(1)−S(3)	119.1	117.8	121.8
P(15)−Pd(1)−S(2)	114.0	118.9	121.8
S(2)−Pd(1)−S(3)	99.3	97.2	91.8
P(14)−Pd(1)−S(2)	114.3	117.6	116.9
P(15)−Pd(1)−S(3)	119.7	115.3	116.9

From the geometrical parameters calculated for **6**, **7** and **8** in Table S4, S5 and S6 respectively with three different functionals in conjunction with BS2, it can be found that B97-D performs better than M06-L in most of the cases when B2PLYP is considered as best functional.

Finally, we have also tested our chosen functional (B97-D) and basis set (BS2) on the basis of known crystal structures taken from literature. The crystal structures chosen are similar to our S-coordinated complexes. The basic difference between the reference crystal structures and our metal-ligand systems is that the S-coordinated ligands are thiolates ($-S^-$) in crystal structures and that are thiols (-SH) in our systems.

Complex S1: $Pd^{II}(SCH_2Ph)_2(dppp)$ [dppp = 1,3-bis(diphenylphosphino)propane][1]. Firstly we built Complex S1 in its trimmed version (–Ph groups are trimmed to –Me) based on its crystal structure. Then Complex S1 is optimized followed by a frequency calculation using both M06-L and B97-D functionals in conjunction with BS2 basis set. Starting from the optimized structure of Complex S1, the full complex is then reconstructed with –Ph groups. Finally the full system for Complex S1 is optimized followed by a frequency calculation at the same level of theories. Figure S4 shows a structural comparison between methods and crystal structure.

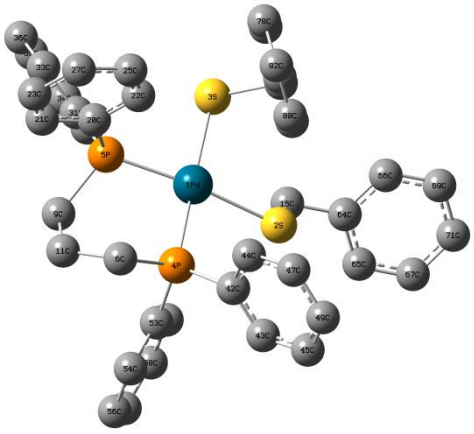


Figure S4. Geometry for $Pd^{II}(SCH_2Ph)_2(dppp)$ [*square planar*] complex (**Complex S1**). (Hydrogens on C-atoms are not shown for clarity)

Table S7. Optimised geometrical parameters for $Pd^{II}(SCH_2Ph)_2(dppp)$ complex with two different functionals along with experimental values.

Parameter	M06-L	B97-D	Experimental
Pd(1)-P(5)	2.310	2.305	2.283
Pd(1)-P(4)	2.304	2.302	2.285
Pd(1)-S(2)	2.411	2.419	2.372
Pd(1)-S(3)	2.402	2.415	2.355
P(5)-C(9)	1.850	1.870	1.834
P(5)-C(20)	1.818	1.828	1.829
P(5)-C(31)	1.821	1.831	1.819
P(4)-C(6)	1.843	1.863	1831
P(4)-C(42)	1.816	1.828	1.824
P(4)-C(53)	1.820	1.830	1.823
S(2)-C(15)	1.843	1.862	1.831

S(3)-C(18)	1.838	1.857	1.846
P(5)-Pd(1)-P(4)	91.1	91.5	92.8
P(5)-Pd(1)-S(3)	88.6	88.3	86.2
P(4)-Pd(1)-S(2)	84.0	85.4	86.7
S(2)-Pd(1)-S(3)	96.3	95.2	94.4
P(5)-Pd(1)-S(2)	172.8	172.3	174.0
P(4)-Pd(1)-S(3)	176.2	175.0	178.9
C(20)-P(5)-C(31)	107.1	107.7	107.3
C(42)-P(4)-C(53)	106.8	107.0	107.8
Pd(1)-S(2)-C(15)	104.9	103.2	100.0
Pd(1)-S(3)-C(18)	101.6	101.0	109.5

Complex S2 and S3: We have also selected two other Pd^{II}-complexes, **$Pd^{II}(PPh_3)_2(Imt)_2$** [Imt = Imidazolidine-2-thione][2] (Complex S2) and **$Pd^{II}(PPh_3)_2(Dmtu)_2$** [Dmtu = N,N′-dimethylthiourea][3] (Complex S3), from the crystal structure database and studied these at the B97-D/BS2 level to test the ability of our chosen method to reproduce their geometries. Natural Bond Orbital (NBO) charges are calculated at the same level to compute the group charges on PPh_3, Pd and Imt/Dmtu. Figure S5 and S6 displays the optimized geometrical parameters for these two complexes along with the NBO group charges on the respective groups.

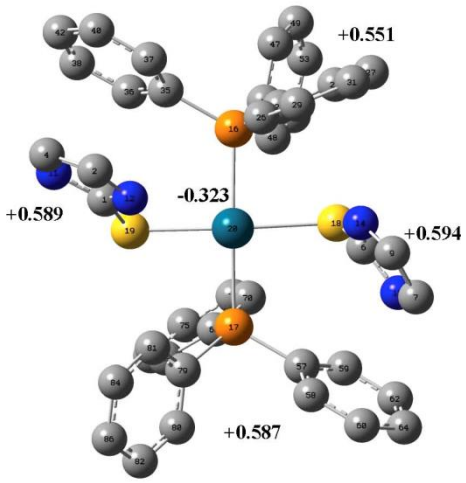


Figure S5. Geometry for $Pd^{II}(PPh_3)_2(Imt)_2$ [*square planar*] complex (**Complex S2**) with NBO group charges.
(Hydrogens on C and N-atoms are not shown for clarity)

Table S8. Optimised geometrical parameters for $Pd^{II}(PPh_3)_2(Imt)_2$ complex with B97-D functional along with experimental values.

Parameters	**PMe_3**	**PPh_3**	**Experimental**
P(16)-Pd(20)	2.395	2.387	2.344
P(17)-Pd(20)	2.395	2.391	2.365
S(18)-Pd(20)	2.402	2.423	2.339
S(19)-Pd(20)	2.402	2.408	2.324

C(1)-S(19)	1.718	1.711	1.714
C(6)-S(18)	1.718	1.722	1.705
P(16)-Pd(20)-P(17)	168.6	173.0	175.1
S(18)-Pd(20)-S(19)	175.3	166.9	159.5
P(16)-Pd(20)-S(19)	92.7	92.0	91.2
P(16)-Pd(20)-S(18)	86.7	86.5	87.1
P(17)-Pd(20)-S(19)	86.7	88.2	89.7
P(17)-Pd(20)-S(18)	92.7	91.5	90.2

We have also examined the trimmed version (L=PMe_3) to reveal the effect of phosphine ligand size on geometry. We have started our optimizations with B97-D/BS2 from the crystal structure and no significant changes are found due to –PMe_3 except the angle S(18)-Pd(20)-S(19). The similar observations were also made with the other complex $Pd^{II}(PPh_3)_2(Dmtu)_2$.

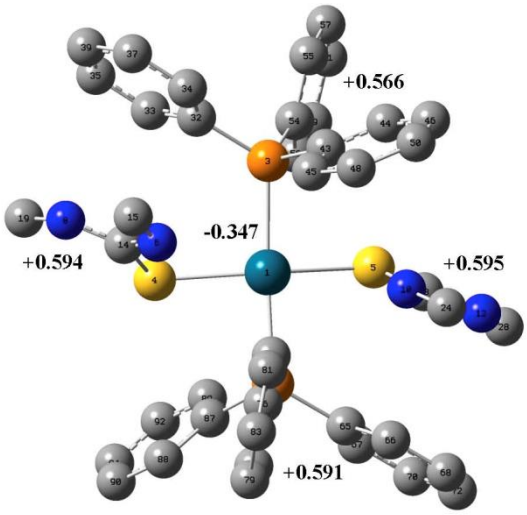


Figure S6. Geometry for $Pd^{II}(PPh_3)_2(Dmtu)_2$ [*square planar*] complex (**Complex S3**) with NBO group charges.
(Hydrogens on C and N-atoms are not shown for clarity)

Table S9. Optimised geometrical parameters for $Pd^{II}(PPh_3)_2(Dmtu)_2$ complex with B97-D functional along with experimental values.

Parameter	**PMe_3**	**PPh_3**	**Experimental**
P(2)-Pd(1)	2.387	2.382	2.353
P(3)-Pd(1)	2.387	2.374	2.360
S(4)-Pd(1)	2.399	2.399	2.336
S(5)-Pd(1)	2.399	2.403	2.323
P(2)-Pd(1)-P(3)	174.4	170.0	177.2
S(4)-Pd(1)-S(5)	172.2	159.8	149.0
P(2)-Pd(1)-S(4)	87.0	88.9	86.7
P(2)-Pd(1)-S(5)	92.5	91.8	91.6
P(3)-Pd(1)-S(4)	92.5	93.9	92.6
P(3)-Pd(1)-S(5)	87.0	88.7	87.5

For complex $Pd^{II}(PPh_3)_2(Dmtu)_2$, the angle S(4)-Pd(1)-S(5) deviates significantly when we move from –PMe_3 to −PPh_3, which is similar to what we observed with former complex. The

NBO group charges on both of the complexes show that charges are symmetrically distributed over the whole complex with a negative charge on the metal centre.

With an overall view on geometrical parameters calculated using three different functionals, it can be observed that B97-D appears to be slightly better than M06-L in producing geometrical parameters considering B2PLYP as the best functional. In summary, there is no significant structural difference between three different functionals chosen and in particular, B97-D is slightly better than M06-L in producing accurate geometry. This is further confirmed with the help of crystal structure (Complex S1) where we find both of the functionals can produce atomic distances within 0.05Å uncertainty compared to crystallographic data. This small uncertainty may be due to the fact that theoretical methods are not capable of accounting crystal-packing effects in this case. Therefore, our chosen functional B97-D in conjunction with BS2, on the basis of binding enthalpies (ΔH) and energies (ΔE), appears to be suitable for further investigation of a wider range of complexes.

Binding parameters (ΔH, ΔG and TΔS) for full set of ligands

Table S10. Binding enthalpies (ΔH, kcal/mol), free energies (ΔG, kcal/mol) and entropies (ΔS, kcal/mol) for full set of ligands with different binding modes to **6**, calculated at B97-D/BS2 level of theory.

