Supplementary Information

Mechanisms of metal-catalyzed cycloisomerizations of *o*-propargylbiaryls and *o*-allenylbiaryls to phenanthrenes: A DFT study

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1. Table S1. ΔZPE, ΔE, ΔH, ΔS, ΔG and ΔG-sol in 1,2-dichloroethane values for the alkyne-allene isomerization, 6-*exo* cyclization and 7-*endo* cyclization of *o*-propargylbiphenyl catalyzed by $InCl_3$ at 298.15 K. (The unit of ΔS is cal/mol-K while kcal/mol is for the rest).

	ΔZPE	Δ*E*	Δ*H*	Δ*S*	Δ*G*	ΔG_{sol}
1b-$InCl_3$	0.0	0.0	0.0	0.0	0.0	0.0
Ts1b	-3.3	22.5	21.8	-7.4	23.9	23.5
Int1b + HCl	-3.1	20.8	21.0	26.1	13.2	13.1
Ts2b	-3.8	32.3	31.8	-3.2	32.8	32.9
Int2b	0.2	-5.6	-5.7	1.0	-6.0	-3.6
Ts1-6b	0.4	12.6	11.8	-7.4	14	11.8
Int1-6b	1.4	11.9	11.1	-6.5	13.1	5.1
Ts2-6b	-0.9	23.1	22.1	-9.4	24.9	20.6
Ts2′-6b	-1.3	26.5	25.2	-13.7	29.3	27.1
Int2′-6b + HCl	-1.1	-0.5	-0.8	24.7	-8.2	-8.7
Int1′-6b	0.8	-34.2	-34	-50.9	-18.8	-2.8
Ts2″-6b	-2	-34	-34.2	-55.8	-17.5	0.6
Int2″-6b	-0.9	-38.7	-38.2	-47.7	-24	-7.8
Ts3″-6b	-3.5	-40.7	-40.4	-49.4	-25.7	-7.5
Ts3′-6b	-1.6	-2.5	-3.7	-9.8	-0.8	0.7
Int2-6b	2.6	-45.9	-46.9	-9.7	-44	-41.1
Ts3-6b	0.2	-15	-16.2	-11.8	-12.7	-16.5
Int3-6b	3.2	-25.5	-27	-14	-22.9	-20.8
Ts4-6b	-0.3	-3.5	-4.7	-10.9	-1.4	-3.1
Ts4′-6b	-1.3	-27.0	-28.4	-12.9	-24.6	-24.5
Int3′-6b + HCl	-1.4	-18.4	-18.8	25.3	-26.3	-26.4
Ts5′-6b	-1.7	-6.4	-7.6	-10.2	-4.6	-4.2
Int4-6b	3.0	-61.4	-62.4	-10	-59.4	-55.7
Ts1-7b	0.4	15.3	14.6	-7.1	16.7	16
Int1-7b	1.7	9.2	8.3	-8.7	10.9	10.8
Ts2-7b	-0.3	26.9	25.8	-10.3	28.9	24.7
Int2-7b	2.2	-18.4	-19.4	-11.8	-15.9	-13.7
Ts3-7b	0.5	-3.2	-4.5	-12.1	-0.9	0.1
Int3-7b	2.9	-41.1	-42.1	-10.7	-38.9	-36.2

1. Table S2 Relative zero-point energy correction ΔZPE, electronic energy ΔE, enthalpy ΔH, entropy ΔS, Gibb's free energy ΔG and Gibb's free energy in solution (1,2-dichloroethane) ΔG-sol for the 6-*exo*, 6-*endo* and 7-*endo* cyclization of *o*-allenylbiphenyl catalyzed by $InCl_3$ at 298.15 K. (The unit of ΔS is cal/mol-K while kcal/mol is for the rest).

	ΔZPE	Δ*E*	Δ*H*	Δ*S*	Δ*G*	ΔG_{sol}
1n′-$InCl_3$	0.0	0.0	0.0	0.0	0.0	0.0
1n-$InCl_3$	0.0	0.4	0.4	3.7	-0.7	0.4
Ts1-6n	-0.2	15.7	15.1	-4.7	16.4	15.2
Int1-6n	1.4	-6.4	-7.3	-8.3	-4.8	-9.2
Ts2-6n	-0.8	5.9	4.8	-10	7.7	1.1
Int2-6n	3.0	-19.6	-20.9	-11.2	-17.6	-16.8
Ts3-6n	-0.5	2.4	1.4	-8.2	3.9	0.9
Ts1′-6n	0.1	21.0	20.1	-10.0	23.1	20.1
Int1′-6n	1.4	3.9	3.1	-8.9	5.7	1.8
Ts2′-6n	-1.5	25	24.1	-10.2	27.1	21.9
Int3-6n	2.8	-55.5	-56.3	-7.3	-54.1	-51.7
Ts1-7n	0.5	20.3	19.7	-3.6	20.7	18.3
Int1-7n	1.7	18.5	17.8	-4.8	19.3	12.7
Ts2-7n	-1.6	24.8	23.8	-8.5	26.3	23.6
Int2-7n	3.1	-34.6	-35.6	-8.9	-32.9	-30.9

1. Table S3 Relative zero-point energy correction ΔZPE, electronic energy ΔE, enthalpy ΔH, entropy ΔS, Gibb's free energy ΔG and Gibb's free energy in solution (1,2-dichloroethane) ΔG-sol for the 6-*exo* cyclization and 7-*endo* cyclization of *o*-propargylbiphenyl catalyzed by $[AuPH_3]^+$ at 298.15 K. (The unit of ΔS is cal/mol-K while kcal/mol is for the rest).

	ΔZPE	Δ*E*	Δ*H*	Δ*S*	Δ*G*	ΔG_{sol}
1b-AuPH$_3$	0.0	0.0	0.0	0.0	0.0	0.0
Ts1-6Au	0.3	3.5	2.8	-6.5	4.8	10.5
Int1-6Au	1.8	-4.2	-4.9	-5.8	-3.1	4.9
Ts2-6Au	-0.8	9.8	9	-6.6	10.9	16.8
Int2-6Au	2.7	-46.9	-47.7	-5.7	-46	-40.1
Ts3-6Au	0.2	-21.5	-22.6	-8.3	-20.1	-12.2
Int3-6Au	2.2	-25.4	-26.2	-7	-24.2	-13.8
Ts4-6Au	-0.4	-6.1	-7	-7.7	-4.7	-1.9
Int4-6Au	2.9	-62.7	-63.5	-8.2	-61	-55.8
Ts1-7Au	0.3	8.4	7.8	-6	9.6	12.3
Int1-7Au	2.2	-2.3	-3.2	-10.1	-0.2	7.1
Ts2-7Au	1.8	-0.4	-1.6	-13.1	2.3	10.2
Int2-7Au	2	-0.3	-1.1	-8.4	1.4	9.6
Ts3-7Au	0.3	12.3	11.2	-11.6	14.7	21
Int3-7Au	2.1	-24	-24.8	-9.8	-21.9	-12.3
Ts4-7Au	0.5	-10.8	-12	-11.1	-8.7	-4
Int4-7Au	3.1	-46.3	-47.2	-10.4	-44.1	-38.7

2. Calculation results obtained by using $InCl_2^+$ as a plausible catalyst for the cycloisomerization of 1b.

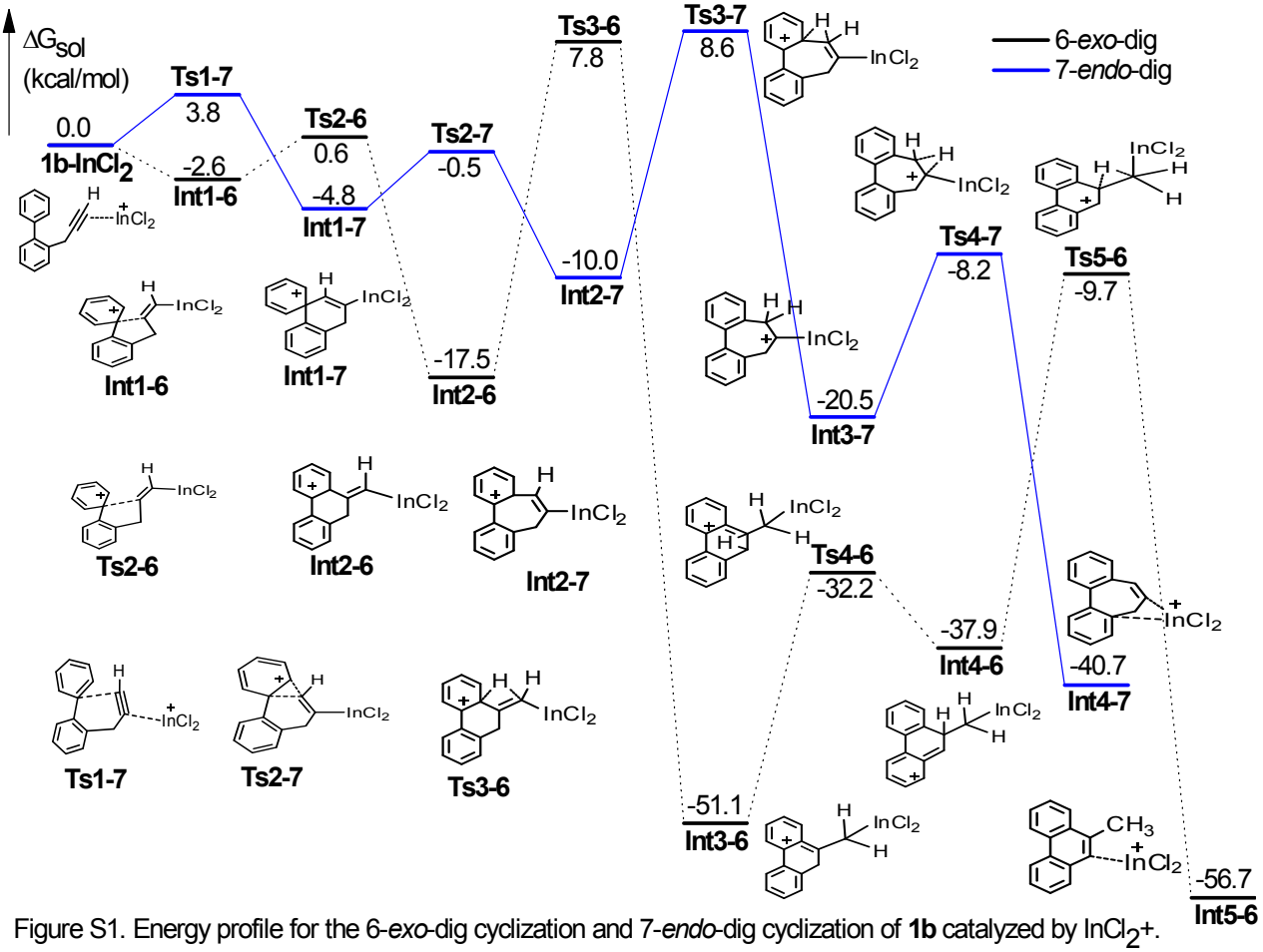

Figure S1. Energy profile for the 6-*exo*-dig cyclization and 7-*endo*-dig cyclization of **1b** catalyzed by $InCl_2^+$.

Results of $InCl_2^+$-catalyzed cyclization of 1b indicate that the 6-*exo*-dig cyclization, upon coordination to the alkyne moiety, instantly gives the spiro cyclic intermediate Int1-6 via a barrierless and exergonic process. Overall, the results depicted above in Figure S1 show that the highest point transition states **Ts3-6** (7.8 kcal/mol) and **Ts3-7** (8.6 kcal) for the 6-*exo*-dig cyclization and 7-*endo*-dig cyclization, respectively, are similar to each other. This suggests that $InCl_2^+$ is inefficient to discriminate the two pathways, contradicting the experimental observation. The calculations were performed with B3LYP hybrid functional in conjunction with 6-31G(d) (for C, H, Cl) and LANL2DZ (for In) for optimization and frequency analysis. Single point energy calculations were performed with larger basis set 6-311+G(d,p) (for C, H, Cl) and Def2-TZVP (for In) in 1,2-dichloroethane using the polarizable continuum model (PCM) based on gas phase optimized structures.