Complexes	**ΔH**	**ΔG**	**TΔS**
6/9	-73.9	-50.8	-23.1
Type 10			
6/10a	-82.7	-59.4	-23.3
6/10b	-71.7	-51.5	-20.3
6/10c	-60.1	-46.1	-13.9
6/10d	-65.8	-51.5	-14.3
Type 11			
6/11a	-82.5	-57.4	-25.1
6/11b	-70.1	-55.5	-14.7
Type 12			
6/12a	-82.6	-56.8	-25.8
6/12b	-74.6	-50.9	-23.7
6/12c	-60.2	-44.4	-15.8
Type 13			
6/13a	-76.4	-52.2	-24.3
6/13b	-44.4	-31.8	-12.6
6/13c	-61.1	-48.0	-13.1
6/13d	-58.7	-46.1	-12.5
6/13e	-51.5	-36.7	-14.8
Type 14			
6/14a	-82.3	-55.8	-26.4
6/14b	-46.6	-33.2	-13.3
6/14c	-54.6	-39.4	-15.3
6/14d-*cis*	-73.1	-55.6	-17.5
6/14d-*trans*	-74.2	-54.1	-20.1
Type 15			
6/15a	-78.7	-54.1	-24.6
6/15b	-44.9	-32.9	-12.0
6/15c	-53.8	-39.3	-14.5
6/15d-*cis*	-72.2	-54.9	-17.3
6/15d-*trans*	-77.8	-60.1	-17.7
6/15e-*cis*	-67.9	-49.9	-18.1
6/15e-*trans*	-87.8	-69.5	-18.2
Type 16			
6/16a	-83.6	-57.7	-25.9
6/16b	-70.6	-54.7	-15.9
6/16c	-59.8	-44.8	-15.0
Type 17			
6/17a	-40.8	-28.1	-12.6

6/17b	-36.6	-23.9	-12.6

Note: Popular commercial set of ligands are coloured in red

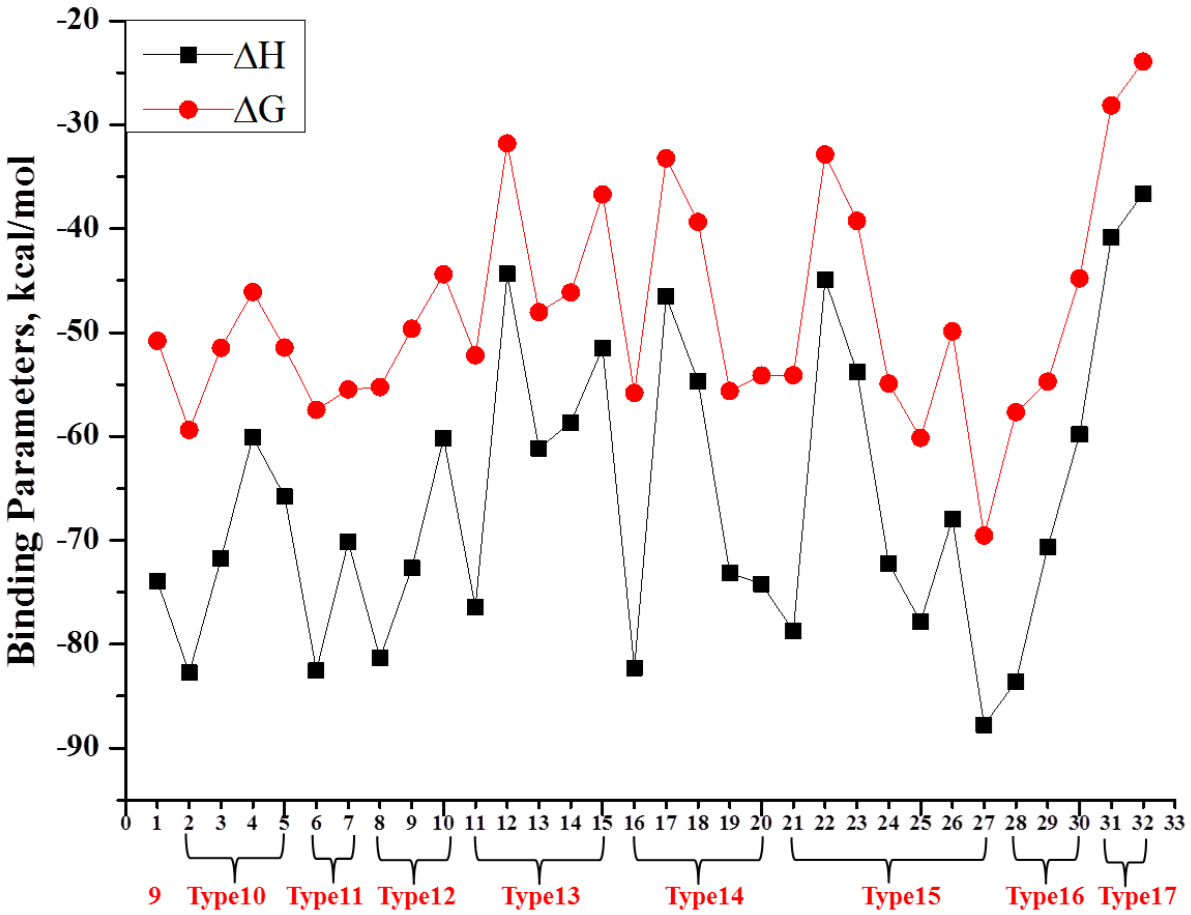


Figure S7. Variation of binding parameters (ΔH and ΔG) with metal-ligand complexes for all ligands (***9*** to ***17***)

Table S11. Binding enthalpies (ΔH, kcal/mol), free energies (ΔG, kcal/mol) and entropies (ΔS, kcal/mol) for full set of ligands with different binding modes to **7**, calculated at B97-D/BS2 level of theory.

Complexes	**ΔH**	**ΔG**	**TΔS**
7/9	-108.9	-86.5	-22.4
Type 10			
7/10a	-121.9	-98.9	-22.9
7/10b	-110.5	-88.7	-21.8
7/10c	-102.7	-88.4	-14.3
Type 11			
7/11a	-125.1	-101.4	-23.6
7/11b	-113.3	-98.7	-14.5
Type 12			
7/12a	-121.7	-97.3	-24.3
7/12b	-111.7	-87.8	-23.8
7/12c	-104.3	-88.9	-15.3
Type 13			
7/13a	-120.6	-94.1	-26.4
7/13b	-94.4	-80.5	-14.0
7/13c	-89.6	-74.8	-14.8
Type 14			
7/14a	-128.0	-101.2	-26.8
7/14b	-97.9	-84.1	-13.8
7/14c	-95.6	-80.4	-15.2
Type 15			
7/15a	-127.3	-103.0	-24.3
7/15b	-97.3	-84.2	-13.2
7/15c	-94.8	-80.3	-14.5
7/15d	-121.3	-103.9	-17.5
7/15e	-128.5	-110.9	-17.6
Type 16			
7/16a	-132.8	-106.4	-26.4
7/16b	-109.4	-93.4	-16.0
7/16c	-117.5	-102.0	-15.5
Type 17			
7/17a	-85.5	-72.1	-13.4
7/17b	-81.8	-68.6	-13.2

Note: Popular commercial set of ligands are coloured in red

Decomposition of complexation energies

Table S12. Ligand strain energies (ΔE_{strain}^{L}, kcal/mol) and complexation energies ($\Delta E_{complex}$, kcal/mol) for ligands **10-17** complexing with **6**.

Complexes	ΔE_{strain}^{L}	$\Delta E_{complex}$
Type 10		
6/10c	2.5	-62.2
Type 11		
6/11b	3.7	-72.4
Type 12		
6/12c	5.5	-62.1
Type 13		
6/13b	9.2	-45.9
6/13e	12.2	-53.4
Type 14		
6/14b	9.9	-48.1
6/14c	9.2	-56.4
6/14d-*cis*	2.5	-76.1
6/14d-*trans*	2.7	-76.6
Type 15		
6/15b	11.5	-46.3
6/15c	11.3	-55.5
6/15d-*cis*	6.3	-75.2
6/15d-*trans*	5.6	-80.3
6/15e-*cis*	8.8	-70.7
6/15e-*trans*	4.6	-90.5
Type 16		
6/16b	5.8	-72.5
6/16c	10.1	-61.7

Structural changes during optimisation

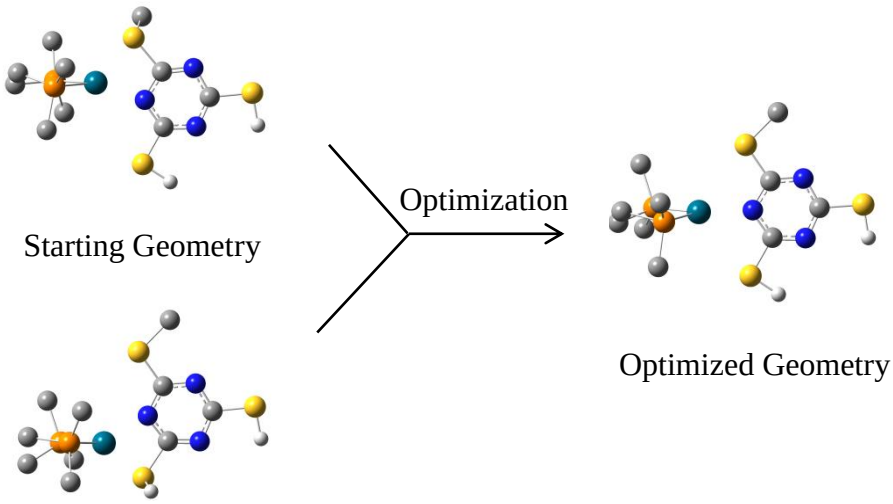


Figure S8. Structural change of **8/17a** and **8/17b** during optimization

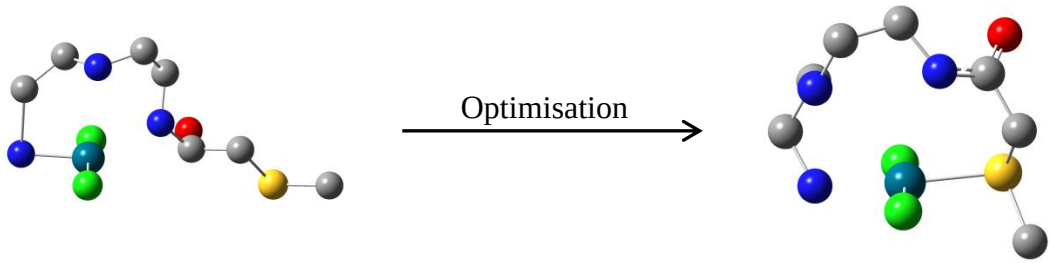


Figure S9. Structural change of **6/15g** during optimization

Optimised Cartesian coordinates at B97-D/BS2 level of theory for popular commercial set of ligands and their metal complexes.

Metals

6

Pd,-1.953604372,-0.0020577743,0.0016640331
Cl,-3.3952296133,1.6947190705,-0.0494146285
Cl,-3.3867007848,-1.7038918133,0.1013615869

7

Pd,-1.0344559183,0.001896811,0.0141865163
O,0.684543149,-1.0674715654,-0.0094305494
O,0.6869879465,1.0683042338,-0.0087025185
C,1.420790411,-0.0002832123,-0.0088819586
C,2.8883085634,-0.0020584402,0.0121496145
H,3.223770539,-0.0207341813,1.0617715565
H,3.266976247,-0.8993224141,-0.4967928987
H,3.2690210625,0.9107097683,-0.466627762

8

C,2.0430445887,0.6950374486,-0.3485020329
C,2.0464659151,-0.6862196767,0.3489521248
H,2.937726501,1.2706517413,-0.0609240602
H,2.0704335498,0.5635210107,-1.4404466596
H,2.0724001905,-0.5545586574,1.4409147767
H,2.9443880269,-1.2570805274,0.0619979635
Pd,-1.0079842148,-0.0036868146,-0.0008762
P,0.4856926407,1.7193088297,0.0282111759
P,0.494829021,-1.7187419914,-0.0288279129
C,0.8382912094,3.2018617057,-1.0603233019
H,0.1024171205,3.9882559164,-0.8462319103
H,1.8524689484,3.5981565996,-0.8921889706
H,0.7327676664,2.9070451151,-2.1126732035
C,0.9518710027,2.4111006452,1.6989447392
H,1.9482632895,2.8800622067,1.6756559135
H,0.2063171112,3.1553872594,2.0079631789
H,0.9468453042,1.5968337377,2.4344601141
C,0.8545024691,-3.1993653695,1.060018484
H,0.1229648035,-3.9896596825,0.8454271939
H,1.8708891746,-3.5902811096,0.892631838
H,0.7466567802,-2.9050753462,2.1122802922
C,0.965858013,-2.4081196609,-1.6991984191
H,1.9647147479,-2.8717718838,-1.6751846006
H,0.2244925706,-3.1563779096,-2.0087022012
H,0.95701683,-1.5939266065,-2.4347594719

Ligands

9

C,-3.0277613131,-0.3842135027,-0.0007113263
C,-1.771430099,0.5014449871,0.0215799166
H,-3.9429480797,0.2162585275,0.0962663205
H,-3.0887766595,-0.9494777675,-0.9422530965
H,-3.0070575966,-1.1100079362,0.8255751512
C,-0.4769229159,-0.3203421168,-0.1153866048
H,-1.8200637566,1.2367818609,-0.7972790604
H,-1.739098497,1.0780553954,0.9598056877
C,0.7724433322,0.5667995886,-0.079333153
H,-0.4258055469,-1.0583078946,0.7012691489
H,-0.493670624,-0.889647917,-1.0565155379
H,0.7500696521,1.2923670401,-0.9035937415
H,0.8227872512,1.13326105,0.8599249733
S,2.3657173636,-0.3479219179,-0.3185525277
H,2.2266481591,-1.1667306169,0.7495962796

10

C,-3.9006432533,0.7696918961,0.0000303794
H,-4.4076607065,1.7417840982,-0.0000730267
H,-4.1925214846,0.211931377,-0.8996411207
H,-4.1924812991,0.212145541,0.8998477271
C,-1.4961017882,-0.6369693098,0.000180736
C,0.0324390012,-0.6622572,0.0001150117
H,-1.8846110417,-1.1433085939,0.8949399365
H,-1.8846922497,-1.1435682766,-0.8943966297
S,-2.0980307598,1.1106143285,-0.0000496868
H,0.4222982122,-0.1593595148,0.8924259481
H,0.4222221679,-0.1596265117,-0.8923792531
H,-0.4792568295,-3.0350871997,0.0003368041
S,0.7136612911,-2.3996168142,0.0003683041

12

C,-3.7796007567,0.6098926162,0.1601675101
H,-4.3775621762,1.528970522,0.1640645281
H,-4.0604456041,0.0029295958,-0.7109273065
H,-3.975093014,0.0508999613,1.0850446375
S,-2.0198676627,1.1156499648,0.0632632537
C,-1.2498593797,-0.5592108956,0.0742264621
C,0.2804727826,-0.4515487158,0.0004612247
H,-1.6324564505,-1.127967276,-0.7861118468
H,-1.5500580967,-1.0782202006,0.9964860638
C,0.9139207111,-1.8500275384,0.0103061427
H,0.5707041493,0.0814464413,-0.9161894089
H,0.6526085656,0.1310284672,0.855254407
H,0.6440248129,-2.3798320067,0.9329272643
H,0.5612404229,-2.429907301,-0.8523189855
H,3.0290145286,-3.0210933545,-0.0544938789
S,2.7631542274,-1.6953780701,-0.0797672874

15

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C,0,-3.4020153741,-0.7957647421,-0.1521375636
C,0,-2.0303871981,-1.1217379839,0.4449093097
H,0,-3.6863716589,-1.4957915048,-0.9489960039
H,0,-4.1472851326,-0.8288338324,0.6502969851
C,0,0.2861961686,-1.7865988073,-0.1047663108
H,0,0.340228379,-2.0865064031,0.9492659268
H,0,0.73240536,-2.5792645559,-0.7178632079
C,0,-3.1179600516,1.9073813916,0.557357263
H,0,-3.9680437236,1.826466791,1.2465022343
H,0,-2.1987522322,1.5992429693,1.0669531676
H,0,-3.0257818624,2.9421802342,0.2065700431
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C,0,3.2712761124,0.5431201542,-0.1817143811
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H,0,5.2594532678,2.2436854395,0.5772507815
H,0,6.5131605941,1.3111835724,0.1189389918

17

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C,-1.7400588498,0.5868843534,-0.3425566059
N,0.9207940769,0.8183793276,-0.0200766877
N,-1.219801066,1.8220385647,-0.4407401075
N,-1.0532637083,-0.5457126585,-0.0977852512
S,1.1949824388,-1.8283244086,0.3752064431
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H,2.384338373,-1.1890644473,0.4465482983
C,-4.0477280327,2.06338705,-0.8497910109
H,-5.1332270458,1.9889633674,-0.9840824616
H,-3.8107422433,2.7020272522,0.0065696365
H,-3.5767893844,2.4633787169,-1.7529064806
S,0.8224163828,3.4794929312,-0.3939156767
H,2.0888673322,3.0622464924,-0.1692835889

Complexes

6/9-*cis*

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S,0.9305767531,4.8801269843,0.7994959392
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Cl,-1.3833016044,2.608242723,1.2564852985
Cl,0.6752184365,0.2188985077,0.052396639
H,0.0001609062,4.9005509678,1.788128417
H,2.8442915137,1.335924454,-1.1713112446
C,-0.2123944653,5.5132334606,-0.528347003
C,-0.7185310599,6.9281462643,-0.2410243183
H,-1.0294711481,4.7869426285,-0.5911049145
H,0.3822435811,5.4713301197,-1.4492322298
C,-1.638952362,7.4216339048,-1.3736242225
H,-1.277941558,6.9308578818,0.7071560645
H,0.1285305398,7.6210834856,-0.1231187984
C,-2.1860475872,8.8311134165,-1.0968983548
H,-1.0796887288,7.4169426543,-2.3223057365
H,-2.4728639324,6.7134068958,-1.4932204858
H,-2.8405388926,9.1682643336,-1.9120467138
H,-2.7680747863,8.84630168,-0.1640892199
H,-1.3655099629,9.5565168493,-0.9956239408
C,3.9012453699,1.5330810431,0.980587625
C,5.2195695324,0.8974374502,0.5348722135
H,3.1847861414,0.7880949783,1.3421548158
H,4.0561303117,2.2939619424,1.755474927
C,5.9091736424,0.1824917082,1.712492164
H,5.0215650698,0.1680082265,-0.2655798702
H,5.8928883571,1.6632368595,0.1204236619
C,7.2234782614,-0.4908403328,1.2861809362
H,6.1052491598,0.9119711196,2.5138724537
H,5.2215224206,-0.5692518095,2.1288045048
H,7.7022039712,-0.9967067637,2.1355440807
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6/9-*trans*

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Cl,-0.3856650273,0.799653326,-2.2922221773
Cl,-0.2122633386,2.2192710961,2.2204338893
H,-1.9333726084,3.0788860192,-1.7929624482
H,1.1993888412,-0.1354230506,1.7754204063
C,-2.9802799395,3.403071761,0.378570627
C,-3.6895476923,2.0542683862,0.2625294582
H,-3.6164035423,4.2355516215,0.0488517463
H,-2.6427246028,3.588054568,1.4046482982
C,-4.9577117815,2.0114906492,1.1324022329
H,-3.9494759975,1.8552588124,-0.7887063313
H,-2.9964156947,1.2607842425,0.5767429386
C,-5.6681641383,0.6516778519,1.0361827244
H,-4.681460033,2.2138610913,2.1787283069
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H,-5.6451999864,2.8148711657,0.8227285194
H,-6.5663608739,0.6271832067,1.6683570828
H,-5.9730096706,0.442294544,0.0004123539
H,-4.9987922875,-0.1580459502,1.3603800991
C,2.4777812425,-0.2361081482,-0.29291261
C,3.492934177,-1.3070298321,0.1139747752
H,2.817197421,0.7738516094,-0.0385874818
H,2.2457143141,-0.2665426716,-1.3633533783
C,4.8327427248,-1.1025777246,-0.6184538094
H,3.6635034596,-1.269373053,1.2013458506
H,3.0951349813,-2.3063560097,-0.1178283999
C,5.8744559446,-2.1596582518,-0.2183509389
H,4.6584806278,-1.1406620201,-1.7047560192
H,5.2175597053,-0.0955242445,-0.3944520094
H,6.8233355,-2.0007410518,-0.7484933986
H,6.0765507309,-2.119294055,0.8619631793
H,5.515620523,-3.1713958004,-0.4572582978