3. Calculation results by B3LYP method for the $InCl_3$-catalyzed cycloisomerization of 1b.

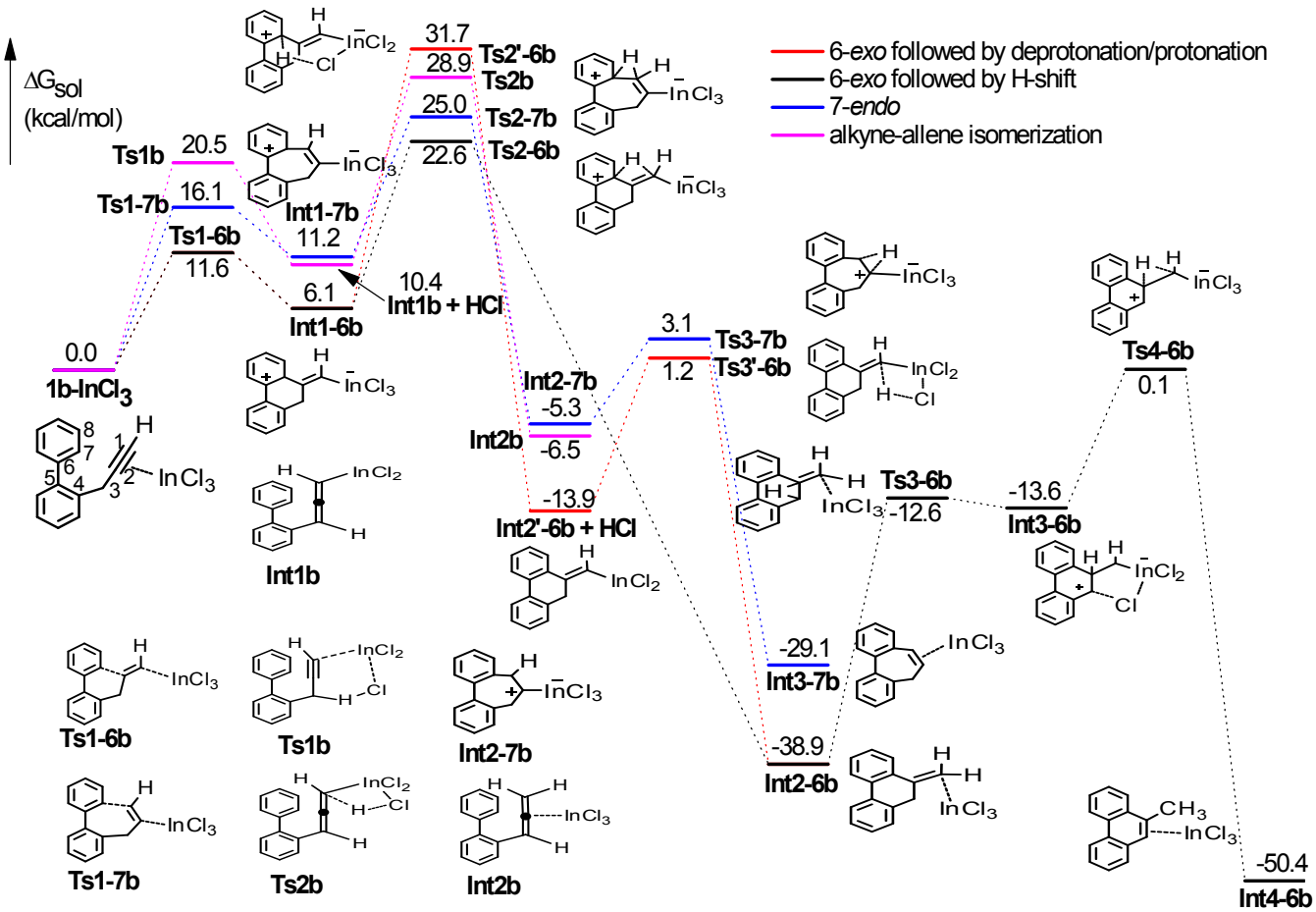

Figure S2. Potential energy profile for the 6-*exo*-dig cyclization and 7-*endo*-dig cyclization pathways and for the alkyne -allene isomerization of **1b** catalyzed by $InCl_3$.

The B3LYP method predicts smaller activation energies for the alkyne-allene isomerization, and higher activation energies for the intramolecular chloride assisted H-abstraction/protonation and the *exo-endo* double bond migration. Overall, the calculation results of B3LYP method are in the same trend with those of M06 method favoring the 6-*exo*-dig cyclization over 7-*endo*-dig cyclization and suggesting the mechanism via allene intermediate is less likely. The B3LYP hybrid functional with 6-31G(d) (for C, H, Cl) and LANL2DZ (for In) was used for optimization and frequency analysis. Single point energy calculations were carried out with larger basis set 6-311+G(d,p) (for C, H, Cl) and Def2-TZVP (for In) in 1,2-dichloroethane using the polarizable continuum model (PCM) based on gas phase optimized structures.

4. Calculation results by B3LYP method for the intermolecular chloride-assisted H-abstraction/protonation steps.

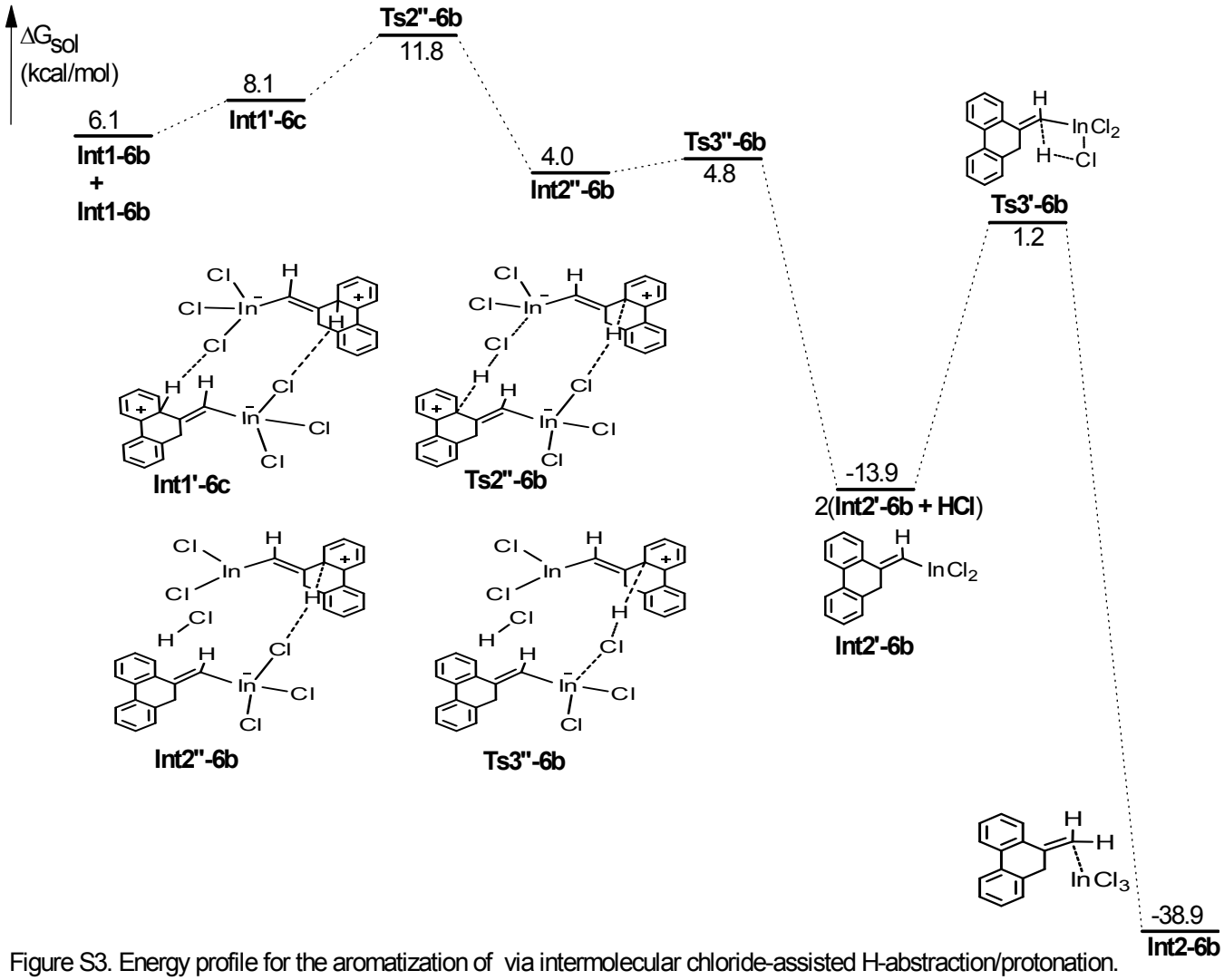

Figure S3. Energy profile for the aromatization of via intermolecular chloride-assisted H-abstraction/protonation.

As can be seen from Figure S3, the B3LYP method gives higher energy values for the intermolecular chloride-assisted H-abstraction step compared to those obtained from M06 method but the conclusion is same as to M06, i.e, the intermolecular chloride-assisted H-abstraction and subsequent proto-demetalation is more favorable than the direct 1,3-H shift for the aromatization of **Int1-6b**. The B3LYP hybrid functional with 6-31G(d) (for C, H, Cl) and LANL2DZ (for In) was used for optimization and frequency analysis. Single point energy calculations were carried out with larger basis set 6-311+G(d,p) (for C, H, Cl) and Def2-TZVP (for In) in 1,2-dichloroethane using the polarizable continuum model (PCM) based on gas phase optimized structures.

5. Calculation results by B3LYP method for the $InCl_3$-catalyzed cyclization of *o*-allenylbiphenyl

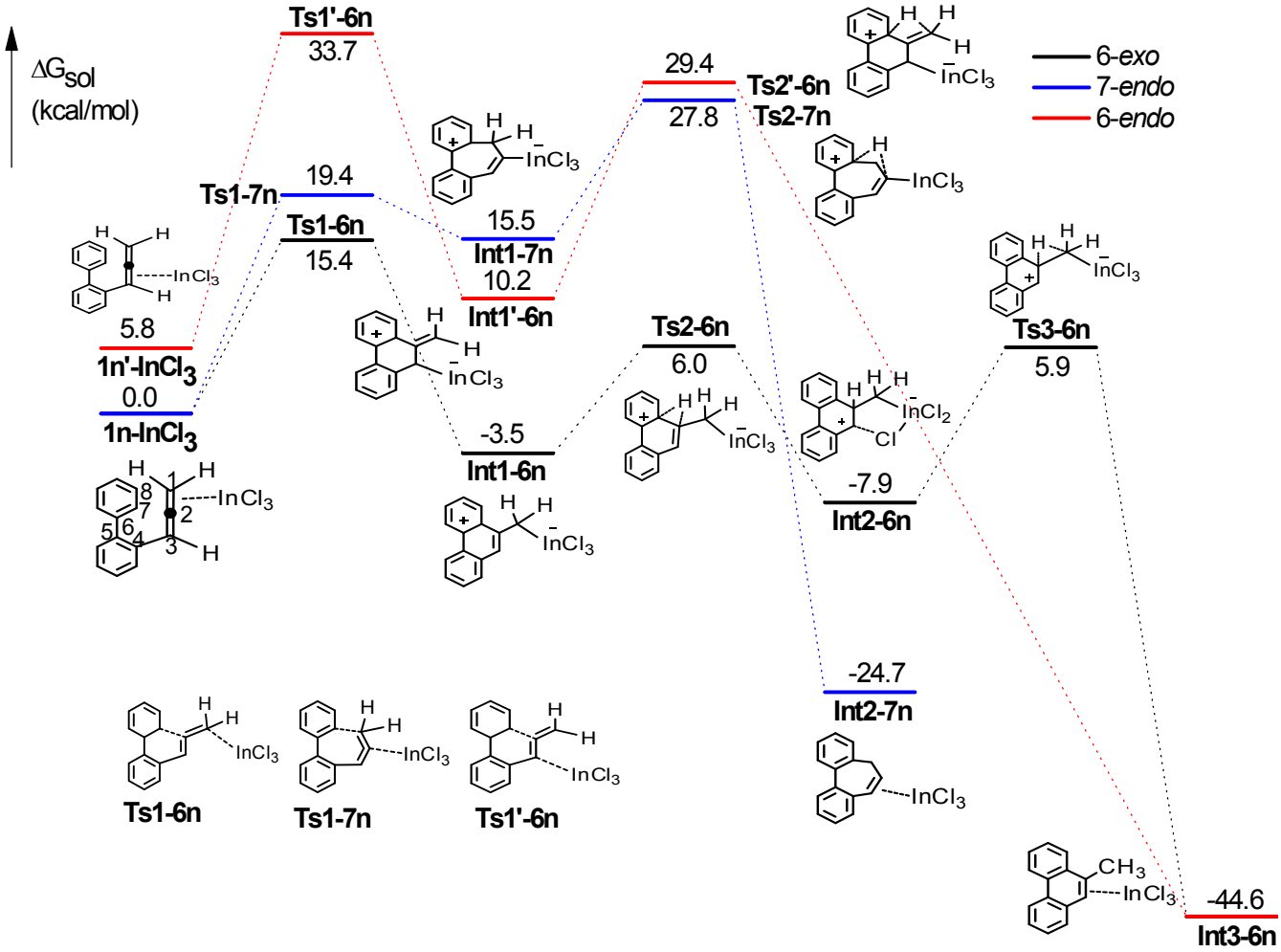

Figure S4. Potential energy profile for the 6-*exo*-dig, 6-*endo*-dig and 7-*endo*-dig cyclization of **1n** catalyzed by $InCl_3$.

6. NBO analysis results for the donor-acceptor bond orbital interaction and E(2) value for 1b-$InCl_3$, 1b-$GaCl_3$, 1b-$PtCl_2$ and 1b-$AuPH_3$

Table S4. Selected donor-acceptor bond orbital interaction between C2–C1 and metal in 1b-$InCl_3$, 1b-$GaCl_3$, 1b-$PtCl_2$ and 1b-$AuPH_3$ and E(2) value (kcal/mol).*

Species	Donor	Acceptor	Interaction	E(2)
1b-$InCl_3$	BD (1) C^2- C^1	LP*(1) In	$\sigma \rightarrow n^*$	0.58
	BD (1) C^2- C^1	LP*(4) In	$\sigma \rightarrow n^*$	3.91
	BD (2) C^2- C^1	LP*(3) In	$\pi \rightarrow n^*$	1.23
	BD (3) C^2- C^1	LP*(1) In	$\pi \rightarrow n^*$	20.27
	BD (3) C^2- C^1	LP*(4) In	$\pi \rightarrow n^*$	21.20
1b-$GaCl_3$	BD (1) C^2- C^1	LP*(1) Ga	$\sigma \rightarrow n^*$	0.63
	BD (1) C^2- C^1	LP*(4) Ga	$\sigma \rightarrow n^*$	6.35
	BD (2) C^2- C^1	LP*(3) Ga	$\pi \rightarrow n^*$	1.92
	BD (3) C^2- C^1	LP*(1) Ga	$\pi \rightarrow n^*$	32.54
	BD (3) C^2- C^1	LP*(2) Ga	$\pi \rightarrow n^*$	0.10
	BD (3) C^2- C^1	LP*(4) Ga	$\pi \rightarrow n^*$	33.49
1b-$PtCl_2$	BD (1) C^2- C^1	LP*(1) C^2	$\sigma \rightarrow n^*$	12.79
	BD (1) C^2- C^1	LP*(5) Pt	$\sigma \rightarrow n^*$	3.40
	BD (1) C^1-Pt	LP*(1) C^2	$\sigma \rightarrow n^*$	193.93
	BD (1) C^1-Pt	BD*(1) C^2- C^1	$\sigma \rightarrow \sigma^*$	1.47
	LP (3) Pt	LP*(1) C^2	$n \rightarrow n^*$	3.54
	LP (3) Pt	BD*(2) C^2- C^1	$n \rightarrow \pi^*$	3.47
	LP (4) Pt	LP*(1) C^2	$n \rightarrow n^*$	78.72
	LP (4) Pt	BD*(1) C^1-Pt	$n \rightarrow \sigma^*$	22.68
1b-$AuPH_3$	BD (1) C^2- C^1	LP*(6) Au	$\sigma \rightarrow n^*$	3.85
	BD (3) C^2- C^1	LP*(6) Au	$\pi \rightarrow n^*$	101.73
	LP (3) Au	BD*(3) C^2- C^1	$n \rightarrow \pi^*$	0.80
	LP (4) Au	BD*(2) C^2- C^1	$n \rightarrow \pi^*$	3.27
	LP (5) Au	BD*(3) C^2- C^1	$n \rightarrow \pi^*$	6.11

* NBO analysis was performed at the M06/6-311++G(d,p)/ LANL2DZ //M06/6-31G(d)/LANL2DZ level. BD and BD* denote the occupied bond and formally empty antibonding orbital, respectively. LP suggests the occupied lone pair

7. Comparison between real $[AuP(C_6F_5)_3]^+$ and model $[AuPH_3]^+$catalysts

Table S5. Comparison between the results of real $[AuP(C_6F_5]^+$ and model $[AuPH_3]^+$ catalyst systems for the 6-*exo* and 7-*endo* cyclization steps.