6/10a

Pd,-0.2425008397,0.797406329,-0.6273105112
S,-1.6361917666,2.6359312358,-1.199444063
S,1.2253685847,-0.9887573379,-0.1133158521
Cl,-1.0387910629,-0.5260171634,-2.4034307837
Cl,0.5257115505,2.0864570429,1.2255915961
C,-2.6311692821,2.9023546071,0.3442107702
C,-3.1530402126,1.6046477959,0.9595202815
H,-3.4478747748,3.5844733564,0.076386451
H,-1.9373808344,3.4052866565,1.0240010287
C,2.8750033612,-0.1723595941,0.0647737683
C,3.9583715179,-1.1966684848,0.4112981324
H,2.7752807093,0.6165477711,0.8178777099
H,3.0612867193,0.2907138061,-0.9109683944
C,0.8499575079,-1.3671498597,1.6439523962
H,1.5541895119,-2.1270297609,2.0018911402
H,0.9079441661,-0.4470689614,2.2337872438
H,-0.16885761,-1.7682229652,1.6601476295
C,-2.9642446994,2.0678365759,-2.3264663026
H,-3.4132469849,1.140271554,-1.9628828673
H,-3.7003213829,2.8783551617,-2.3984226452
H,-2.4986439741,1.8773101421,-3.2966823229
H,-3.1071291317,2.3749239782,3.2300943348
H,3.7379441753,-1.6872905831,1.366687227
H,4.0361882062,-1.9522788283,-0.3789442694
H,-2.3169269781,0.9377900971,1.1959314159
H,-3.834790688,1.0816220533,0.2797214443
H,6.3449424637,-1.4015410607,0.6634716431
S,5.5780804232,-0.2929625275,0.5563524999
S,-4.145156545,1.9297882341,2.4852231589

6/10b

Pd,-0.021724309,-1.4625838401,0.0088769809
S,-2.3440802596,-1.4664192644,-0.3569511579
S,2.2993369792,-1.5417248449,0.3743397717

Cl,0.372461963,-1.3751356623,-2.3209379299
Cl,-0.4133722711,-1.3849103552,2.3394736359
H,-2.318451869,-1.2275294235,-1.6939923053
H,2.2809081744,-1.3146082581,1.7135493507
C,-2.8193814422,0.2529408019,0.1742217329
C,-4.3105420466,0.5020964263,-0.053352241
H,-2.187390414,0.9548876054,-0.3793898305
H,-2.5488400187,0.2841920683,1.2348433944
H,-4.5649834194,0.4017583519,-1.1180410675
H,-4.9090920919,-0.2140815267,0.5256663673
C,2.8278098169,0.1669290718,-0.1408741772
C,4.3259323324,0.3676004185,0.0888701342
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H,2.5585681463,0.2164056295,-1.2011334822
H,4.5769160877,0.2495835696,1.1525668492
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C,-6.5324315386,2.157700698,0.1929568751
H,-6.9320082182,3.1364902068,0.4831800784
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H,-7.0058197104,1.3795910757,0.8056670294
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H,7.0279768288,2.9242656784,-0.4233664692
H,6.804362351,1.7656745571,0.9193468314
H,7.0473564563,1.1689403468,-0.7618751116

6/10c

Pd,0.1289259725,0.7342750921,-0.5138624173
S,-1.1747156687,-1.1109159622,-1.1677097914
S,1.8198550657,-0.7319196589,0.2293435016
Cl,-1.638539578,2.1328350149,-1.1482820418
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H,2.3108747984,-1.2906497533,2.5425038726
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H,0.585737205,-0.7702104173,2.339339137
C,1.0247756217,-2.3875443367,-0.0712905773
C,-0.4985299539,-2.3672226409,0.0456375968
H,1.3422240974,-2.6743251229,-1.0818058726
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H,-0.9163045587,-3.3517533879,-0.2008635008
H,-0.8171819966,-2.0727760538,1.0505133231
H,-2.3119811226,-0.8087207437,-0.4964008286

6/10d

Pd,-0.5250627506,0.0078965609,-0.1695786348
S,0.6894006016,-2.00139081,-0.0593547353
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H,-0.870871078,-3.1288123729,1.332822887
H,0.814887247,-3.6890164472,1.6766044127
H,0.2090950038,-2.1029687269,2.319742666

6/12a

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Cl,-0.9798317961,-0.0778357457,-2.9304281045
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H,-3.2982347309,1.6529736861,-2.6052523402
H,-3.5153248746,3.4244840792,-2.9333615306
H,-2.2688926881,2.4604425064,-3.8099427749
C,0.6570087577,-1.1221883681,1.2235390406
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H,0.7657105048,-0.2246864739,1.8400390572
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H,3.8642117597,-1.8773723767,-0.4660027682
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C,-4.1121475848,2.192751925,1.6230419089
H,-4.8714940149,2.9713838332,1.4726800458
H,-3.4213106222,2.5086842634,2.4144380269
H,-5.4935167247,1.1016888523,3.2794967931
C,5.1947608424,-0.3517224993,0.3134075105
H,5.1641980642,0.517317927,0.9826819941
H,5.522500007,-0.0008424627,-0.6738139004
H,6.0373373404,-1.7234818664,2.1032256319
S,6.5343606,-1.5008104751,0.8645607329
S,-4.9514468135,0.6185841853,2.1388517518

6/12b

Pd,-0.0028822453,-1.5443556993,0.1190955108
S,2.32097137,-1.6026929547,0.4815230065
S,-2.3288641846,-1.5720581668,-0.2305610521

Cl,-0.3747711647,-1.0851394192,2.4125962224
Cl,0.3751529912,-1.8137525982,-2.2005713525
C,2.8708467187,-0.0071963057,-0.2968663149
C,4.3349604112,0.3217664097,0.0170060023
H,2.1865780195,0.7751888616,0.0492180739
H,2.6996221381,-0.1721810101,-1.366567564
H,4.4640120699,0.4434958315,1.1019543567
H,4.9891418473,-0.4994876877,-0.3041948573
C,-2.7809528474,0.2109194731,0.0339988884
C,-4.2424679972,0.5027100563,-0.326469248
H,-2.0809072177,0.814271747,-0.5544032064
H,-2.5730333431,0.3716548739,1.097836756
H,-4.4250065525,0.2994939279,-1.3907861815
H,-4.9033917429,-0.1545285179,0.2544969874
C,-4.5723261981,1.9756920024,-0.0264734002
C,4.7491266684,1.618016763,-0.7029944387
H,4.6800277594,1.485475691,-1.7908697321
H,4.0831813573,2.4478487551,-0.4233272001
H,-3.945486538,2.6394251143,-0.6371058846
H,-4.3757345293,2.2073988057,1.0306854257
S,6.486215374,2.1283025227,-0.3850829398
S,-6.3036693104,2.4509278987,-0.4222263099
H,-2.3120979082,-1.5394847182,-1.5883211028
H,2.3129706985,-1.1643025285,1.7671610895
C,6.3396558605,2.6233390548,1.3753971156
H,5.5700353566,3.397901281,1.4935193459
H,6.111742754,1.7644901955,2.0190523473
H,7.3116451653,3.0371021094,1.6684850678
C,-7.1856593805,1.4985069922,0.8745620604
H,-7.0732912103,0.4171113312,0.7275432513
H,-6.8258408595,1.7829629658,1.8723160268
H,-8.2470503302,1.7591709424,0.7886132502

6/12c

Pd,0.1552516793,0.3661926977,-0.463891603
S,-1.118202275,-1.5301109203,-1.1107205911
S,1.8333190795,-0.9182814147,0.5811160419
Cl,-1.5117421494,1.7067395304,-1.4260563629
Cl,1.3501134271,2.2306939501,0.3106550557
C,1.5160552236,-0.6542164625,2.3689173111
H,2.216260443,-1.2662652268,2.9507610256
H,1.6927650049,0.4128166633,2.5348832363
H,0.477879693,-0.9005667106,2.6125835926
H,-2.3125593112,-0.8846616483,-1.1189444642
C,1.3465092731,-2.6906772639,0.3949028809
C,-1.2665008557,-2.2967917211,0.5834207161
C,-0.0257489602,-3.1433560271,0.9371169803
H,-0.1703390304,-4.1679681343,0.5659760775
H,0.0174232526,-3.208417961,2.0327103606
H,-2.1633306907,-2.926460597,0.5961849378
H,-1.3993859403,-1.4621692221,1.2781696681
H,2.1348437917,-3.2872154477,0.8715667974
H,1.4133595452,-2.858655244,-0.6874306906

6/15a

Pd,-0.346477749,-0.2307976487,1.342727194
S,-2.354867449,-0.4513405628,0.1072570656
S,1.6647459592,-0.0111625062,2.5850100768
Cl,-1.4542541686,0.8462977323,3.1220808613
Cl,0.7748052129,-1.2290665816,-0.514495604
C,-2.9984935858,1.2820399493,0.0491286645
C,-4.2739481454,1.3195595314,-0.8000827661
H,-2.1763383555,1.8789914098,-0.3621991905
H,-3.203740683,1.5951401565,1.0768979816
C,-5.1732221043,1.7599567429,-3.0631770761
H,-6.1105303408,1.9539027484,-2.5271179482
H,-5.010773356,2.5655891689,-3.7889426471
C,2.4651091016,-1.6959887243,2.4423405414
C,3.8904207803,-1.6159656191,1.8778897757
H,1.7990196544,-2.3171565356,1.8389191042
H,2.5185844867,-2.0624309697,3.4721156268
C,5.2268794545,-1.8793858682,-0.1856856317
H,6.0488222742,-2.0317587843,0.5246189391
H,5.254876707,-2.6793300652,-0.9356466892
C,2.6811027311,1.0367507228,1.4686560275
H,3.7082835407,1.0410586552,1.8489201484
H,2.6266891681,0.6558655292,0.4456031026
H,2.2381786756,2.036280701,1.5348905972
C,-3.5715859542,-1.2060214909,1.253711567
H,-3.4959329566,-0.7150492687,2.2284657788
H,-4.5647838414,-1.0727000671,0.8123351853
H,-3.3057127871,-2.2660708159,1.3278363929
O,4.836619719,-1.2570603941,2.573894602
N,3.9787176408,-1.9698871997,0.5661596899
C,5.3882476138,-0.517676582,-0.8828440395
H,5.324657445,0.2841530798,-0.1185809379
H,4.5528566461,-0.3674168617,-1.5835993016
C,6.8222800117,0.7406703057,-2.4049197493
C,8.1290735231,0.6918477169,-3.2029865395
H,5.9841433864,0.8526177285,-3.1070634313
H,6.8224965724,1.6455702576,-1.7563346471
H,8.9668751407,0.4958011242,-2.4998196848
H,8.0806389736,-0.1624236535,-3.8915923814
H,3.1131984388,-2.0957924863,0.0490338545
N,6.6344390467,-0.4994923886,-1.6467859487
H,7.4135439628,-0.6031017379,-0.99641254
N,8.2809456639,1.9263709202,-3.9916854522
H,8.4661902936,2.705300443,-3.3600347898
H,9.1024282388,1.8465521905,-4.5883106326
O,-5.3560114233,0.9488323818,-0.3528833436
N,-4.0963003649,1.7818169082,-2.0731158497
H,-3.1575692653,1.9792495305,-2.3923776515
C,-5.2648614092,0.40739354,-3.7899464004
H,-5.3456375916,-0.397631626,-3.0315363073
H,-4.3357944673,0.2317267304,-4.3538837939
C,-6.4650017598,-0.7863407983,-5.5469288863
C,-7.659811098,-0.7164085644,-6.5027672341
H,-5.5440892687,-0.8832410432,-6.1390543984

H,-6.5472133577,-1.7056806377,-4.9251515767
H,-8.5813835299,-0.5461775194,-5.9054916956
H,-7.5319600039,0.1591319757,-7.1537021081
N,-6.3766456171,0.4346961086,-4.739061822
H,-7.2445149362,0.5360141102,-4.2122363395
N,-7.6998651876,-1.9260738698,-7.3412532168
H,-7.953181447,-2.7260767111,-6.7617912858
H,-8.4411405991,-1.8334913174,-8.0333806185

6/15b

Pd,0.2427320813,0.6085953761,0.4782971128
S,1.9164379234,0.0878908437,2.0399077616
Cl,-1.561040411,1.1087390666,-0.8740795139
Cl,1.7472791642,0.7690905747,-1.2658326731
O,-1.0371142461,0.3611307818,2.2233802989
C,0.8242327898,-0.8093131695,3.2542418099
C,-0.5781462393,-0.2081862646,3.2381679448
H,0.7449567942,-1.8526887337,2.9198349213
H,1.2847219688,-0.7889931077,4.247327609
C,-1.0544293208,-1.0952442137,5.5622470531
C,-2.0158135177,-0.6766404382,6.6820438222
H,-1.1537596661,-2.1767050152,5.3699924529
H,-0.0285619973,-0.9029238112,5.8956452272
H,-1.8530597461,0.3866375138,6.9103868933
H,-3.0646541006,-0.7752865751,6.3240659447
C,2.8354284564,-1.3301515035,1.3184179931
H,2.122248851,-2.0834582536,0.9685570267
H,3.3659336374,-0.9109933116,0.4571121556
H,3.5359050039,-1.7344049233,2.0587531646
N,-1.3430311499,-0.3315826182,4.342276493
N,-1.7289044861,-1.4555715828,7.8807718858
C,-2.4793660473,-1.0038988787,9.0610284785
C,-2.1603126098,-1.8827938446,10.2855652273
H,-3.5788590455,-0.9990173823,8.8958784444
H,-2.1823733247,0.0353675298,9.2742182144
H,-2.4331644996,-2.9261473529,10.0581425133
H,-1.0749883836,-1.866955201,10.4561282842
H,-2.2922151644,0.0113047569,4.2209748154
H,-1.9634612698,-2.4323855388,7.7042536672
N,-2.8412103363,-1.4949900442,11.5256769035
H,-2.5838307808,-0.5393907859,11.7703038579
H,-3.8497198976,-1.490149263,11.3757296004

6/15c

Pd,0.3118985639,0.0931404536,-0.040849507
S,1.819485535,0.1695565333,1.7810989979
Cl,-1.3471045364,0.0107471125,-1.6694073028
Cl,2.0891509295,-0.0665791736,-1.5159557311
C,2.2809494959,-1.6074072667,1.916457937
H,1.3741088178,-2.2194894631,1.9615250481
H,2.8368828073,-1.8266543694,0.9991785185
H,2.9072851312,-1.7495686151,2.8050610663
C,0.5359113183,0.2666999495,3.1265589907

C,-0.710081581,-0.4350280154,2.5970376231
N,-1.286251351,0.2102707685,1.4334578907
H,-2.04807121,-0.3742380675,1.0754301096
O,-1.100948447,-1.5094330886,2.9890008004
C,-1.7463642037,1.6305963355,1.5558746952
C,-2.8896918877,1.7753787887,2.5652435168
H,-2.058273896,1.9212241566,0.5465405391
H,-0.8945682159,2.2570411372,1.837143792
H,-3.7184727379,1.0915426163,2.2784840581
H,-2.5470010416,1.4531230627,3.5622127058
C,-4.3531050032,3.4034612724,3.6334459013
H,-5.2545028429,2.7856664122,3.4281771957
H,-3.9847229868,3.1127443205,4.627310804
N,-3.2845653428,3.1766192332,2.6512341128
H,-3.6167208753,3.4790617258,1.7352387387
C,-4.7502222292,4.8824852148,3.6673694805
H,-5.0444289941,5.1941937482,2.6424169622
H,-3.8660909899,5.4733754864,3.9420339093
N,-5.7917396692,5.0907402983,4.6855034673
H,-5.9703780134,6.087727967,4.7890144525
H,-6.6663094333,4.6785178562,4.3617951031
H,0.3767142247,1.3326042562,3.3190013032
H,0.8949279745,-0.2377717161,4.0272716308

6/15d-*cis*

Pd,-0.8925064885,-0.043045744,-0.0038090313
C,2.4290625459,0.0096729088,-0.6613591095
C,1.9817586875,-1.4337097989,-0.8533285471
H,2.8159410215,-2.116244927,-0.6627704874
S,0.6222214423,-1.8083231791,0.3653158788
N,0.3115818402,1.5045719592,0.9899767686
C,1.4723544884,-1.5381501221,1.9738461244
H,2.0632748196,-2.4318661484,2.2063101038
H,2.130106389,-0.6647792798,1.9462265447
H,0.6741040035,-1.4141651357,2.713317395
H,1.5199238671,-1.6359087225,-1.8264451987
O,3.2791337825,0.2972233311,0.1847904739
N,1.7547936794,0.942317827,-1.4025959096
Cl,-2.0863698812,-1.6175800799,-1.2442660426
Cl,-2.5411790626,1.5755926368,-0.4030365922
C,1.7313037532,2.3356739868,-0.9525275877
C,0.6030812191,2.6517928699,0.0646770748
H,0.9441146342,0.6186627535,-1.92298433
H,1.61134887,2.9911703013,-1.8228868358
H,2.7102662141,2.5306237155,-0.5036484468
H,0.920942824,3.527770175,0.646891716
H,-0.3394270863,2.8873152114,-0.4361360539
H,1.2091593974,1.0962645905,1.2568676111
C,-0.3719513109,1.9140492482,2.2551801217
C,0.5129934631,2.7380605317,3.2047312476
H,-0.6742889458,0.9962298924,2.771644031
H,-1.2844005654,2.4485925031,1.9689156994
H,1.4585558256,2.1962117417,3.3678277758
H,0.7692221292,3.711684786,2.7450363867

N,-0.1770697181,2.8479287,4.4992703471
H,0.4233765542,3.3292039084,5.1660034936
H,-1.0071602221,3.429907789,4.3903092886

6/15d-*trans*

Pd,-0.146881367,-0.5158737128,0.5646713343
Cl,0.1104687697,-2.1634280741,-1.0750992707
C,-1.8101824056,1.4595757806,-1.0582710383
C,-2.8359370876,1.0427313109,0.0208895531
H,1.851038638,1.1371812799,0.6482584504
H,-3.840124444,1.0170322726,-0.4156527469
S,-2.5051409236,-0.6778794358,0.6850462283
N,1.6875139938,0.422598833,-0.0684141878
Cl,-0.1789022925,1.0210861931,2.4002648138
C,-3.0831122572,-1.6512545443,-0.7589571232
H,-4.1781583307,-1.5856410343,-0.7797358673
H,-2.6348818898,-1.2486290488,-1.6703710975
H,-2.7521535497,-2.6813390893,-0.6012187461
H,-2.8105816436,1.6886916059,0.904743208
O,-1.9282984801,1.1268106503,-2.230783759
N,-0.7752237373,2.2161338561,-0.5647583912
H,-0.7077961316,2.2659160805,0.449941423
C,0.497303909,2.3592453004,-1.269285844
C,1.3728545237,1.0886833437,-1.3811971349
H,0.2950751028,2.6901926363,-2.2951075421
H,1.0543730904,3.1545586698,-0.7559145177
H,0.8831974965,0.336489112,-2.0053685746
H,2.3121118055,1.3914073164,-1.8687659911
C,2.8896289393,-0.4600633646,-0.1275706612
C,4.20634028,0.33236284,-0.1740525722
H,2.7879793233,-1.1164682975,-0.99582155
H,2.8687327479,-1.0889335265,0.7708277913
H,4.2540144793,0.9305163555,-1.094804355
H,4.2198449576,1.0429649398,0.6802893383
N,5.3242907167,-0.6183482781,-0.1984697846
H,6.2003194301,-0.1177882389,-0.3320791701
H,5.3927073365,-1.0875597317,0.7036957848

6/15e-*cis*

Pd,-1.4445332097,-1.2119274286,1.0443588211
C,0.7738620389,-1.5252595013,-1.3297882137
C,2.073330108,-0.6643832454,-1.5244793091
C,3.4558981778,0.638093882,0.113546987
C,2.5641075164,1.2860785,1.1966625721
C,0.7213606222,2.0025004985,-0.2824995655
C,-0.6857304623,1.6911666025,-0.8159787773
H,4.4544022971,0.4899661409,0.5458635003
H,0.9188645521,-2.5251391556,-1.7573766397
H,1.8056839435,0.3702209789,-1.7560885176
H,1.2404440832,-1.2968682412,0.6222059623
H,2.9146553205,2.3092524406,1.3878085661
H,-0.5648939775,0.9950112414,-1.6563735351
S,-1.9349280035,0.9983208285,0.3553277493

N,0.4302039152,-1.6861176315,0.1120192472
C,-3.2851765173,0.7292278078,-0.8638418443
H,-3.5970652418,1.7029311027,-1.2606417136
H,-2.9356914356,0.0679082319,-1.6642896336
H,-4.0952242503,0.2549309433,-0.3027139034
H,-1.0974128921,2.6288414482,-1.2066765313
O,1.429104154,2.7744541192,-0.9233615724
N,1.1499221903,1.3157546444,0.8085446619
H,2.6213379514,0.7103593304,2.1276605144
H,3.550389647,1.3384259722,-0.7286306488
N,2.9284808497,-0.6700969034,-0.3245217682
H,2.6066158692,-1.0506501284,-2.4066436213
H,-0.0638608117,-1.0647901894,-1.8655406172
H,0.42456642,-2.6834021768,0.3506258231
H,0.5196676269,0.6714955221,1.2732410492
H,3.6797783461,-1.3421719094,-0.4222977695
Cl,-3.4755011661,-0.9505003029,2.1860661844
Cl,-1.1930550714,-3.3904140717,1.8980136932