Cat	$[AuP(C_6F_5)_3]^+$		$[AuPH_3]^+$	
	ΔG_{gas}	ΔG_{sol}	ΔG_{gas}	ΔG_{sol}
1b-cat	0.0	0.0	0.0	0.0
Ts1-6Au	5.8	10.4	4.8	10.5
Int1-6Au	0.5	4.5	-3.1	4.9
Ts1-7Au	8.9	11.8	9.6	12.3
Int1-7Au	0.6	6.2	-0.2	7.1

As can be seen from Table S5, the calculation results of the model catalyst $[AuPH_3]^+$ are comparable to those of the real catalyst $[AuP(C_6F_5)_3]^+$, especially, the relative free energies in solution. The relative free energies in gas phase are also comparable, except the energies of the intermediates in which the model catalyst $[AuPH_3]^+$ gives lower energy than the real catalyst $[AuP(C_6F_5)_3]^+$.

8. Calculation results with $H_3PAuNTf_2$ as a possible Catalytic Species

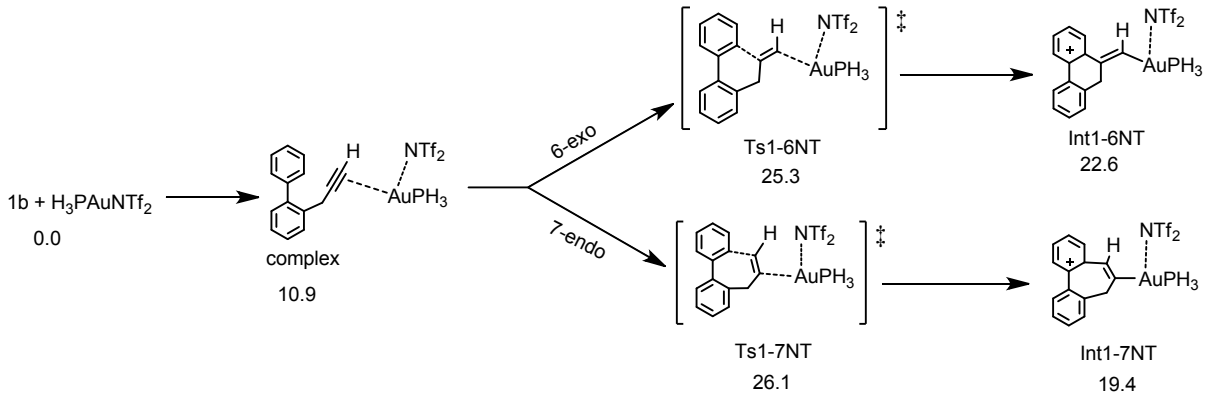

Figure S5. Energy profile of the 6-exo-cyclization and 7-endo cyclization steps with the neutral catalyst (relative free energies are in kcal/mol).

9. Cartesian coordinates (Å) for optimized structures in gas phase at M06/6-31G(d)/LANL2DZ level.

1b-$InCl_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.856022	3.526265	-0.150692
2	6	0	3.935743	2.867354	-0.726176
3	6	0	4.013937	1.481926	-0.656729
4	6	0	3.031643	0.731740	-0.005387
5	6	0	1.937045	1.403005	0.566709
6	6	0	1.860400	2.791964	0.482675
7	1	0	2.777536	4.610154	-0.205380
8	1	0	4.717703	3.430250	-1.232542
9	1	0	4.858460	0.957001	-1.103110
10	1	0	0.996417	3.303903	0.906513
11	6	0	3.146006	-0.745739	0.023140
12	6	0	3.204446	-1.460050	-1.178012
13	6	0	3.180512	-1.454628	1.228340
14	6	0	3.263803	-2.848407	-1.174769
15	1	0	3.173259	-0.912372	-2.120050
16	6	0	3.243184	-2.843617	1.232957
17	1	0	3.176801	-0.907010	2.171405
18	6	0	3.274985	-3.544565	0.031327
19	1	0	3.297609	-3.390767	-2.118369
20	1	0	3.271876	-3.380633	2.179552
21	1	0	3.318083	-4.632188	0.034439
22	6	0	0.810900	0.658845	1.258442
23	1	0	-0.005988	1.365592	1.476174
24	1	0	1.114494	0.253592	2.235784
25	6	0	0.264934	-0.440948	0.472695
26	6	0	-0.267065	-1.326570	-0.176610
27	1	0	-0.496202	-2.214350	-0.737986
28	49	0	-2.399567	-0.010296	-0.096908
29	17	0	-1.817359	2.103728	-0.830917
30	17	0	-3.439282	-1.454923	-1.560542

31	17	0	-2.929255	-0.105165	2.149965

Ts1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.657787	-2.214076	-0.362404
2	6	0	-5.004633	-1.024632	-0.993378
3	6	0	-4.190579	0.093388	-0.847466
4	6	0	-3.026378	0.051765	-0.080432
5	6	0	-2.665373	-1.158339	0.543748
6	6	0	-3.495556	-2.275873	0.392647
7	1	0	-5.287099	-3.096234	-0.462125
8	1	0	-5.909129	-0.965158	-1.595730
9	1	0	-4.457517	1.034128	-1.328492
10	1	0	-3.211562	-3.212356	0.873920
11	6	0	-2.214081	1.284443	0.067483
12	6	0	-1.394701	1.725250	-0.973428
13	6	0	-2.271071	2.024949	1.251855
14	6	0	-0.616381	2.868406	-0.819923
15	1	0	-1.355515	1.155042	-1.902700
16	6	0	-1.499905	3.171267	1.402593
17	1	0	-2.921835	1.686173	2.058819
18	6	0	-0.662326	3.588628	0.370831
19	1	0	0.033233	3.191142	-1.630904
20	1	0	-1.552351	3.742720	2.328239
21	1	0	-0.052523	4.482690	0.488652
22	6	0	-1.412586	-1.358865	1.298237
23	1	0	-0.382782	-1.687476	-0.001103
24	1	0	-1.351249	-2.312375	1.835462
25	6	0	-0.425437	-0.488468	1.560420
26	6	0	0.672570	0.181172	1.641390
27	1	0	0.850008	0.925162	2.417644
28	49	0	2.128690	-0.183679	0.097529
29	17	0	0.468816	-1.864932	-1.145059
30	17	0	2.600879	1.385170	-1.534316
31	17	0	3.899590	-1.564784	0.645633

Int1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.324136	-0.832107	-0.030598
2	6	0	-5.229109	0.495322	-0.434595
3	6	0	-3.981891	1.107402	-0.477117
4	6	0	-2.821794	0.419376	-0.117150
5	6	0	-2.920073	-0.911936	0.338697
6	6	0	-4.181381	-1.520527	0.350473
7	1	0	-6.291211	-1.331176	-0.004495
8	1	0	-6.118348	1.048963	-0.729633
9	1	0	-3.889928	2.136829	-0.824665
10	1	0	-4.256979	-2.553600	0.690232
11	6	0	-1.519457	1.115431	-0.256775
12	6	0	-0.580222	0.699491	-1.206698
13	6	0	-1.224660	2.233462	0.527871
14	6	0	0.638763	1.375616	-1.342801
15	1	0	-0.793982	-0.163274	-1.838553
16	6	0	-0.012390	2.907664	0.402780
17	1	0	-1.956599	2.562211	1.265571
18	6	0	0.926293	2.483636	-0.530489
19	1	0	1.327532	1.090885	-2.141861
20	1	0	0.200741	3.765500	1.037302
21	1	0	1.879589	2.998077	-0.634558
22	6	0	-1.778720	-1.692619	0.831410
23	1	0	-1.900247	-2.778901	0.819412
24	6	0	-0.665069	-1.217444	1.354063
25	6	0	0.478934	-0.756564	1.764714
26	1	0	0.673018	-0.512940	2.809892
27	49	0	1.874694	-0.425362	0.219528
28	17	0	3.881566	0.723931	0.471499
29	17	0	1.908779	-1.950816	-1.544925

HC1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.215960
2	17	0	0.000000	0.000000	0.071527

Ts2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.170652	-2.907448	0.279799
2	6	0	4.778273	-1.852646	0.951728
3	6	0	4.266803	-0.566944	0.819084
4	6	0	3.146067	-0.303872	0.029205
5	6	0	2.511303	-1.381190	-0.622872
6	6	0	3.048586	-2.667547	-0.500441
7	1	0	4.565847	-3.917701	0.366759
8	1	0	5.657081	-2.027336	1.569486
9	1	0	4.754927	0.269591	1.319014
10	1	0	2.553467	-3.493745	-1.010852
11	6	0	2.679778	1.096726	-0.107195
12	6	0	2.292320	1.821140	1.022504
13	6	0	2.645541	1.727583	-1.356958
14	6	0	1.841150	3.132571	0.905055
15	1	0	2.319185	1.336338	1.998592
16	6	0	2.204179	3.039592	-1.474054
17	1	0	2.967945	1.176167	-2.240139
18	6	0	1.789817	3.742506	-0.343876
19	1	0	1.435555	4.767636	-0.437597
20	6	0	1.280165	-1.235742	-1.414452
21	1	0	-0.294477	0.684710	0.518112
22	1	0	1.086665	-2.005365	-2.167177
23	6	0	0.359117	-0.311513	-1.288649
24	6	0	-0.608885	0.553179	-1.049738
25	49	0	-2.396409	-0.234744	-0.114667
26	17	0	-4.288489	1.056511	0.066173
27	17	0	-2.591748	-2.527076	-0.050785
28	17	0	-0.717292	0.451806	1.916026
29	1	0	2.187383	3.519193	-2.451627
30	1	0	1.523390	3.675467	1.793737
31	1	0	-0.604106	1.518031	-1.568508

Int2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.175091	-3.068301	-0.011034
2	6	0	5.138432	-2.071717	0.101909
3	6	0	4.756713	-0.733257	0.099599
4	6	0	3.417395	-0.368927	-0.015270
5	6	0	2.441694	-1.379240	-0.113559
6	6	0	2.835324	-2.721946	-0.115017
7	1	0	4.465355	-4.116894	-0.012907
8	1	0	6.190808	-2.335044	0.189551
9	1	0	5.506536	0.052855	0.182749
10	1	0	2.073962	-3.497556	-0.193312
11	6	0	3.030552	1.061701	-0.034465
12	6	0	2.916903	1.781653	1.158040
13	6	0	2.768824	1.704404	-1.248904
14	6	0	2.526994	3.116318	1.138121
15	1	0	3.125100	1.280476	2.103317
16	6	0	2.382966	3.039376	-1.268283
17	1	0	2.863688	1.142183	-2.178267
18	6	0	2.254786	3.745307	-0.074334
19	1	0	1.950068	4.790281	-0.089285
20	6	0	1.010341	-1.083878	-0.185567
21	1	0	-0.640302	1.618314	0.837354
22	1	0	0.342520	-1.950103	-0.281003
23	6	0	0.381199	0.062519	-0.144075
24	6	0	-0.433295	1.116515	-0.115686
25	49	0	-2.494060	-0.208106	0.031870
26	17	0	-3.851506	1.458368	-0.810240
27	17	0	-2.231447	-2.110564	-1.268949
28	17	0	-2.464119	-0.576996	2.315574
29	1	0	2.184304	3.532672	-2.218403
30	1	0	2.435368	3.667748	2.072290
31	1	0	-0.611756	1.705339	-1.021115

Ts1-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.656555	-3.087141	-0.181617
2	6	0	-4.533543	-2.172781	-0.760158

3	6	0	-4.260743	-0.814985	-0.685177
4	6	0	-3.126634	-0.359424	-0.004927
5	6	0	-2.246597	-1.282929	0.586367
6	6	0	-2.516017	-2.643028	0.477777
7	1	0	-3.853584	-4.154540	-0.258108
8	1	0	-5.424895	-2.519833	-1.278446
9	1	0	-4.945329	-0.092912	-1.129633
10	1	0	-1.809325	-3.360242	0.894341
11	6	0	-2.791018	1.063386	0.055480
12	6	0	-2.937904	1.905897	-1.055903
13	6	0	-2.172408	1.587279	1.231497
14	6	0	-2.524228	3.222248	-0.988428
15	1	0	-3.338190	1.499680	-1.982875
16	6	0	-1.855268	2.971088	1.305120
17	1	0	-2.339690	1.068001	2.175868
18	6	0	-1.981853	3.766162	0.196497
19	1	0	-2.619156	3.856290	-1.868399
20	1	0	-1.463936	3.370913	2.238378
21	1	0	-1.694279	4.814538	0.226586
22	6	0	-0.986685	-0.802524	1.259008
23	1	0	-0.165501	-1.497088	1.019734
24	1	0	-1.087225	-0.802250	2.355968
25	6	0	-0.577096	0.545183	0.785469
26	6	0	0.400105	1.123946	0.179398
27	1	0	0.422774	2.149316	-0.183952
28	49	0	2.209756	-0.145012	-0.135335
29	17	0	1.335865	-2.071992	-1.175229
30	17	0	3.641962	1.148054	-1.435078
31	17	0	2.942112	-0.685506	2.023220