6/15e-*trans*

Pd,-0.1090023356,-1.398813931,-0.1981974229
Cl,-0.2965100971,-1.457309999,2.1492939628
C,-2.8584690405,-0.1231908793,0.4972875906
C,-2.1022866501,1.2040782503,0.4933535582
C,-1.1209614656,2.9394375435,-0.9557363089
C,0.1782961981,2.6234635417,-1.7222048436
C,1.6160646725,1.666017967,0.0395597165
C,2.3450400973,0.4492292439,0.6586904861
H,-1.6225115926,3.7560347677,-1.4959353427
H,-3.9019901213,0.0246988582,0.1718589388
H,-1.0804602196,1.0213154623,0.8422349707
H,-2.275068342,-0.7595716525,-1.3790414934
H,0.7982506114,3.5307614907,-1.7453100586
H,1.9402246717,0.3271875786,1.669408202
S,2.2218166316,-1.22374069,-0.1574321883
N,-2.2111108382,-1.1092863187,-0.4187066132
Cl,-0.0224366786,-1.4548935468,-2.5744141318
C,2.8997468,-2.2485466917,1.2056913405
H,3.9532509682,-1.9761829765,1.3437557694
H,2.3130952635,-2.0870471389,2.1145437691
H,2.8188508348,-3.2907831677,0.8795078925
H,3.4123900292,0.6984567032,0.7187340652
O,1.6780308859,2.7158288285,0.6740702015
N,0.9595832865,1.5315396911,-1.1383298654
H,-0.05939826,2.3200585375,-2.7481137027
H,-0.8501266082,3.3227581542,0.0399880762
N,-2.0354568956,1.7793830883,-0.8574162359
H,-2.5838302254,1.8771208344,1.2307686713
H,-2.8505760181,-0.5441092317,1.5065076216
H,-2.6916374884,-2.0080292606,-0.3718848124
H,0.8870269474,0.6355236556,-1.6077624799
H,-2.9697173911,2.0776572276,-1.1263545133

6/15f

Pd,0.6234619248,-0.5246047752,-0.9454681438
S,-2.7579404852,1.4705836178,-3.6800079641
S,5.0853388227,0.7006554832,0.7605442685
Cl,-0.018486595,-2.5545849431,-0.0114802725
Cl,1.2838088508,1.5458367541,-1.9096038019
C,-1.7928044667,-0.0644577223,-3.3241837766
C,-2.1338268304,-0.5036978853,-1.9161245395
H,-0.7382092497,0.2147678651,-3.4231474299
H,-2.0592742889,-0.8584470141,-4.0293987863
C,-1.9835527987,0.2082995447,0.4841641343
H,-2.2030272334,-0.8351325485,0.7249366378
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C,3.3572805424,0.0816253979,0.9809892418
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6/15h

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6/15i

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6/15j

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6/15k

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6/17a

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6/17b

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O,-0.973538629,2.2090590354,-0.4488412371
C,-0.0026668892,2.9045634468,0.0337035336
C,-0.0389477333,4.3964872843,0.0482901505
H,-0.6571919697,4.7676344214,-0.7765816656
H,-0.4880681943,4.7266611887,0.9967092557
H,0.9787132279,4.798637976,-0.010649375
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7/10b

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S,-1.6275341949,-1.7629800346,-0.33172384
S,1.6845426877,-1.6514551619,0.4748899179
H,-1.4150910964,-1.8908983968,-1.6669949492
H,1.4847954061,-1.8178906853,1.8078558691
C,-3.2260580251,-0.7822583482,-0.4612824505
C,-4.2987897756,-1.5560804195,-1.2408025134
H,-2.984955526,0.1779264661,-0.9239947672
H,-3.5140673481,-0.6174249656,0.5823286125
H,-4.0003788622,-1.6844548593,-2.2889515862
H,-4.4870004741,-2.5455707148,-0.8051435035
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H,2.9007225641,0.369942358,1.1034824897
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S,5.8210315318,-0.1925390191,1.4196663064
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C,-0.1161877701,2.385647549,0.1057250495
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H,-0.434555799,4.1837240837,1.1764513678

7/10c

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H,2.7582500742,2.4009319462,1.1714630456
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H,2.5547361088,-0.4772277642,-1.5667808714
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H,2.3453661674,-1.0315871875,1.4766336771
H,0.2790974984,-2.3914573143,1.3417218123
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H,-5.0587049153,0.4526917664,0.1190938359
H,-4.6189385846,1.1042506581,1.7121374815
H,-4.5465896818,2.1760552709,0.2789992864

7/12a

Pd,-0.0018052876,0.3264244015,-0.012082222
S,1.5978827435,-1.2701899133,0.561378656
S,-1.6316195621,-1.2301693268,-0.6113767917
C,3.0742139825,-0.5541250181,-0.30124969
C,4.3880048731,-1.2294106276,0.1254326821
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O,1.0445401886,2.1250064797,0.389962692
O,-1.0104208851,2.1537600361,-0.3808987372
C,0.0263379455,2.8127912318,0.0040514065
C,0.0576413731,4.3058922898,-0.0212976793
H,0.7032302905,4.6827021823,0.7800961379
H,0.4767842816,4.6320608969,-0.9846034194
H,-0.9575681553,4.7071687765,0.0706788076

7/12b

Pd,0.0001675297,0.0443513968,0.0061067295
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S,1.7127210745,-1.5586778467,0.1354166604
H,-1.6991861115,-1.7571680061,-1.446260422
H,1.7050520019,-1.7367860966,1.4815612842
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C,-4.4572058359,-1.2709528373,-0.6432144693
H,-3.0393342928,0.4126317897,-0.5877413958
H,-3.3902727242,-0.2918516152,1.0091523814
H,-4.2743723535,-1.5098338499,-1.6998558721
H,-4.6152072336,-2.216415978,-0.1075157776
C,3.2547390025,-0.5215317933,0.0622480364
C,4.4599035964,-1.2671761782,0.6518644866
H,3.0433913608,0.4173067879,0.5833518296
H,3.3821574821,-0.3095881683,-1.0059678207
H,4.2845588714,-1.4917033677,1.7129124054
H,4.6129477079,-2.219948821,0.1278038095
O,1.0920903126,1.8722589057,0.0996888194
O,-1.0880768572,1.8722859153,-0.1226122877

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C,5.72491447,-0.3868830279,0.5256149838
H,5.5778736783,0.5649497109,1.0526491956
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C,-5.7220558905,-0.3876936683,-0.5379781156
H,-5.9433654768,-0.1514464029,0.5123559524
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S,-7.1972138262,-1.1550886341,-1.302732776
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H,-8.5196890734,-2.9057366717,-0.3601514919

7/12c

Pd,-0.7992094153,0.009710337,-0.1034620986
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H,0.5141989626,2.6940634666,1.4857671893
H,1.5804327653,1.3114848103,1.9118965473
H,-0.2586150511,-2.6597783732,0.716391654
C,2.4922014608,0.3653652406,-0.7986691483
C,1.8588155602,-1.4885094247,0.982775969
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H,3.474649158,-0.1016130159,1.0842375233
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H,1.3900397469,-0.9610554293,1.8183000266
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C,-3.1971547433,0.4874171916,0.2502591229
C,-4.642021968,0.7723195606,0.4744385934
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H,-4.819749805,0.8650919531,1.5561214802
H,-4.9162150865,1.718825615,-0.0055130798

7/15a

Pd,-0.0244906329,0.3278588222,0.052906725
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C,2.6685050751,-0.1760415294,-1.6948352021
C,3.5876873813,0.0476044277,-0.479046872
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H,3.2164091252,-0.7493017383,-2.4504944788
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H,3.5111499847,2.2103379484,2.0267889148
H,4.3770806658,0.6544360431,1.9329609006
C,-2.7581859615,-0.3491310821,1.66262221
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H,-2.4024017051,0.5421887993,2.1913259174
H,-3.3361809674,-0.9911430021,2.3361845861
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H,-3.4248789667,2.3203848546,-1.8936303797
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H,-2.7080001661,-3.0451846977,0.5447920229
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H,-0.8182690202,4.7246778538,-0.5622550018
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C,-5.4119648297,2.3061735333,-1.0212240259
H,-5.224881918,3.1954319295,-0.4002421969
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C,-7.2612412022,3.5372575657,-2.063987081
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H,-7.0020137089,4.4047592814,-1.4364655982
H,-7.0160889589,4.5991942605,-3.9309100391
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H,-8.8119378333,5.7320010163,-2.8037808016
H,-9.7689678264,4.393289921,-2.8751975434
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7/15b

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C,-0.6439597016,0.8103643103,0.539643281
C,-0.5467019026,-0.5953799402,1.1154711288
H,-0.400695951,1.5278284219,1.3342460198
H,-1.6324706455,1.0416505771,0.1322012731
C,-2.9591023179,-0.5348592855,1.8027469107
C,-3.8333016798,-0.8421108924,0.5729306128
H,-3.4167888056,-0.9318102044,2.7164270695
H,-2.8718754974,0.5499576486,1.928210029
H,-3.2984850179,-0.5196154086,-0.3347981452
H,-3.9753247064,-1.9391380574,0.4828825006
C,1.3024572967,2.6742849239,-0.4219745037
H,1.6142981003,2.7172557616,0.6260137916
H,2.1679933164,2.8042654514,-1.0806026431
H,0.5371225015,3.4247966789,-0.6510396496
N,-1.614577544,-1.1337008864,1.7017712254
N,-5.0669587811,-0.0727393869,0.6670513918
C,-5.9092862529,-0.1740891458,-0.5386076719
C,-7.207238373,0.6430646006,-0.3657512585
H,-6.1690458331,-1.2231997224,-0.790811633
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H,-6.9385739678,1.6844505094,-0.1412153368
H,-1.4746527429,-2.071217281,2.0688912859
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C,4.5912046368,-0.9468909962,-0.2352822503
C,6.0533294675,-1.1697639457,-0.4129436669
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H,6.3810011552,-0.7794487336,-1.3830814482