Int1-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-3.294250	-3.274905	-0.146034
2	6	0	-4.280071	-2.461335	-0.712118
3	6	0	-4.153687	-1.088885	-0.642440
4	6	0	-3.059120	-0.505412	0.026889
5	6	0	-2.074743	-1.333676	0.617199

6	6	0	-2.202464	-2.714326	0.502948
7	1	0	-3.375392	-4.357179	-0.225093
8	1	0	-5.136811	-2.906583	-1.212626
9	1	0	-4.926948	-0.451938	-1.069171
10	1	0	-1.417137	-3.351229	0.907579
11	6	0	-2.880425	0.924462	0.069207
12	6	0	-3.408206	1.778542	-0.913172
13	6	0	-2.008624	1.490160	1.109354
14	6	0	-3.156246	3.131080	-0.864387
15	1	0	-3.971120	1.363963	-1.746156
16	6	0	-1.846684	2.942916	1.130463
17	1	0	-2.296783	1.131966	2.112036
18	6	0	-2.381902	3.732378	0.169272
19	1	0	-3.554916	3.767327	-1.653670
20	1	0	-1.230319	3.359867	1.925819
21	1	0	-2.230004	4.808609	0.170071
22	6	0	-0.868569	-0.732195	1.276880
23	1	0	0.006671	-1.359042	1.058391
24	1	0	-0.999673	-0.749839	2.374609
25	6	0	-0.643151	0.689925	0.838571
26	6	0	0.420401	1.197838	0.236358
27	1	0	0.406875	2.235199	-0.103885
28	49	0	2.188956	-0.026801	-0.137219
29	17	0	1.337446	-1.924546	-1.293982
30	17	0	3.726324	1.222651	-1.380204
31	17	0	2.965241	-0.759120	1.967824

Ts2-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.246551	-3.438282	-0.114448
2	6	0	4.400444	-2.739485	-0.459553
3	6	0	4.408168	-1.353386	-0.412168
4	6	0	3.266086	-0.651026	-0.008312
5	6	0	2.104103	-1.361795	0.341281
6	6	0	2.103145	-2.750121	0.279221
7	1	0	3.232312	-4.525176	-0.162500
8	1	0	5.290784	-3.275825	-0.780889

9	1	0	5.298107	-0.809969	-0.726902
10	1	0	1.193290	-3.291621	0.536054
11	6	0	3.232983	0.812037	0.019801
12	6	0	4.383769	1.596160	0.139530
13	6	0	1.989246	1.493354	-0.129606
14	6	0	4.318629	2.979295	0.072964
15	1	0	5.344575	1.110892	0.297695
16	6	0	1.935669	2.904417	-0.200080
17	1	0	1.379174	0.893223	-1.042147
18	6	0	3.096426	3.639635	-0.106259
19	1	0	5.233434	3.560592	0.171328
20	1	0	0.971070	3.398817	-0.292661
21	1	0	3.058317	4.725463	-0.140082
22	6	0	0.895217	-0.608726	0.818160
23	1	0	1.024978	-0.321568	1.875989
24	1	0	0.010248	-1.255449	0.769576
25	6	0	0.645318	0.645486	0.032305
26	6	0	-0.548297	1.079008	-0.436355
27	1	0	-0.540653	1.983109	-1.055637
28	49	0	-2.446756	0.025927	-0.053034
29	17	0	-4.125131	1.154047	-1.207448
30	17	0	-1.972204	-2.156456	-0.838620
31	17	0	-2.636155	0.005801	2.289007

Ts2′-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-4.148475	-3.009373	-0.168400
2	6	0	-5.052106	-1.961036	-0.001352
3	6	0	-4.586784	-0.660121	0.070539
4	6	0	-3.212384	-0.379191	-0.019803
5	6	0	-2.307556	-1.442353	-0.201754
6	6	0	-2.788522	-2.745596	-0.270595
7	1	0	-4.507632	-4.034950	-0.229204
8	1	0	-6.119592	-2.160120	0.062679
9	1	0	-5.308086	0.148748	0.165253
10	1	0	-2.078559	-3.561107	-0.404050
11	6	0	-2.707816	0.988020	0.016507

12	6	0	-3.511749	2.061413	0.410278
13	6	0	-1.342110	1.270369	-0.388081
14	6	0	-3.082360	3.372042	0.275532
15	1	0	-4.503522	1.876973	0.814801
16	6	0	-0.985299	2.651541	-0.606459
17	1	0	-0.619445	1.315901	0.687590
18	6	0	-1.824416	3.678981	-0.258492
19	1	0	-3.740360	4.178667	0.595084
20	1	0	0.034133	2.864034	-0.920762
21	1	0	-1.503012	4.711911	-0.361398
22	6	0	-0.835794	-1.170949	-0.240905
23	1	0	-0.308757	-1.990071	-0.744999
24	1	0	-0.475644	-1.173470	0.806927
25	6	0	-0.468912	0.145938	-0.879779
26	6	0	0.728597	0.355077	-1.452621
27	1	0	0.919229	1.365640	-1.831360
28	49	0	2.312277	-0.289836	-0.195444
29	17	0	4.304331	0.878650	-0.406555
30	17	0	0.971676	1.078286	1.690662
31	17	0	2.468921	-2.443334	0.670511

Int2′-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.860675	3.514836	-0.354445
2	6	0	3.976483	2.820550	-0.811699
3	6	0	4.031269	1.437876	-0.694492
4	6	0	2.980661	0.724066	-0.109368
5	6	0	1.853608	1.431942	0.339619
6	6	0	1.801613	2.816095	0.214604
7	1	0	2.807903	4.597457	-0.453588
8	1	0	4.802885	3.355854	-1.275909
9	1	0	4.895373	0.905800	-1.089526
10	1	0	0.913816	3.347098	0.560769
11	6	0	3.000979	-0.742923	0.033506
12	6	0	4.187977	-1.477942	-0.042551
13	6	0	1.787091	-1.442959	0.220872
14	6	0	4.185527	-2.862512	0.049238

15	1	0	5.136310	-0.955372	-0.155916
16	6	0	1.799104	-2.837328	0.308523
17	6	0	2.986375	-3.549070	0.222108
18	1	0	5.126039	-3.408203	-0.003319
19	1	0	0.861482	-3.363967	0.483017
20	1	0	2.979787	-4.633798	0.308322
21	6	0	0.723873	0.669329	0.974455
22	1	0	-0.195367	1.270192	0.961783
23	1	0	0.965443	0.497065	2.039708
24	6	0	0.532088	-0.674251	0.333766
25	6	0	-0.655181	-1.151676	-0.091125
26	1	0	-0.676851	-2.143679	-0.549049
27	49	0	-2.469137	-0.143620	-0.048994
28	17	0	-4.437134	-1.144417	-0.719305
29	17	0	-2.794748	2.056929	0.602619

Int1′-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.695582	-1.806174	3.629452
2	6	0	-4.872141	-2.151266	2.957895
3	6	0	-4.880413	-2.204307	1.580828
4	6	0	-3.714707	-1.918420	0.836744
5	6	0	-2.527363	-1.579658	1.527540
6	6	0	-2.538817	-1.526416	2.917972
7	1	0	-3.684857	-1.760491	4.716642
8	1	0	-5.777095	-2.376727	3.517325
9	1	0	-5.802202	-2.479473	1.074237
10	1	0	-1.619264	-1.263767	3.439748
11	6	0	-3.709649	-1.967634	-0.605416
12	6	0	-4.862342	-2.216466	-1.365395
13	6	0	-2.469286	-1.647226	-1.335661
14	6	0	-4.811318	-2.270600	-2.742405
15	1	0	-5.818229	-2.377468	-0.875683
16	6	0	-2.466714	-1.841395	-2.781261
17	1	0	-2.611932	-0.494626	-1.341540
18	6	0	-3.610379	-2.095976	-3.469509
19	1	0	-5.734434	-2.458932	-3.289182

20	1	0	-1.524724	-1.664196	-3.298067
21	1	0	-3.615546	-2.158537	-4.554300
22	6	0	-1.274984	-1.225655	0.788658
23	1	0	-0.398082	-1.456086	1.408204
24	1	0	-1.286582	-0.124352	0.671640
25	6	0	-1.183617	-1.865261	-0.562850
26	6	0	-0.127528	-2.530481	-1.042158
27	1	0	-0.224104	-2.949074	-2.049452
28	49	0	1.777653	-2.914332	-0.139995
29	17	0	2.015036	-2.125550	2.091759
30	17	0	2.507662	-5.119402	-0.366922
31	17	0	3.343769	-1.508225	-1.402762
32	6	0	3.694725	1.807893	3.629407
33	6	0	4.871336	2.152956	2.957923
34	6	0	4.879923	2.205186	1.580826
35	6	0	3.714457	1.918545	0.836658
36	6	0	2.527000	1.580071	1.527363
37	6	0	2.538170	1.527539	2.917829
38	1	0	3.683773	1.762793	4.716619
39	1	0	5.776065	2.379058	3.517458
40	1	0	5.801658	2.480597	1.074261
41	1	0	1.618548	1.265009	3.439542
42	6	0	3.709745	1.966781	-0.605550
43	6	0	4.862890	2.213814	-1.365431
44	6	0	2.469281	1.647112	-1.335890
45	6	0	4.812156	2.267584	-2.742470
46	1	0	5.818926	2.373567	-0.875605
47	6	0	2.467059	1.841093	-2.781519
48	1	0	2.611825	0.494396	-1.342140
49	6	0	3.611101	2.094321	-3.469671
50	1	0	5.735619	2.454476	-3.289152
51	1	0	1.524992	1.664635	-3.298433
52	1	0	3.616456	2.156641	-4.554473
53	6	0	1.274808	1.225659	0.788326
54	1	0	0.397757	1.455979	1.407705
55	1	0	1.286640	0.124344	0.671395
56	6	0	1.183592	1.865194	-0.563229
57	6	0	0.127524	2.530384	-1.042661

58	1	0	0.224262	2.948957	-2.049950
59	49	0	-1.777660	2.914533	-0.140631
60	17	0	-2.014793	2.126289	2.091305
61	17	0	-2.507155	5.119630	-0.368845
62	17	0	-3.344087	1.507863	-1.402427

Ts2″-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	4.603937	-2.593421	-2.892594
2	6	0	5.646460	-2.561089	-1.967486
3	6	0	5.428847	-2.035985	-0.706847
4	6	0	4.168311	-1.534180	-0.339172
5	6	0	3.115862	-1.578446	-1.278696
6	6	0	3.351269	-2.107369	-2.544513
7	1	0	4.766623	-3.010609	-3.884569
8	1	0	6.626988	-2.952321	-2.229965
9	1	0	6.247629	-2.042117	0.009138
10	1	0	2.529566	-2.141299	-3.259145
11	6	0	3.926753	-0.985727	0.991058
12	6	0	4.953478	-0.711947	1.904176
13	6	0	2.579590	-0.613040	1.369597
14	6	0	4.679916	-0.203380	3.161821
15	1	0	5.989500	-0.895030	1.631943
16	6	0	2.336925	-0.178019	2.713855
17	1	0	2.778706	0.634042	0.955886
18	6	0	3.367240	0.062508	3.584327
19	1	0	5.508829	0.005283	3.836162
20	1	0	1.307166	0.061617	2.976985
21	1	0	3.180329	0.465236	4.576506
22	6	0	1.754762	-1.042927	-0.932314
23	1	0	0.983726	-1.542104	-1.535394
24	1	0	1.718150	0.025932	-1.227123
25	6	0	1.470712	-1.178541	0.533987
26	6	0	0.416229	-1.814392	1.065150
27	1	0	0.379367	-1.854906	2.160983
28	49	0	-1.079181	-3.029919	0.125113
29	17	0	-0.827777	-5.323493	0.471702

30	17	0	-3.122841	-2.315355	1.275530
31	17	0	-1.479325	-2.526469	-2.162495
32	6	0	-4.402004	1.076329	-3.372810
33	6	0	-5.527385	1.205327	-2.553156
34	6	0	-5.376223	1.212354	-1.183476
35	6	0	-4.097649	1.097185	-0.593738
36	6	0	-2.964385	0.977904	-1.434734
37	6	0	-3.137174	0.965495	-2.815675
38	1	0	-4.517172	1.066078	-4.454909
39	1	0	-6.517902	1.296349	-2.992772
40	1	0	-6.263058	1.310012	-0.562505
41	1	0	-2.257891	0.867388	-3.451371
42	6	0	-3.925267	1.085695	0.838340
43	6	0	-4.996530	1.136028	1.743391
44	6	0	-2.571780	0.897095	1.396341
45	6	0	-4.782065	1.100879	3.104878
46	1	0	-6.018256	1.204700	1.382753
47	6	0	-2.415997	0.989936	2.843646
48	1	0	-2.563936	-0.262162	1.311051
49	6	0	-3.488146	1.035150	3.675473
50	1	0	-5.646885	1.126809	3.766574
51	1	0	-1.402848	0.912086	3.234579
52	1	0	-3.369626	1.017672	4.755451
53	6	0	-1.585370	0.833604	-0.870705
54	1	0	-0.854391	1.267607	-1.564849
55	1	0	-1.354273	-0.249442	-0.847282
56	6	0	-1.452115	1.395400	0.508200
57	6	0	-0.502138	2.245373	0.915121
58	1	0	-0.545303	2.589001	1.953899
59	49	0	0.978472	3.202566	-0.283454
60	17	0	1.246284	5.469561	0.174167
61	17	0	3.188880	2.228828	0.466675
62	17	0	1.040268	2.677142	-2.576402