7/15c

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H,3.6563899142,2.5118929739,-0.2133302029
H,2.5653494081,3.9206812325,-0.4629087685
C,-0.1115398459,2.3590437672,-0.5156271129
C,-0.2693265077,1.7309386983,0.8607226543
N,-0.2237627614,0.2567435472,0.8264552515
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C,-2.7198665529,-0.0858403508,0.6521290792
H,-1.1308090215,-1.5015234634,0.134291703
H,-1.2828324613,-0.1341163403,-0.9809575257
H,-2.7427669854,-0.3397429985,1.7340691505
H,-2.8829248353,1.0015882497,0.5815619823
C,-5.1022748706,-0.2875141442,0.1492087672
H,-5.3666091694,-0.4204195592,1.2184239242
H,-5.1660196459,0.7866043676,-0.0717560326
N,-3.734745951,-0.7477188126,-0.1522355964
H,-3.686002328,-1.7537921618,0.0072245148
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H,-8.1146084777,-0.7851958167,-1.1861953753
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H,-0.8421427883,1.9879361486,-1.2419831545
H,-0.1531710126,3.4488297821,-0.4456203656
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O,2.148879531,-2.1588904022,0.7017512822
C,3.2414843157,-2.1454519217,0.0224634523
C,4.1820587168,-3.3012226329,0.0085439554
H,3.8731501384,-3.9953501711,-0.7869413265
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7/15d

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S,-2.1501315808,0.9872309082,-1.2730653912
N,0.6930754612,-0.2973566187,0.2022384183
C,-0.882283779,1.6757023556,-2.4074922834
H,-1.3265970388,2.5270966833,-2.9359492805
H,-0.000717651,1.9957862563,-1.8457263631
H,-0.6448632275,0.8756259428,-3.1164960151
H,-3.0747296026,2.0362894611,0.6730872378
O,0.1540620049,2.6967754499,0.383404701
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H,1.1232334469,1.6356880413,2.3699748627
H,1.9392328669,-0.556347969,1.919409863
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H,0.8766903773,0.6751610984,-0.0632070075
C,1.6200543998,-1.1743190287,-0.5857710202
C,3.0982007777,-0.7213125744,-0.5297859248
H,1.2964052716,-1.1413639407,-1.6314866909
H,1.4931777069,-2.1991645752,-0.2174741812
H,3.1467248179,0.3382425426,-0.822172611
H,3.4828008017,-0.7950531197,0.5045059283
N,3.843803375,-1.5074200499,-1.5096290224
H,4.7050327496,-1.0354021358,-1.7703395142
H,4.0982390909,-2.4159779224,-1.1290808178
C,-2.349651522,-3.1284556182,0.0893806813
O,-1.1437271565,-2.8994318002,0.4832120716
O,-2.9705666991,-2.1483677169,-0.466442737
C,-2.9848111375,-4.4703791657,0.2411116036
H,-4.0761101042,-4.375179959,0.247164111
H,-2.6909607813,-5.0952876722,-0.6150710691
H,-2.6265891735,-4.9538235742,1.1574491149

7/15e

Pd,1.1394803341,-0.5038043938,-0.3251010185
C,-1.131555677,-2.4319540825,0.1428893026
C,-2.5936117382,-2.7667018367,-0.2182967076
C,-3.7529887888,-0.7720955438,0.6575262712
C,-3.9285930233,0.7302273642,0.3835968342
C,-1.5234928581,1.4214859439,0.5076253
C,-0.4521085928,2.3158997605,-0.1541496102
H,-4.7123256832,-1.1516235699,1.0508583575
H,-0.5142329519,-3.3271969878,0.2618172518
H,-3.0422897958,-3.3359963171,0.6149826645
H,-1.3319303978,-0.965367533,-1.2324518946
H,-4.2416315424,1.2153704147,1.319678088
H,0.285641597,2.5803916448,0.6084636632
S,0.4263509156,1.3710110661,-1.4896974187
N,-0.5479925185,-1.5722337987,-0.9393535971
C,1.9690206245,2.3570811883,-1.6296718825
H,1.6971414815,3.384183287,-1.8992047396
H,2.5122286378,2.3129981032,-0.6806869826
H,2.5604799615,1.8989403582,-2.4289588162
H,-0.8686379192,3.217257011,-0.6228178952
O,-1.2571289452,0.7703325511,1.5117223072
N,-2.7226310675,1.4014986699,-0.136208075
H,-4.7155302135,0.8937652091,-0.3627242777
H,-3.0056159545,-0.8881567847,1.4463901403
N,-3.3013889116,-1.513159729,-0.5303813296
H,-2.6185928378,-3.4047316494,-1.112511073
H,-1.0875709921,-1.847636541,1.0676658154
H,-0.3038805044,-2.1495703946,-1.7480834086
H,-2.8523674294,2.0297736889,-0.9178101285

H,-4.084328323,-1.7001326197,-1.1497786144
C,4.288932701,-1.2762565474,1.9519443864
H,4.701885368,-0.3387293283,2.3398167199
H,5.0517511149,-1.7724316354,1.3342488821
H,4.0184659409,-1.953454089,2.7703982282
C,3.0909669339,-1.002716386,1.1047145996
O,2.9083924576,0.1498235407,0.54757719
O,2.2028469678,-1.897392344,0.8724360974

7/17a

C,1.4233222338,1.2867815281,0.0365873382
C,3.1271926808,-0.229890058,-0.1415520699
C,1.0296868536,-0.95899151,-0.2519761989
N,2.7389784131,1.0497541056,0.0025814404
N,2.2816714281,-1.3038766996,-0.2836141394
N,0.5100499728,0.2745197691,-0.0874178432
S,0.7786808067,2.8904204334,0.2448397215
S,-0.4022026864,-2.0814543291,-0.4332817939
H,2.0022196692,3.4660473678,0.3165467887
C,-0.2658444083,-3.0463049341,1.1369744621
H,-1.1646060418,-3.6706413595,1.1791985237
H,0.6331412677,-3.6680924722,1.0672880327
H,-0.2259175336,-2.3642112868,1.9906520688
S,4.8186185579,-0.6389174085,-0.1683545078
H,5.2464469702,0.6355419495,-0.0075039099
Pd,-1.5205706102,-0.0341228353,0.053352897
O,-2.6215616175,1.7058371169,0.4254214528
O,-3.566015756,-0.2496383135,0.2416243998
C,-3.7091756505,1.017399243,0.4392881045
C,-5.0413481581,1.6322305993,0.6875350751
H,-5.2975843407,1.5019808169,1.7492770494
H,-5.0104102058,2.7029586021,0.4577703339
H,-5.803643545,1.1230886147,0.0858901045

7/17b

C,0.8426692583,-1.4523961104,-0.0478955525
C,2.9971384471,-0.9196100814,-0.0110466953
C,1.4462596363,0.7675315254,-0.0236131568
N,2.0544376903,-1.9222054114,-0.0379428412
N,2.7291064473,0.3947662744,-0.0115708837
N,0.4373929455,-0.174108637,-0.0392336401
S,-0.6967854057,-2.4722158207,-0.1336344472
S,0.9450786626,2.4231533053,-0.0187285614
H,-0.6869313028,-2.8172750401,1.1820360248
C,2.564538851,3.2906343974,0.0031923358
H,2.3084390947,4.355708177,0.0075769869
H,3.1184597272,3.0236545674,0.9075957698
H,3.1359942559,3.0353831919,-0.8936120217
S,4.6843546595,-1.3486497629,0.0203844869
H,4.4652888226,-2.6844082793,0.0031531086
Pd,-1.6171483439,-0.2490286915,0.0043892459

O,-2.5287138756,1.6300787104,0.0695891321
O,-3.6775527043,-0.2187801546,0.0630828188
C,-3.6884452576,1.0707145571,0.0927977053
C,-4.9510044359,1.8525790355,0.1725249322
H,-5.766783417,1.2943254522,-0.301049761
H,-5.2019982058,2.008757793,1.2321354637
H,-4.8160160198,2.8310486723,-0.3025194299

8/10a

Pd,-0.0185285709,0.4084766723,0.1852958795
S,-1.6074055933,-1.3608090672,-0.6907934357
S,1.8008290731,-1.1720813191,0.9300373001
C,-3.2294755371,-0.7921707683,-0.0150639093
C,-4.4198260044,-1.613173471,-0.5125323524
H,-3.3402063644,0.2699303821,-0.2618319059
H,-3.1186190283,-0.8756688276,1.0724476307
C,3.2842304147,-0.5758092737,0.0106171406
C,4.5618188118,-1.3353328951,0.3702556537
H,3.3809128118,0.500024067,0.2017860354
H,3.0276502139,-0.710871388,-1.0464545028
C,2.2545004384,-0.5745814141,2.6083497281
H,3.1053695787,-1.1308255674,3.0237733286
H,2.4794361322,0.4979797224,2.5601566664
H,1.3704033392,-0.7273686132,3.2356445901
C,-1.8591896917,-0.8764361338,-2.4454679454
H,-2.6289078711,-1.489926756,-2.9325070753
H,-2.1214608716,0.1875291255,-2.4872189464
H,-0.8967509908,-1.0255902569,-2.9455839788
H,-5.7722345649,-1.2224531931,1.4454384243
H,4.785975993,-1.2313507781,1.4379666037
H,4.4522346963,-2.397009838,0.1215605488
H,-4.3051382204,-2.6727239112,-0.2554944111
H,-4.5213860036,-1.5354001743,-1.6016979542
H,6.9274570182,-1.4602378186,-0.1474092415
S,5.9785891642,-0.6140156391,-0.6081384074
S,-6.0410657676,-0.9854316678,0.1407775543
P,-0.825793259,1.932245113,1.7179153507
P,0.5860731635,2.0993678982,-1.2813672736
C,-0.2589993763,3.6121752433,-0.5177490001
C,-0.2080231018,3.581930008,1.0211077591
C,-2.6553950952,2.3135129858,1.8593374508
H,-3.1658641636,1.4856315057,2.3684681239
H,-2.8366691413,3.2465323238,2.4162395923
H,-3.0821649841,2.405617968,0.8522994557
C,-0.3308761506,2.1757138673,3.5097496023
H,-0.6710936355,3.1473800116,3.902491253
H,-0.7651492395,1.3718310382,4.1195883398
H,0.7624139116,2.1165755294,3.590402508
C,2.3516336085,2.7258596772,-1.3457461401
H,2.9819789718,2.0043298806,-1.8815792753
H,2.4210800881,3.706021848,-1.8439209351
H,2.7332230618,2.8153771376,-0.3203228616
C,0.1052972083,2.3739812337,-3.0735812763
H,-0.9685245032,2.1767192871,-3.191983631

H,0.3240679771,3.4017964106,-3.4044330226
H,0.6562798095,1.6680663277,-3.7097215837
H,-0.7873452572,4.4160937646,1.4486139543
H,0.832289256,3.6894588637,1.3638144176
H,-1.3049482108,3.588389455,-0.859951462
H,0.1970601365,4.5370047043,-0.9061957939