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.587829	2.346753	3.554046

2	6	0	4.755967	2.655012	2.862505
3	6	0	4.800016	2.521882	1.482037
4	6	0	3.683588	2.071463	0.768625
5	6	0	2.504228	1.774117	1.471763
6	6	0	2.467159	1.914555	2.855428
7	1	0	3.545626	2.456314	4.636138
8	1	0	5.633337	3.011124	3.399411
9	1	0	5.708976	2.801126	0.951116
10	1	0	1.540580	1.685183	3.382971
11	6	0	3.695914	1.918104	-0.697397
12	6	0	4.891302	1.860630	-1.429687
13	6	0	2.466292	1.849487	-1.404205
14	6	0	4.887996	1.755949	-2.812221
15	1	0	5.842697	1.878198	-0.901258
16	6	0	2.485500	1.736211	-2.801592
17	1	0	3.213798	-0.219729	-1.253581
18	6	0	3.679219	1.694727	-3.505201
19	1	0	5.831972	1.704398	-3.351475
20	1	0	1.535252	1.661646	-3.329671
21	1	0	3.670923	1.596413	-4.588879
22	6	0	1.301871	1.287068	0.714301
23	1	0	0.390486	1.444002	1.306389
24	1	0	1.398583	0.187868	0.589613
25	6	0	1.196348	1.919897	-0.644100
26	6	0	0.094077	2.517429	-1.128915
27	1	0	0.189934	2.956387	-2.128577
28	49	0	-1.797801	2.865918	-0.221361
29	17	0	-2.713749	4.994223	-0.472825
30	17	0	-3.360037	1.362826	-1.454006
31	17	0	-2.066217	2.080715	2.014855
32	6	0	-3.830610	-1.726123	3.596841
33	6	0	-4.962231	-2.146306	2.893317
34	6	0	-4.910610	-2.256124	1.519797
35	6	0	-3.725473	-1.960548	0.812609
36	6	0	-2.579836	-1.561382	1.537980
37	6	0	-2.653769	-1.439178	2.921723
38	1	0	-3.870744	-1.624274	4.679394
39	1	0	-5.883023	-2.377980	3.423499

40	1	0	-5.802165	-2.579194	0.988213
41	1	0	-1.772821	-1.100619	3.465794
42	6	0	-3.667265	-2.032911	-0.629713
43	6	0	-4.784764	-2.314996	-1.427379
44	6	0	-2.417532	-1.676703	-1.320247
45	6	0	-4.688475	-2.359646	-2.803485
46	1	0	-5.751682	-2.501542	-0.969581
47	6	0	-2.356105	-1.866656	-2.761955
48	1	0	-2.619181	-0.512025	-1.341334
49	6	0	-3.471385	-2.145120	-3.488975
50	1	0	-5.587412	-2.570993	-3.380932
51	1	0	-1.405471	-1.656394	-3.249833
52	1	0	-3.438683	-2.196941	-4.573758
53	6	0	-1.300193	-1.210159	0.841824
54	1	0	-0.444253	-1.427097	1.496368
55	1	0	-1.301479	-0.109776	0.720450
56	6	0	-1.161748	-1.851957	-0.500864
57	6	0	-0.084583	-2.513449	-0.943140
58	1	0	-0.123307	-2.947507	-1.945716
59	49	0	1.678589	-2.946998	0.125886
60	17	0	2.798162	-4.912006	-0.361112
61	17	0	3.543274	-1.495625	-1.381091
62	17	0	2.146986	-2.039417	2.210132

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-3.706342	-2.144764	3.615834
2	6	0	-4.889601	-2.413015	2.933374
3	6	0	-4.931874	-2.305612	1.550777
4	6	0	-3.798012	-1.923419	0.825019
5	6	0	-2.603105	-1.670596	1.519042
6	6	0	-2.569012	-1.781059	2.905506
7	1	0	-3.665983	-2.232467	4.699936
8	1	0	-5.780883	-2.716296	3.479659
9	1	0	-5.855203	-2.551509	1.028368
10	1	0	-1.631163	-1.583761	3.425959
11	6	0	-3.811224	-1.792780	-0.642853

12	6	0	-5.007005	-1.694318	-1.369497
13	6	0	-2.584600	-1.783958	-1.357436
14	6	0	-5.007441	-1.606626	-2.753303
15	1	0	-5.955459	-1.664651	-0.836533
16	6	0	-2.606723	-1.686622	-2.756238
17	1	0	-3.210695	0.325501	-1.284343
18	6	0	-3.801852	-1.603621	-3.453957
19	1	0	-5.951920	-1.521540	-3.287369
20	1	0	-1.658141	-1.656432	-3.291376
21	1	0	-3.795735	-1.517546	-4.538588
22	6	0	-1.378084	-1.261892	0.752240
23	1	0	-0.475180	-1.471411	1.341588
24	1	0	-1.406590	-0.160357	0.626500
25	6	0	-1.313588	-1.901358	-0.605191
26	6	0	-0.238615	-2.538969	-1.100019
27	1	0	-0.352276	-2.976619	-2.097730
28	49	0	1.635009	-2.933367	-0.195520
29	17	0	2.634397	-4.993544	-0.601625
30	17	0	3.221775	-1.371700	-1.461370
31	17	0	2.001427	-2.189752	2.023742
32	6	0	3.825662	1.704131	3.656666
33	6	0	4.986151	2.061956	2.969863
34	6	0	4.975586	2.118495	1.589672
35	6	0	3.806683	1.826241	0.862449
36	6	0	2.632650	1.489390	1.567081
37	6	0	2.661046	1.423742	2.956518
38	1	0	3.829851	1.650255	4.743385
39	1	0	5.897773	2.294211	3.515861
40	1	0	5.886828	2.407945	1.071095
41	1	0	1.751061	1.150020	3.489483
42	6	0	3.789293	1.852475	-0.591798
43	6	0	4.950465	2.001126	-1.361063
44	6	0	2.546053	1.599976	-1.302158
45	6	0	4.901062	2.018243	-2.742359
46	1	0	5.916261	2.100727	-0.873924
47	6	0	2.531851	1.739589	-2.735277
48	1	0	2.748498	0.329499	-1.341324
49	6	0	3.688890	1.897312	-3.446015

50	1	0	5.831236	2.122757	-3.298551
51	1	0	1.579998	1.593447	-3.243669
52	1	0	3.679276	1.917656	-4.532388
53	6	0	1.365844	1.149826	0.839285
54	1	0	0.495286	1.397232	1.463127
55	1	0	1.340033	0.048919	0.733418
56	6	0	1.278605	1.775995	-0.515973
57	6	0	0.220652	2.449614	-0.991610
58	1	0	0.295662	2.874637	-1.996083
59	49	0	-1.529187	2.985378	0.047155
60	17	0	-2.540716	4.997494	-0.485354
61	17	0	-3.493189	1.609859	-1.420363
62	17	0	-2.069477	2.141419	2.142728

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.141065	3.510113	0.015733
2	6	0	4.257283	2.844101	-0.481584
3	6	0	4.277135	1.456863	-0.526190
4	6	0	3.189666	0.708419	-0.063222
5	6	0	2.065894	1.389627	0.429124
6	6	0	2.046331	2.779426	0.463959
7	1	0	3.115653	4.597769	0.039552
8	1	0	5.112209	3.407931	-0.850151
9	1	0	5.142263	0.953385	-0.954292
10	1	0	1.156416	3.288389	0.835680
11	6	0	3.167000	-0.763684	-0.098315
12	6	0	4.336134	-1.515028	-0.253658
13	6	0	1.932769	-1.453183	-0.018119
14	6	0	4.299139	-2.898622	-0.339524
15	1	0	5.298048	-1.007188	-0.289404
16	6	0	1.911355	-2.849058	-0.116349
17	6	0	3.081445	-3.573170	-0.273772
18	1	0	5.227604	-3.456020	-0.449505
19	1	0	0.960074	-3.372102	-0.027824
20	1	0	3.048027	-4.659129	-0.328504
21	6	0	0.898094	0.592932	0.937305

22	1	0	-0.006395	1.214273	0.956607
23	1	0	1.094276	0.304679	1.988549
24	6	0	0.697370	-0.683092	0.177320
25	6	0	-0.538813	-1.118214	-0.206156
26	1	0	-0.577323	-2.065229	-0.753919
27	49	0	-2.307740	0.068887	-0.319453
28	17	0	-4.169821	-0.788232	-1.362523
29	17	0	-2.310233	2.355416	0.038622
30	17	0	-2.218352	-1.085667	2.283041
31	1	0	-1.189895	-1.332560	1.301726

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	4.752727	-2.522937	-0.039036
2	6	0	5.430971	-1.309612	0.035192
3	6	0	4.722514	-0.117368	0.020451
4	6	0	3.324869	-0.109925	-0.063088
5	6	0	2.652997	-1.337375	-0.161498
6	6	0	3.367295	-2.530333	-0.141309
7	1	0	5.303350	-3.461542	-0.032451
8	1	0	6.517153	-1.291179	0.097316
9	1	0	5.271472	0.821722	0.052198
10	1	0	2.827577	-3.474717	-0.213784
11	6	0	2.540608	1.135028	-0.067526
12	6	0	3.106534	2.358591	0.306931
13	6	0	1.188235	1.132190	-0.493826
14	6	0	2.378591	3.536422	0.255395
15	1	0	4.130869	2.390110	0.670507
16	6	0	0.470085	2.338041	-0.556162
17	1	0	-0.855257	-1.204573	-2.016102
18	6	0	1.053534	3.532537	-0.180703
19	1	0	2.845041	4.468750	0.568419
20	1	0	-0.577583	2.331525	-0.857453
21	1	0	0.475472	4.453073	-0.205842
22	6	0	1.155742	-1.354194	-0.243254
23	1	0	0.757764	-1.383640	0.792670
24	1	0	0.786709	-2.263092	-0.737086

25	6	0	0.559973	-0.128416	-0.852130
26	6	0	-0.587518	-0.225107	-1.611799
27	1	0	-0.940915	0.633973	-2.184548
28	49	0	-2.260810	-0.275455	0.095794
29	17	0	-3.510863	1.556523	-0.591688
30	17	0	-3.069586	-2.419222	-0.266249
31	17	0	-1.211604	-0.014264	2.159493

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.295519	-2.629466	-0.255090
2	6	0	-4.905930	-1.465889	-0.739892
3	6	0	-4.303143	-0.228594	-0.599359
4	6	0	-3.055624	-0.097755	0.028290
5	6	0	-2.458614	-1.278604	0.533124
6	6	0	-3.079887	-2.530932	0.384784
7	1	0	-4.775370	-3.596686	-0.383564
8	1	0	-5.870097	-1.533391	-1.240345
9	1	0	-4.812349	0.645705	-0.995527
10	1	0	-2.574232	-3.417173	0.766563
11	6	0	-2.361026	1.177295	0.174675
12	6	0	-2.896165	2.365233	-0.349454
13	6	0	-1.104830	1.242820	0.828951
14	6	0	-2.217526	3.563951	-0.249258
15	1	0	-3.855093	2.350251	-0.860842
16	6	0	-0.428882	2.464865	0.916697
17	1	0	1.160017	-0.938471	2.349461
18	6	0	-0.972598	3.615771	0.378923
19	1	0	-2.651959	4.466384	-0.674538
20	1	0	0.554353	2.509361	1.376853
21	1	0	-0.420989	4.551220	0.433744
22	6	0	-1.180963	-1.203143	1.154505
23	1	0	-0.713767	-2.115311	1.529327
24	1	0	-1.215667	-0.327488	2.343079
25	6	0	-0.494941	0.023180	1.400154
26	6	0	0.930568	-0.027087	1.783038
27	1	0	1.265902	0.837291	2.361517

28	49	0	2.090451	-0.256473	-0.087901
29	17	0	4.108240	-1.345295	0.354566
30	17	0	0.531035	-1.685332	-1.231865
31	17	0	2.327056	1.806251	-1.183826

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-4.490500	-2.449688	-0.270187
2	6	0	-5.145684	-1.227289	-0.401377
3	6	0	-4.447714	-0.035228	-0.262637
4	6	0	-3.075461	-0.030586	0.006940
5	6	0	-2.431363	-1.270741	0.168849
6	6	0	-3.132778	-2.464609	0.016392
7	1	0	-5.037492	-3.383510	-0.381073
8	1	0	-6.213788	-1.202407	-0.609898
9	1	0	-4.981998	0.909408	-0.347468
10	1	0	-2.602445	-3.410726	0.129552
11	6	0	-2.289641	1.208864	0.114531
12	6	0	-2.736274	2.406020	-0.450235
13	6	0	-1.043729	1.185215	0.776710
14	6	0	-1.981108	3.567316	-0.358214
15	1	0	-3.674657	2.421797	-1.002442
16	6	0	-0.300372	2.357537	0.866285
17	1	0	1.055174	-1.129348	2.356754
18	6	0	-0.759167	3.543690	0.301699
19	1	0	-2.341704	4.486613	-0.815586
20	1	0	0.665473	2.357872	1.368252
21	1	0	-0.148515	4.441897	0.364826
22	6	0	-0.990518	-1.283422	0.510652
23	1	0	-0.669159	-2.242223	0.933899
24	1	0	-1.209211	-0.289285	2.290548
25	6	0	-0.580300	-0.117095	1.391056
26	6	0	0.879281	-0.185811	1.820658
27	1	0	1.123436	0.619020	2.522805
28	49	0	2.210129	-0.187193	0.144605
29	17	0	3.698733	-1.955943	-0.105685
30	17	0	0.002727	-1.232259	-1.116197

31	17	0	2.821512	1.680455	-1.088855

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.520471	-2.514804	-0.179686
2	6	0	-5.073367	-1.326461	-0.682092
3	6	0	-4.398242	-0.127530	-0.571695
4	6	0	-3.135465	-0.055219	0.042266
5	6	0	-2.585372	-1.261219	0.555038
6	6	0	-3.291413	-2.477504	0.434005
7	1	0	-5.059842	-3.454265	-0.277547
8	1	0	-6.046767	-1.348550	-1.168495
9	1	0	-4.859951	0.768985	-0.977283
10	1	0	-2.837834	-3.385837	0.829695
11	6	0	-2.383411	1.181512	0.168584
12	6	0	-2.869942	2.401934	-0.334941
13	6	0	-1.108166	1.180781	0.793578
14	6	0	-2.133954	3.564295	-0.243606
15	1	0	-3.842546	2.436811	-0.819680
16	6	0	-0.367208	2.371099	0.866711
17	1	0	1.166163	-1.154425	2.224222
18	6	0	-0.869201	3.549072	0.353259
19	1	0	-2.534182	4.491028	-0.649787
20	1	0	0.632263	2.371545	1.295980
21	1	0	-0.271334	4.456387	0.400874
22	6	0	-1.325218	-1.237260	1.193363
23	1	0	-0.921635	-2.168827	1.594172
24	1	0	-0.221091	-0.054227	2.487497
25	6	0	-0.597341	-0.070796	1.327701
26	6	0	0.920804	-0.188414	1.768329
27	1	0	1.358790	0.653317	2.313709
28	49	0	2.121393	-0.302316	-0.182170
29	17	0	3.720014	-1.901147	0.394094
30	17	0	0.492992	-1.045130	-1.683125
31	17	0	2.958613	1.844195	-0.550494

Ts4′-6b

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.568503	-2.550160	0.160400
2	6	0	5.187255	-1.364350	0.579778
3	6	0	4.522081	-0.159312	0.485905
4	6	0	3.214158	-0.085285	-0.030158
5	6	0	2.602067	-1.285143	-0.460142
6	6	0	3.289890	-2.506640	-0.350993
7	1	0	5.095905	-3.499068	0.236202
8	1	0	6.198198	-1.392004	0.981724
9	1	0	5.031178	0.743334	0.815486
10	1	0	2.793936	-3.418373	-0.684674
11	6	0	2.469147	1.157977	-0.143240
12	6	0	2.994971	2.376732	0.324548
13	6	0	1.167392	1.168936	-0.721578
14	6	0	2.281524	3.553116	0.238275
15	1	0	3.982603	2.398523	0.778565
16	6	0	0.459205	2.386433	-0.796265
17	1	0	-0.963218	-1.024463	-2.319055
18	6	0	0.999554	3.561432	-0.323613
19	1	0	2.715542	4.476227	0.618137
20	1	0	-0.544697	2.403914	-1.214478
21	1	0	0.426677	4.484414	-0.376745
22	6	0	1.262782	-1.245211	-0.981933
23	1	0	0.403976	-1.261914	0.470555
24	1	0	0.845218	-2.175959	-1.377207
25	6	0	0.577857	-0.062455	-1.200193
26	6	0	-0.798211	-0.113602	-1.731310
27	1	0	-1.057045	0.747173	-2.356935
28	49	0	-2.260667	-0.182601	-0.120874
29	17	0	-3.884889	-1.834165	-0.175821
30	17	0	-0.475954	-1.278337	1.588193
31	17	0	-2.871194	1.787256	0.943768

Int3′-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.156143	-1.428512	0.144048

2	6	0	5.275339	-0.118204	0.629448
3	6	0	4.204611	0.749560	0.565276
4	6	0	2.973613	0.350453	0.011327
5	6	0	2.859364	-0.973714	-0.480904
6	6	0	3.962373	-1.845994	-0.400261
7	1	0	6.003328	-2.109713	0.197006
8	1	0	6.217509	0.219813	1.057076
9	1	0	4.331459	1.761685	0.943828
10	1	0	3.851040	-2.861237	-0.781668
11	6	0	1.821258	1.227671	-0.086728
12	6	0	1.816954	2.528932	0.449725
13	6	0	0.642471	0.767205	-0.732782
14	6	0	0.716308	3.357887	0.357042
15	1	0	2.698678	2.895096	0.971013
16	6	0	-0.453874	1.654317	-0.865038
17	1	0	-0.748414	-2.211582	-1.805240
18	6	0	-0.425853	2.926656	-0.322056
19	1	0	0.748506	4.351471	0.799162
20	1	0	-1.297492	1.393007	-1.507916
21	1	0	-1.282815	3.586671	-0.441117
22	6	0	1.621080	-1.422309	-1.033228
23	1	0	1.548720	-2.468640	-1.336020
24	6	0	0.540755	-0.606675	-1.176727
25	6	0	-0.783609	-1.133524	-1.617899
26	1	0	-1.183251	-0.641937	-2.515228
27	49	0	-2.096877	-0.592917	-0.007794
28	17	0	-1.596009	-1.104328	2.191262
29	17	0	-4.151161	0.453492	-0.299875

Ts5′-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.158103	-1.613124	0.243252
2	6	0	5.342948	-0.275535	0.622209
3	6	0	4.325003	0.641897	0.462349
4	6	0	3.085373	0.265748	-0.086892
5	6	0	2.906296	-1.085025	-0.477948
6	6	0	3.955069	-2.007717	-0.298033

7	1	0	5.962045	-2.334625	0.375529
8	1	0	6.294456	0.043869	1.043172
9	1	0	4.502294	1.674343	0.756116
10	1	0	3.794370	-3.043507	-0.597354
11	6	0	1.985484	1.192184	-0.276369
12	6	0	2.019725	2.514246	0.201820
13	6	0	0.806879	0.753186	-0.934929
14	6	0	0.958382	3.385244	0.039624
15	1	0	2.895376	2.861802	0.745546
16	6	0	-0.239796	1.683287	-1.159224
17	1	0	-0.660683	-2.168251	-1.981407
18	6	0	-0.173421	2.978224	-0.667875
19	1	0	1.016818	4.391072	0.449606
20	1	0	-1.060791	1.435896	-1.835430
21	1	0	-0.996926	3.666895	-0.847529
22	6	0	1.654302	-1.507685	-1.020168
23	1	0	1.521775	-2.572355	-1.223127
24	6	0	0.626733	-0.645226	-1.253746
25	6	0	-0.738821	-1.130488	-1.616310
26	1	0	-1.230580	-0.587251	-2.435461
27	49	0	-1.815134	-0.101785	0.175942
28	17	0	-0.734502	-0.011831	2.202584
29	17	0	-3.725495	1.099425	-0.314624
30	17	0	-2.683656	-2.688415	0.172020
31	1	0	-1.688052	-2.061766	-0.757051

Int4-6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	1.193822	3.806600	0.543121
2	6	0	2.353766	3.469261	-0.169179
3	6	0	2.744856	2.153069	-0.295935
4	6	0	1.991819	1.112650	0.279690
5	6	0	0.830475	1.465787	1.007735
6	6	0	0.442044	2.812104	1.126347
7	1	0	0.889526	4.847360	0.630323
8	1	0	2.949091	4.252746	-0.633985
9	1	0	3.645420	1.928693	-0.862215

10	1	0	-0.469125	3.048925	1.676983
11	6	0	2.332264	-0.293277	0.139308
12	6	0	3.444141	-0.718643	-0.611998
13	6	0	1.524063	-1.291940	0.754653
14	6	0	3.750524	-2.055457	-0.750510
15	1	0	4.076173	0.015063	-1.105439
16	6	0	1.856637	-2.652941	0.596394
17	1	0	-1.255524	-1.449423	2.830292
18	6	0	2.952754	-3.034042	-0.143343
19	1	0	4.614793	-2.349614	-1.343145
20	1	0	1.225460	-3.412203	1.052661
21	1	0	3.191160	-4.088499	-0.264252
22	6	0	0.028622	0.430181	1.601199
23	1	0	-0.791030	0.733285	2.258381
24	1	0	0.234381	-2.383022	3.080963
25	6	0	0.373750	-0.907282	1.537893
26	6	0	-0.406506	-1.918894	2.318834
27	1	0	-0.799441	-2.721187	1.681048
28	49	0	-1.526137	-0.107951	-0.393885
29	17	0	-3.333977	0.743610	0.786189
30	17	0	-0.605125	1.186920	-2.065455
31	17	0	-1.661387	-2.365567	-0.915235

Ts1-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.944150	-3.534599	-0.078918
2	6	0	-3.953160	-2.742347	-0.614932
3	6	0	-3.854020	-1.363819	-0.529133
4	6	0	-2.769418	-0.737204	0.104892
5	6	0	-1.754210	-1.545530	0.665113
6	6	0	-1.859827	-2.932668	0.541508
7	1	0	-2.995889	-4.619000	-0.150215
8	1	0	-4.814416	-3.195700	-1.101286
9	1	0	-4.654961	-0.745614	-0.932200
10	1	0	-1.057025	-3.553075	0.938610
11	6	0	-2.772695	0.738463	0.127901
12	6	0	-3.236752	1.466929	-0.983463

13	6	0	-2.317089	1.481630	1.249282
14	6	0	-3.308848	2.847692	-0.950563
15	1	0	-3.513366	0.932354	-1.889884
16	6	0	-2.484372	2.884945	1.302641
17	1	0	-2.090720	0.953453	2.174799
18	6	0	-2.947599	3.567348	0.200153
19	1	0	-3.651991	3.384209	-1.833326
20	1	0	-2.192337	3.416311	2.205984
21	1	0	-3.036412	4.651073	0.216428
22	6	0	-0.518080	-1.017984	1.353719
23	1	0	0.219191	-1.827337	1.433307
24	1	0	-0.738533	-0.723607	2.394448
25	6	0	0.070545	0.178249	0.679790
26	6	0	-0.449101	1.303652	0.391543
27	1	0	-0.360621	2.234546	-0.152637
28	49	0	2.166559	0.009124	-0.151592
29	17	0	2.570215	1.978347	-1.331094
30	17	0	3.439203	-0.339479	1.768641
31	17	0	1.832839	-1.928470	-1.415972

Int1-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-3.813973	-3.192720	0.022615
2	6	0	-4.610172	-2.171365	-0.486910
3	6	0	-4.122013	-0.873091	-0.532214
4	6	0	-2.836505	-0.578922	-0.068880
5	6	0	-2.036959	-1.604460	0.446618
6	6	0	-2.535235	-2.905545	0.480374
7	1	0	-4.186012	-4.214681	0.055515
8	1	0	-5.614288	-2.384081	-0.847937
9	1	0	-4.755680	-0.070757	-0.909139
10	1	0	-1.896821	-3.704054	0.858536
11	6	0	-2.373420	0.835212	-0.076631
12	6	0	-2.863828	1.754579	-1.088093
13	6	0	-1.895550	1.429517	1.176644
14	6	0	-2.845819	3.096665	-0.887537
15	1	0	-3.224812	1.331621	-2.023857

16	6	0	-2.015640	2.857346	1.378355
17	1	0	-1.860715	0.788602	2.057354
18	6	0	-2.433588	3.656781	0.365980
19	1	0	-2.495964	4.733180	0.509627
20	6	0	-0.624304	-1.337306	0.902412
21	1	0	0.004252	-2.222092	0.720323
22	1	0	-0.586799	-1.202404	2.003668
23	6	0	0.001051	-0.124779	0.326072
24	6	0	-0.735257	1.010090	0.123229
25	1	0	-0.318387	1.880255	-0.386784
26	49	0	2.173952	-0.123351	-0.122276
27	17	0	2.516598	-1.989867	-1.485678
28	17	0	2.555708	1.969330	-1.102621
29	17	0	3.033668	-0.393157	2.046303
30	1	0	-1.755458	3.265460	2.352053
31	1	0	-3.187236	3.763934	-1.676146

Ts2-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.329792	3.649639	-0.294898
2	6	0	-3.548847	3.100993	-0.683176
3	6	0	-3.791634	1.749562	-0.484559
4	6	0	-2.819564	0.928735	0.104638
5	6	0	-1.606157	1.497940	0.529587
6	6	0	-1.366244	2.850314	0.310354
7	1	0	-2.128922	4.706366	-0.459226
8	1	0	-4.305661	3.723233	-1.156121
9	1	0	-4.727599	1.309681	-0.828024
10	1	0	-0.412386	3.274136	0.623264
11	6	0	-3.082766	-0.514944	0.210592
12	6	0	-4.350144	-0.974632	0.588517
13	6	0	-2.137995	-1.497466	-0.247021
14	6	0	-4.691130	-2.314209	0.504639
15	1	0	-5.074021	-0.249663	0.956371
16	6	0	-2.537187	-2.857420	-0.393708
17	1	0	-1.682727	-0.994476	-1.230663
18	6	0	-3.789075	-3.261857	-0.004354

19	1	0	-4.077223	-4.307322	-0.080608
20	6	0	-0.602225	0.634293	1.243782
21	1	0	-1.122685	0.014750	1.998680
22	1	0	0.116234	1.259443	1.790258
23	6	0	0.089180	-0.289817	0.299869
24	6	0	-0.587858	-1.235219	-0.386297
25	1	0	-0.089176	-1.960596	-1.035721
26	49	0	2.260541	-0.141286	-0.028212
27	17	0	3.351835	-0.471100	2.011380
28	17	0	2.667383	-1.771680	-1.675337
29	17	0	2.400782	2.099051	-0.749231
30	1	0	-1.812098	-3.571021	-0.782791
31	1	0	-5.681610	-2.633583	0.823398

Int2-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.461951	3.409252	-0.003391
2	6	0	1.730418	3.455905	-0.595893
3	6	0	2.577441	2.356637	-0.582913
4	6	0	2.187971	1.161267	0.023029
5	6	0	0.889558	1.099907	0.622354
6	6	0	0.046925	2.245190	0.596414
7	1	0	-0.193106	4.275636	-0.032203
8	1	0	2.055436	4.368533	-1.092994
9	1	0	3.541818	2.408798	-1.084668
10	1	0	-0.934635	2.184589	1.071558
11	6	0	3.059693	-0.009904	0.021621
12	6	0	4.451560	0.117143	0.126040
13	6	0	2.483960	-1.289263	-0.090447
14	6	0	5.261238	-1.007672	0.125429
15	1	0	4.893589	1.105428	0.248333
16	6	0	3.310108	-2.409793	-0.089396
17	1	0	0.642388	-2.396611	-0.012682
18	6	0	4.689330	-2.273784	0.014115
19	1	0	5.322103	-3.159268	0.011200
20	6	0	0.648252	0.047352	1.782275
21	1	0	-0.072250	0.428516	2.508820