8/10b

Pd,0.1464986102,0.8201551379,-0.1745384791
S,-1.5503728287,-0.9422109703,-0.8688776767
S,1.7295989122,-0.8542623045,0.901832918
H,-1.9268246347,-0.5568183512,-2.1109211611
H,2.1323319059,-0.2273663271,2.0321110062
C,-3.1100876675,-0.3857719124,-0.0321711515
C,-4.3431898235,-1.1699960326,-0.4801036416
H,-3.2184466221,0.6887316083,-0.2083120404
H,-2.9071053253,-0.5359459986,1.034592542
H,-4.5087433797,-1.0428590365,-1.559612786
H,-4.2143731805,-2.239436721,-0.2662924203
C,-7.0785723858,-1.7035383876,-0.2801109978
H,-8.0421304274,-1.4571595925,0.1816827674
H,-7.1584443723,-1.5760510205,-1.36785327
H,-6.8215786193,-2.7443423015,-0.042901184
C,3.3199830949,-0.5950730171,-0.0179263739
C,4.5042076738,-1.3231329371,0.6174435552
H,3.4905193343,0.4831892574,-0.0923975743
H,3.1103850474,-0.9760629888,-1.0242674131
H,4.6748282737,-0.9592995076,1.6409138191
H,4.3131658783,-2.4039487586,0.6543498443
C,7.2035410638,-2.043022603,0.5890971461
H,8.1808044655,-1.966076791,0.0977430562
H,7.2890031149,-1.6716746095,1.6189641519
H,6.8856390234,-3.0939705658,0.5951267318
S,6.0331184041,-1.0157885938,-0.3804520781
S,-5.8364235191,-0.5511655886,0.4228538431
P,-0.6619454985,2.6039302245,1.063996687
P,1.0586498005,2.2447473981,-1.7570461822
C,-0.3611525689,3.0411021544,2.8599588817
H,-0.6392948368,4.0834923157,3.0831399329
H,-0.9469338791,2.3676734606,3.5000416624
H,0.703330248,2.8945244152,3.0878587098
C,0.2025838944,4.0784801771,0.2504826392
C,-2.44496374,3.1604450654,0.9047601562
H,-3.0997678986,2.4683639424,1.4502676862
H,-2.5919028126,4.1796273869,1.2961968664
H,-2.7290748357,3.1372817048,-0.1556781121
C,2.876003051,2.7030482995,-1.7107362349
H,3.0867751799,3.6027985157,-2.3104835227
H,3.1679967503,2.8887236284,-0.6685901284
H,3.4787292517,1.8682820805,-2.0919121004
C,0.7717181312,2.3132219044,-3.606453352
H,1.3106804137,1.4859561071,-4.0875966816
H,-0.3013210533,2.1881332374,-3.8050946013
H,1.1121603182,3.2665513739,-4.0411000384

C,0.3002235934,3.912037619,-1.2775317487
H,0.8795284457,4.7354362595,-1.7256298324
H,-0.7061010275,3.9310138073,-1.7230204942
H,1.2110325314,4.1240993599,0.689159245
H,-0.317536915,5.0145430356,0.5107072397

8/10c

Pd,-0.2266634179,0.1435935543,-0.1235442807
S,1.2341400046,-1.9600877991,-0.0561857381
S,1.8775838442,1.4716286414,-0.1144505251
C,2.2420927531,1.8757081242,1.645588282
H,3.2815131497,2.2142727464,1.7670906319
H,1.5547439323,2.6844366347,1.9174161956
H,2.0312058519,1.0092526276,2.282883152
C,3.1183342214,0.1226244626,-0.3516503541
C,2.8500176685,-1.1623250221,0.4380152492
H,3.1215796062,-0.0750288802,-1.4312541572
H,4.1083162014,0.5091576502,-0.0673616774
H,3.6659164218,-1.872422504,0.2481791962
H,2.8041008883,-0.9488774803,1.5114675873
H,1.0390599505,-2.5682372927,1.1379684744
P,-1.7223441544,0.3983331075,-1.8856526422
P,-1.908888307,0.4403408129,1.4293620315
C,-1.8420317316,2.0702758829,-2.7171729086
H,-2.7726370322,2.1800362327,-3.2970887443
H,-1.7969829111,2.8493626164,-1.945317966
H,-0.9799185005,2.205247304,-3.3840800286
C,-2.135518047,-0.7075837508,-3.3411223024
H,-3.0881699155,-0.4261336947,-3.8184759442
H,-1.3285743355,-0.6404939025,-4.083407141
H,-2.1966827464,-1.7474774174,-2.9935477295
C,-3.3992282745,0.3562813054,-1.0022806789
C,-3.34959667,1.0592523134,0.3683513749
C,-2.7191504987,-1.0411406777,2.2393613899
H,-2.0476059831,-1.4528279811,3.0053753401
H,-3.6825696122,-0.7805508757,2.7063925051
H,-2.880963694,-1.8137739156,1.4765003293
C,-2.0322386255,1.672999151,2.8366339799
H,-3.0596230687,1.7621666449,3.2258364284
H,-1.3667773744,1.3580126104,3.6520631215
H,-1.6960020095,2.6545327403,2.4761177668
H,-3.1888858014,2.1393277889,0.2309223131
H,-4.3011042662,0.9300561953,0.9092795734
H,-3.6511261342,-0.7070285792,-0.8696849888
H,-4.1759460825,0.8050311056,-1.6426902356

8/10d

Pd,0.2981906083,-0.0631919555,-0.2095570191
S,-1.1699292454,2.0133924754,-0.1966447786
S,-1.8018857923,-1.4084087397,-0.5376108719
C,-2.2730149521,-1.9915684872,1.1432469936
H,-3.317658302,-2.3347546539,1.1652208792
H,-1.6035350962,-2.8286687863,1.3704079991

H,-2.1005745716,-1.1955161193,1.8765264746
C,-3.0292553094,-0.0348929872,-0.7123038746
C,-2.7756124291,1.1748313522,0.1927995597
H,-2.9900958143,0.2530727597,-1.7707661779
H,-4.0302123832,-0.4397645383,-0.5026974642
H,-3.5978268984,1.8950378972,0.0699406541
H,-2.7321085775,0.8631582063,1.2445044671
C,-0.8758690881,2.7875344853,1.4432951821
H,0.0835662194,3.3121492493,1.3711974548
H,-1.6690224904,3.505723539,1.6937596316
H,-0.798943299,1.9989364181,2.2017383019
P,2.1471201626,-0.1333802082,-1.5952226168
P,1.5950761081,-0.5032982947,1.6591046208
C,3.4945673623,-0.8175379075,-0.4516148309
C,3.3516062439,-0.2836257428,0.9857970169
C,1.702618802,-2.2725296924,2.2660686529
H,2.5796301358,-2.4382255433,2.9123890521
H,0.7909856536,-2.5236029459,2.8254871338
H,1.7607080636,-2.9351688527,1.3931006552
C,1.8141153639,0.3918468852,3.2968040571
H,1.8669591936,1.4732324919,3.1117843161
H,0.9444869521,0.1933025053,3.9385300348
H,2.7274434883,0.0697591337,3.8230519807
C,2.9510574269,1.4804867991,-2.0997435808
H,3.9662130566,1.3310162513,-2.5016995524
H,2.3285706258,1.975179146,-2.8572989265
H,2.9994738851,2.1358002658,-1.2201004095
C,2.5120970268,-1.1578948523,-3.1205909558
H,1.9244248797,-0.7693932713,-3.9632784261
H,3.5815333727,-1.1381586871,-3.386524425
H,2.2023294803,-2.1949937873,-2.9345388744
H,4.0776664392,-0.767643337,1.6592614499
H,3.5494811825,0.7989680967,1.0034225486
H,4.492084625,-0.5815398836,-0.8564283143
H,3.3845622909,-1.9126112941,-0.459981308

8/12a

Pd,0.004470195,-0.074107051,-0.0643261035
S,-1.776788133,-1.6539377631,-0.9365297782
S,1.6677761719,-1.842946903,0.6331442191
C,-3.2543041856,-1.0756689973,0.0004044928
C,-4.567427715,-1.7770517337,-0.3729002205
H,-3.322360636,0.011239201,-0.1427072236
H,-2.9926106827,-1.2517035901,1.0508784268
C,-5.7220820272,-1.2353499222,0.4820867458
H,-4.7915490115,-1.6122852404,-1.4362772639
H,-4.460917897,-2.8603097788,-0.2220560405
H,-5.5257502817,-1.4271698195,1.544850347
H,-5.8308014928,-0.1538100915,0.3287287765
H,-8.1079781663,-1.4148967353,0.8639666518
C,3.2452203366,-1.1442052357,-0.0144977165
C,4.5033477945,-1.9455200576,0.3477321321
H,3.3114082789,-0.1081758338,0.3455462681
H,3.0982296538,-1.1085536432,-1.1008024543

C,5.7446686726,-1.2925715425,-0.2772282888
H,4.6219403987,-1.985919455,1.4396755221
H,4.398058773,-2.9785119292,-0.0122936859
H,5.6524180447,-1.2792836392,-1.3709373534
H,5.8510805322,-0.2615912165,0.0846232139
H,8.1550537603,-1.4663448034,-0.4483119126
P,0.7545299295,1.585954547,-1.4819980308
P,-0.6735995645,1.4808704507,1.5068525756
C,0.7190777856,3.1175567832,-0.3695054443
C,-0.5063160063,3.1162539813,0.5636551281
H,0.7440907138,4.0335451917,-0.9817862997
H,1.644867693,3.0883859568,0.2250726025
H,-1.4277951601,3.2273274573,-0.0280406846
H,-0.4624151745,3.9594584922,1.2717124928
C,-2.3636518868,1.7700474732,2.2722827519
H,-2.5708126695,0.9791997863,3.0061644887
H,-2.4259703036,2.7495735884,2.7729642797
H,-3.1283864013,1.7173331902,1.4861069018
C,0.3900993092,1.8798348643,3.0000829681
H,0.0773108224,2.8193757484,3.4830582922
H,0.3253936059,1.0605433556,3.7280036226
H,1.4353761563,1.971536798,2.6769458602
C,-0.3182550906,2.2045924189,-2.89072251
H,0.034535392,3.1735107365,-3.278956129
H,-0.3192949349,1.4679917951,-3.7049434489
H,-1.3492614165,2.3151098077,-2.5290088569
C,2.4425882436,1.8382051436,-2.2628094022
H,2.5636892411,1.136340325,-3.0992494004
H,2.5754425102,2.866282525,-2.636533702
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8/12b

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8/15a

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8/15e

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8/17c

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