22	1	0	1.587665	-0.318155	2.207448
23	6	0	0.168314	-0.423122	0.521108
24	6	0	1.002346	-1.389974	-0.280933
25	49	0	-1.963027	-0.365966	-0.074547
26	17	0	-2.560710	-2.594143	-0.434740
27	17	0	-3.034105	0.694243	1.742733
28	17	0	-1.959802	0.963159	-2.013617
29	1	0	2.862439	-3.399002	-0.182567
30	1	0	0.757306	-1.276233	-1.351138
31	1	0	6.339670	-0.900147	0.220818

Ts3-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208927	3.648239	0.087012
2	6	0	-2.371936	3.374448	0.801199
3	6	0	-2.959118	2.119271	0.723335
4	6	0	-2.398790	1.108550	-0.067781
5	6	0	-1.236803	1.406137	-0.805331
6	6	0	-0.642127	2.662212	-0.709359
7	1	0	-0.738565	4.626553	0.157889
8	1	0	-2.813549	4.136809	1.439810
9	1	0	-3.843809	1.899424	1.319579
10	1	0	0.273443	2.856796	-1.269056
11	6	0	-3.040350	-0.221873	-0.110131
12	6	0	-4.439839	-0.303124	-0.137144
13	6	0	-2.319684	-1.439017	-0.035637
14	6	0	-5.099479	-1.521674	-0.099378
15	1	0	-5.013768	0.618836	-0.214247
16	6	0	-2.998042	-2.662060	0.046075
17	1	0	-0.146082	-1.864653	-0.908835
18	6	0	-4.379509	-2.712356	-0.003098
19	1	0	-4.895807	-3.668683	0.039568
20	6	0	-0.608907	0.320438	-1.638085
21	1	0	0.153001	0.726810	-2.314000
22	1	0	-1.371518	-0.205665	-2.234815
23	6	0	0.004300	-0.566664	-0.603067
24	6	0	-0.856222	-1.436759	0.080412

25	49	0	2.114529	-0.273850	0.088392
26	17	0	2.799490	-2.506611	0.282321
27	17	0	3.044651	1.027434	-1.613373
28	17	0	1.869904	0.822695	2.132264
29	1	0	-2.417959	-3.580276	0.140981
30	1	0	-0.416795	-2.076141	0.858757
31	1	0	-6.186707	-1.545595	-0.141593

Int3-7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.334585	3.651545	0.059097
2	6	0	-1.321056	3.337892	0.987892
3	6	0	-2.030738	2.153241	0.866729
4	6	0	-1.778061	1.250433	-0.176944
5	6	0	-0.776824	1.574482	-1.112024
6	6	0	-0.071680	2.772005	-0.981973
7	1	0	0.234994	4.574324	0.147055
8	1	0	-1.525032	4.006463	1.821743
9	1	0	-2.764021	1.890229	1.627172
10	1	0	0.705034	3.005537	-1.708893
11	6	0	-2.559413	-0.003790	-0.217371
12	6	0	-3.915136	0.042726	0.136084
13	6	0	-1.992171	-1.279315	-0.470484
14	6	0	-4.682779	-1.104458	0.264752
15	1	0	-4.375964	1.015530	0.299068
16	6	0	-2.769151	-2.434465	-0.274237
17	1	0	0.994276	-1.065946	-2.210914
18	6	0	-4.104580	-2.357573	0.075243
19	1	0	-4.692453	-3.264530	0.197287
20	6	0	-0.461506	0.639183	-2.249151
21	1	0	0.258295	1.107833	-2.930051
22	1	0	-1.373987	0.430580	-2.834147
23	6	0	0.081058	-0.669967	-1.752002
24	6	0	-0.645400	-1.509664	-0.962462
25	49	0	1.642035	-0.398358	0.278741
26	17	0	2.526626	-2.547948	0.121448
27	17	0	2.970543	1.166550	-0.803076

28	17	0	0.650734	0.109214	2.295476
29	1	0	-2.302986	-3.407369	-0.429678
30	1	0	-0.224003	-2.498691	-0.757186
31	1	0	-5.736104	-1.020951	0.525923

1n-$InCl_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	4.175169	-3.068177	-0.010733
2	6	0	5.138413	-2.071557	0.102680
3	6	0	4.756654	-0.733105	0.100191
4	6	0	3.417365	-0.368861	-0.015338
5	6	0	2.441740	-1.379224	-0.113955
6	6	0	2.835423	-2.721907	-0.115249
7	1	0	4.465515	-4.116749	-0.012547
8	1	0	6.190743	-2.334887	0.190876
9	1	0	5.506393	0.053048	0.183689
10	1	0	2.074104	-3.497535	-0.193788
11	6	0	3.030481	1.061756	-0.034691
12	6	0	2.917377	1.782007	1.157694
13	6	0	2.768113	1.704120	-1.249167
14	6	0	2.527302	3.116605	1.137635
15	1	0	3.126109	1.281039	2.102966
16	6	0	2.382135	3.039068	-1.268690
17	1	0	2.862518	1.141662	-2.178432
18	6	0	2.254435	3.745262	-0.074861
19	1	0	2.436022	3.668277	2.071695
20	1	0	2.183009	3.532119	-2.218836
21	1	0	1.949608	4.790203	-0.089913
22	49	0	-2.493883	-0.208245	0.031743
23	17	0	-2.464147	-0.575720	2.315775
24	17	0	-3.851434	1.458269	-0.810178
25	17	0	-2.231531	-2.111532	-1.268000
26	6	0	1.010417	-1.083860	-0.186156
27	6	0	0.381170	0.062476	-0.144391
28	1	0	0.342562	-1.950074	-0.281622
29	6	0	-0.433377	1.116436	-0.115779
30	1	0	-0.612009	1.705296	-1.021155

31	1	0	-0.640329	1.618086	0.837344

1n′-$InCl_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.410885	3.762556	-0.228186
2	6	0	-1.539185	3.675874	0.580102
3	6	0	-2.259866	2.488199	0.642054
4	6	0	-1.866542	1.362421	-0.079306
5	6	0	-0.698370	1.439699	-0.864351
6	6	0	0.002315	2.650526	-0.946279
7	1	0	0.154210	4.689910	-0.291235
8	1	0	-1.865299	4.538084	1.158741
9	1	0	-3.158434	2.422852	1.254705
10	1	0	0.905417	2.699913	-1.555140
11	6	0	-2.689513	0.132249	-0.005333
12	6	0	-2.747249	-0.607904	1.177440
13	6	0	-3.432440	-0.288164	-1.112663
14	6	0	-3.511576	-1.768555	1.240577
15	1	0	-2.163485	-0.280250	2.037745
16	6	0	-4.205256	-1.441353	-1.044361
17	1	0	-3.399008	0.300466	-2.030299
18	6	0	-4.238541	-2.188953	0.130718
19	1	0	-4.788454	-1.755338	-1.908937
20	1	0	-4.839971	-3.095049	0.183151
21	49	0	1.771598	-0.380124	0.185588
22	17	0	2.394127	-2.609736	0.239242
23	17	0	3.248652	0.997340	-0.947383
24	17	0	0.787007	0.400313	2.120737
25	6	0	-0.118656	0.284290	-1.573223
26	6	0	-0.374266	-1.016113	-1.407669
27	1	0	0.587949	0.537013	-2.374089
28	6	0	-0.649162	-2.286932	-1.355569
29	1	0	-0.085424	-2.985708	-0.736844
30	1	0	-3.538410	-2.347721	2.162044
31	1	0	-1.488616	-2.679706	-1.931481

Ts1-6n

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.936434	-3.150860	0.037640
2	6	0	4.964420	-2.219585	0.199878
3	6	0	4.685361	-0.864919	0.135449
4	6	0	3.385951	-0.411204	-0.125710
5	6	0	2.344063	-1.354232	-0.287589
6	6	0	2.640588	-2.720478	-0.188981
7	1	0	4.149850	-4.215844	0.100712
8	1	0	5.983529	-2.555841	0.379117
9	1	0	5.485958	-0.134742	0.249524
10	1	0	1.831661	-3.442828	-0.290597
11	6	0	3.059629	1.003480	-0.155870
12	6	0	3.641436	1.920850	0.726900
13	6	0	2.045936	1.449650	-1.044217
14	6	0	3.247884	3.247387	0.714316
15	1	0	4.375929	1.573333	1.451565
16	6	0	1.688953	2.822256	-1.062584
17	1	0	1.949403	0.899209	-1.988933
18	6	0	2.268370	3.705482	-0.184990
19	1	0	3.691206	3.944617	1.423022
20	1	0	0.935462	3.162875	-1.771627
21	1	0	1.976872	4.753156	-0.182530
22	49	0	-2.402141	-0.138926	0.096306
23	17	0	-1.823466	0.317897	2.310906
24	17	0	-4.274541	0.967373	-0.731748
25	17	0	-2.278947	-2.434579	-0.392324
26	6	0	0.960907	-0.947361	-0.430143
27	6	0	0.453135	0.243492	-0.734460
28	1	0	0.204000	-1.706575	-0.189820
29	6	0	-0.743472	0.854341	-1.120792
30	1	0	-1.057561	0.711715	-2.162879
31	1	0	-0.890789	1.886759	-0.785811

Int1-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.779120	-2.165221	-0.167326

2	6	0	-5.205132	-0.912511	-0.663650
3	6	0	-4.386982	0.179951	-0.554596
4	6	0	-3.111846	0.083716	0.064488
5	6	0	-2.687295	-1.187060	0.572812
6	6	0	-3.554024	-2.296729	0.434358
7	1	0	-5.430493	-3.031682	-0.265242
8	1	0	-6.182813	-0.817959	-1.130623
9	1	0	-4.735704	1.139090	-0.929993
10	1	0	-3.221019	-3.262317	0.812134
11	6	0	-2.222127	1.181503	0.160999
12	6	0	-2.441518	2.417921	-0.475622
13	6	0	-1.032643	1.067451	1.062380
14	6	0	-1.502958	3.419709	-0.442616
15	1	0	-3.335260	2.562809	-1.075916
16	6	0	-0.015892	2.139148	0.934757
17	1	0	-1.515007	1.322512	2.046650
18	6	0	-0.267675	3.273903	0.242680
19	1	0	-1.698243	4.340676	-0.989376
20	1	0	0.932104	2.028838	1.455921
21	1	0	0.487517	4.053440	0.179356
22	49	0	2.030422	-0.403305	-0.092419
23	17	0	0.390090	0.074920	-1.761415
24	17	0	3.438393	1.476824	0.172085
25	17	0	3.114391	-2.435407	-0.447134
26	6	0	-1.411048	-1.354990	1.158552
27	6	0	-0.534942	-0.319615	1.363842
28	1	0	-1.086785	-2.368772	1.397458
29	6	0	0.822009	-0.517268	1.804399
30	1	0	0.996314	-1.506351	2.240140
31	1	0	1.257032	0.264492	2.435161

Ts2-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	4.751840	-2.309561	0.139023
2	6	0	5.216147	-1.073729	0.638612
3	6	0	4.444567	0.058448	0.549530
4	6	0	3.161614	0.021297	-0.044009

5	6	0	2.699278	-1.229557	-0.557933
6	6	0	3.519337	-2.383143	-0.450297
7	1	0	5.374701	-3.197210	0.223284
8	1	0	6.198567	-1.017354	1.102981
9	1	0	4.837039	0.992454	0.942546
10	1	0	3.139822	-3.325995	-0.841729
11	6	0	2.311457	1.169894	-0.133197
12	6	0	2.638445	2.412121	0.449174
13	6	0	1.047145	1.076582	-0.819810
14	6	0	1.777696	3.481184	0.394175
15	1	0	3.578432	2.523535	0.982220
16	6	0	0.185194	2.213151	-0.889107
17	1	0	1.272168	0.578647	-2.034766
18	6	0	0.538470	3.378923	-0.270508
19	1	0	2.052032	4.414916	0.880359
20	1	0	-0.789668	2.131072	-1.363252
21	1	0	-0.151789	4.218996	-0.276118
22	49	0	-2.096430	-0.374068	0.074382
23	17	0	-3.241103	1.698071	-0.030451
24	17	0	-3.487184	-2.244372	0.218761
25	17	0	-0.470954	-0.308251	1.820149
26	6	0	1.430575	-1.330537	-1.145125
27	6	0	0.561864	-0.246416	-1.321809
28	1	0	1.071419	-2.314772	-1.447950
29	6	0	-0.833067	-0.427047	-1.752890
30	1	0	-0.962546	-1.385314	-2.267799
31	1	0	-1.211384	0.368095	-2.403298

Int2-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-4.489964	-2.450310	-0.270166
2	6	0	-5.145305	-1.228028	-0.401706
3	6	0	-4.447548	-0.035844	-0.263018
4	6	0	-3.075351	-0.030927	0.006862
5	6	0	-2.431095	-1.270948	0.169100
6	6	0	-3.132300	-2.464952	0.016673
7	1	0	-5.036796	-3.384234	-0.380981

8	1	0	-6.213364	-1.203338	-0.610479
9	1	0	-4.981983	0.908677	-0.348167
10	1	0	-2.601812	-3.410959	0.130041
11	6	0	-2.289764	1.208662	0.114493
12	6	0	-2.736648	2.405781	-0.450183
13	6	0	-1.043897	1.185261	0.776753
14	6	0	-1.981804	3.567255	-0.357985
15	1	0	-3.675004	2.421395	-1.002440
16	6	0	-0.300892	2.357802	0.866572
17	1	0	-1.208894	-0.289116	2.290746
18	6	0	-0.759927	3.543889	0.302085
19	1	0	-2.342601	4.486498	-0.815306
20	1	0	0.664889	2.358332	1.368665
21	1	0	-0.149522	4.442251	0.365385
22	49	0	2.210335	-0.187032	0.144633
23	17	0	2.820285	1.680498	-1.089734
24	17	0	3.699209	-1.955525	-0.105544
25	17	0	0.002929	-1.232373	-1.115997
26	6	0	-0.990253	-1.283402	0.510906
27	6	0	-0.580167	-0.116915	1.391115
28	1	0	-0.668800	-2.242107	0.934303
29	6	0	0.879481	-0.185329	1.820694
30	1	0	1.055384	-1.128688	2.357096
31	1	0	1.123491	0.619703	2.522660

Ts3-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.520327	-2.514899	-0.179701
2	6	0	-5.073246	-1.326585	-0.682155
3	6	0	-4.398176	-0.127624	-0.571750
4	6	0	-3.135432	-0.055248	0.042269
5	6	0	-2.585312	-1.261220	0.555085
6	6	0	-3.291299	-2.477539	0.434044
7	1	0	-5.059657	-3.454383	-0.277571
8	1	0	-6.046620	-1.348725	-1.168607
9	1	0	-4.859901	0.768862	-0.977385
10	1	0	-2.837698	-3.385845	0.829770

11	6	0	-2.383430	1.181511	0.168593
12	6	0	-2.870006	2.401912	-0.334941
13	6	0	-1.108192	1.180828	0.793601
14	6	0	-2.134054	3.564296	-0.243624
15	1	0	-3.842617	2.436751	-0.819670
16	6	0	-0.367264	2.371167	0.866701
17	1	0	-0.221140	-0.054096	2.487548
18	6	0	-0.869295	3.549116	0.353229
19	1	0	-2.534312	4.491013	-0.649814
20	1	0	0.632217	2.371648	1.295947
21	1	0	-0.271451	4.456448	0.400821
22	49	0	2.121373	-0.302303	-0.182154
23	17	0	2.958617	1.844184	-0.550603
24	17	0	3.719992	-1.901148	0.394092
25	17	0	0.492963	-1.045171	-1.683077
26	6	0	-1.325179	-1.237204	1.193423
27	6	0	-0.597331	-0.070718	1.327763
28	1	0	-0.921569	-2.168764	1.594223
29	6	0	0.920837	-0.188291	1.768339
30	1	0	1.166194	-1.154261	2.224324
31	1	0	1.358775	0.653482	2.313697

Ts1′-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.288810	3.742568	-0.455431
2	6	0	-1.487259	3.824623	0.240543
3	6	0	-2.254414	2.676795	0.419506
4	6	0	-1.816896	1.454539	-0.084054
5	6	0	-0.586124	1.358965	-0.761994
6	6	0	0.159567	2.519536	-0.950737
7	1	0	0.319284	4.632294	-0.604878
8	1	0	-1.831053	4.776167	0.640058
9	1	0	-3.216852	2.732054	0.927991
10	1	0	1.125095	2.461049	-1.452589
11	6	0	-2.662570	0.261018	-0.013328
12	6	0	-3.248472	-0.201966	1.164416
13	6	0	-2.815730	-0.496573	-1.218989

14	6	0	-4.033171	-1.345108	1.136326
15	1	0	-3.059876	0.326528	2.097051
16	6	0	-3.704846	-1.600933	-1.233066
17	1	0	-2.615368	0.007900	-2.165400
18	6	0	-4.270477	-2.046969	-0.060313
19	1	0	-3.901078	-2.110988	-2.174613
20	1	0	-4.919489	-2.919831	-0.054205
21	49	0	1.729838	-0.365379	0.124407
22	17	0	2.544300	-2.546092	-0.220341
23	17	0	3.356188	1.194690	-0.496289
24	17	0	0.756828	-0.093338	2.242908
25	6	0	-0.104467	0.016651	-1.216004
26	6	0	-0.967066	-1.099146	-0.962225
27	1	0	0.261099	0.032137	-2.253322
28	6	0	-0.907494	-2.382123	-0.668475
29	1	0	0.076896	-2.817452	-0.468269
30	1	0	-4.479808	-1.706588	2.061279
31	1	0	-1.765937	-3.040390	-0.612826

Int1′-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.619782	3.843539	-0.719235
2	6	0	-1.842133	3.746600	-0.016973
3	6	0	-2.409508	2.517850	0.179643
4	6	0	-1.797619	1.335706	-0.325641
5	6	0	-0.563071	1.442090	-1.045072
6	6	0	-0.000345	2.725232	-1.218466
7	1	0	-0.162174	4.820242	-0.866232
8	1	0	-2.325725	4.643989	0.361134
9	1	0	-3.363289	2.449163	0.697988
10	1	0	0.953050	2.808499	-1.738617
11	6	0	-2.337478	0.047923	-0.096660
12	6	0	-3.338006	-0.204891	0.865788
13	6	0	-1.947115	-1.094946	-0.993768
14	6	0	-3.736956	-1.484117	1.156913
15	1	0	-3.725102	0.612522	1.467865
16	6	0	-2.256647	-2.447361	-0.458460

17	1	0	-2.714969	-0.966144	-1.796931
18	6	0	-3.157013	-2.625287	0.532046
19	1	0	-1.780503	-3.298090	-0.939823
20	1	0	-3.412098	-3.621053	0.885395
21	49	0	1.519809	-0.234372	0.294718
22	17	0	3.053402	-1.781351	-0.539511
23	17	0	2.467543	1.741579	1.102869
24	17	0	-0.057368	-1.179429	1.788467
25	6	0	0.150993	0.266235	-1.469820
26	6	0	-0.594328	-0.982455	-1.691512
27	1	0	0.924519	0.455161	-2.224706
28	6	0	-0.125652	-1.967487	-2.467304
29	1	0	0.835209	-1.866617	-2.969049
30	1	0	-4.478115	-1.634791	1.940673
31	1	0	-0.654275	-2.904011	-2.628797

Ts2′-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.387870	3.824521	0.550358
2	6	0	2.610479	3.454704	-0.014281
3	6	0	2.923229	2.114167	-0.145244
4	6	0	2.034190	1.120613	0.290689
5	6	0	0.819910	1.498371	0.905791
6	6	0	0.507092	2.858465	1.007981
7	1	0	1.125719	4.877080	0.639799
8	1	0	3.310778	4.213457	-0.356330
9	1	0	3.881146	1.830266	-0.577684
10	1	0	-0.447487	3.147232	1.448071
11	6	0	2.288480	-0.297743	0.063905
12	6	0	3.197720	-0.748070	-0.904212
13	6	0	1.571620	-1.294120	0.784478
14	6	0	3.394073	-2.095001	-1.137668
15	1	0	3.721192	-0.019636	-1.517890
16	6	0	1.769318	-2.671020	0.530249
17	1	0	1.639136	-0.930861	2.121962
18	6	0	2.676287	-3.065564	-0.424661
19	1	0	1.159405	-3.408646	1.046301

20	1	0	2.804670	-4.121100	-0.650735
21	49	0	-1.538016	-0.050279	-0.315751
22	17	0	-2.331962	-2.154159	0.445816
23	17	0	-3.136952	1.647423	-0.351628
24	17	0	-0.262059	-0.292858	-2.271537
25	6	0	-0.125754	0.473513	1.376187
26	6	0	0.453219	-0.822937	1.739941
27	1	0	-0.814242	0.850906	2.143268
28	6	0	-0.038591	-1.673210	2.696428
29	1	0	-0.897944	-1.385606	3.297137
30	1	0	4.094650	-2.405536	-1.910250
31	1	0	0.397468	-2.650910	2.883433

Int3-6n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	1.191258	3.807037	0.543738
2	6	0	2.351388	3.470618	-0.168679
3	6	0	2.743352	2.154712	-0.295698
4	6	0	1.991047	1.113686	0.279780
5	6	0	0.829468	1.465904	1.007878
6	6	0	0.440150	2.811924	1.126773
7	1	0	0.886289	4.847580	0.631201
8	1	0	2.946161	4.254578	-0.633392
9	1	0	3.644026	1.931025	-0.862081
10	1	0	-0.471158	3.048057	1.677480
11	6	0	2.332462	-0.291994	0.139232
12	6	0	3.444597	-0.716511	-0.612163
13	6	0	1.525005	-1.291306	0.754534
14	6	0	3.751839	-2.053101	-0.750915
15	1	0	4.076175	0.017658	-1.105500
16	6	0	1.858485	-2.652054	0.596051
17	1	0	0.236192	-2.383581	3.080655
18	6	0	2.954771	-3.032315	-0.143854
19	1	0	4.616253	-2.346597	-1.343671
20	1	0	1.227876	-3.411810	1.052290
21	1	0	3.193845	-4.086595	-0.264983
22	49	0	-1.525939	-0.108533	-0.393866

23	17	0	-1.658595	-2.366081	-0.916249
24	17	0	-3.334746	0.739994	0.786919
25	17	0	-0.607263	1.188174	-2.065277
26	6	0	0.028295	0.429639	1.601182
27	6	0	0.374488	-0.907543	1.537869
28	1	0	-0.791491	0.732156	2.258483
29	6	0	-0.405109	-1.919809	2.318653
30	1	0	-1.254335	-1.450959	2.830304
31	1	0	-0.797510	-2.722186	1.680652

Ts1-7n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	3.745775	-3.324020	-0.116514
2	6	0	4.745973	-2.379967	0.090228
3	6	0	4.409953	-1.034760	0.138719
4	6	0	3.090695	-0.604017	-0.041751
5	6	0	2.064067	-1.557685	-0.236455
6	6	0	2.429656	-2.911660	-0.255442
7	1	0	3.988772	-4.383906	-0.157393
8	1	0	5.782213	-2.687541	0.213689
9	1	0	5.186450	-0.284546	0.288569
10	1	0	1.643186	-3.655964	-0.377824
11	6	0	2.853307	0.847713	-0.017030
12	6	0	3.322773	1.633599	1.032355
13	6	0	2.153020	1.485931	-1.083132
14	6	0	3.173268	3.017959	1.006150
15	1	0	3.803480	1.152251	1.882344
16	6	0	2.112504	2.903964	-1.138938
17	1	0	2.025950	0.917951	-2.006713
18	6	0	2.578284	3.661512	-0.083328
19	1	0	3.530801	3.608119	1.848133
20	1	0	1.639307	3.382238	-1.995714
21	1	0	2.491177	4.745016	-0.100050
22	49	0	-2.280402	-0.153822	0.083456
23	17	0	-2.500340	1.128779	2.028910
24	17	0	-3.159164	0.946682	-1.793220
25	17	0	-2.777949	-2.420850	0.270674

26	6	0	0.618515	-1.290177	-0.258303
27	6	0	-0.036346	-0.129569	-0.314725
28	1	0	0.016398	-2.193976	-0.121575
29	6	0	0.250305	1.223574	-0.551258
30	1	0	-0.143832	1.636123	-1.486517
31	1	0	0.141989	1.918711	0.292054

Int1-7n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-3.541391	3.447537	-0.142868
2	6	0	-4.581202	2.574262	0.192370
3	6	0	-4.320291	1.224919	0.273816
4	6	0	-3.038440	0.690369	-0.001835
5	6	0	-1.970503	1.581924	-0.328974
6	6	0	-2.272294	2.955448	-0.376396
7	1	0	-3.727812	4.517112	-0.218491
8	1	0	-5.584971	2.950929	0.374158
9	1	0	-5.139801	0.542131	0.489063
10	1	0	-1.461054	3.646574	-0.600482
11	6	0	-2.905383	-0.743810	0.011261
12	6	0	-3.712879	-1.537072	0.843432
13	6	0	-1.933041	-1.419442	-0.864911
14	6	0	-3.709325	-2.912791	0.743722
15	1	0	-4.337084	-1.061649	1.595814
16	6	0	-2.099300	-2.871267	-1.015085
17	1	0	-1.851889	-0.905574	-1.835049
18	6	0	-2.925160	-3.596218	-0.219167
19	1	0	-4.331167	-3.491516	1.425435
20	1	0	-1.438139	-3.365907	-1.726421
21	1	0	-2.974899	-4.679180	-0.294590
22	49	0	2.282106	0.103581	0.089300
23	17	0	2.988641	2.333335	0.009946
24	17	0	2.556645	-0.990394	2.154975
25	17	0	3.071549	-1.262472	-1.671873
26	6	0	-0.551672	1.257642	-0.435131
27	6	0	0.106543	0.096776	-0.262489
28	1	0	0.068528	2.157141	-0.510694

29	6	0	-0.437716	-1.269201	-0.283206
30	1	0	0.173377	-1.875651	-0.969783
31	1	0	-0.352109	-1.752305	0.706267

Ts2-7n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.109367	-3.010231	-0.017143
2	6	0	4.967464	-1.938215	0.261145
3	6	0	4.469040	-0.654659	0.330167
4	6	0	3.091190	-0.388220	0.188889
5	6	0	2.211469	-1.490309	-0.039108
6	6	0	2.762488	-2.778441	-0.190105
7	1	0	4.504512	-4.020706	-0.097101
8	1	0	6.030109	-2.114952	0.413994
9	1	0	5.144493	0.172765	0.541435
10	1	0	2.085382	-3.601740	-0.414017
11	6	0	2.642155	0.993347	0.098951
12	6	0	3.439230	1.960708	-0.528787
13	6	0	1.327523	1.393779	0.548465
14	6	0	2.994110	3.261808	-0.687598
15	1	0	4.405558	1.672022	-0.936837
16	6	0	0.923146	2.763483	0.412885
17	1	0	0.598896	0.790113	-0.426970
18	6	0	1.730368	3.667779	-0.228799
19	1	0	3.632083	3.978978	-1.201130
20	1	0	-0.067626	3.039824	0.772387
21	1	0	1.400733	4.694163	-0.369588
22	49	0	-2.166174	-0.249832	-0.057169
23	17	0	-2.469058	-1.556718	-1.978054
24	17	0	-3.325606	-0.899322	1.864256
25	17	0	-2.397249	2.085017	-0.419307
26	6	0	0.797205	-1.315275	-0.264431
27	6	0	-0.016759	-0.411165	0.378317
28	1	0	0.348900	-1.943480	-1.042021
29	6	0	0.590364	0.445833	1.471668
30	1	0	-0.171402	0.970069	2.061467
31	1	0	1.263229	-0.089239	2.155356

Int2-7n

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.927243	3.634255	-0.076358
2	6	0	-2.120105	3.461259	0.622636
3	6	0	-2.748220	2.225251	0.640057
4	6	0	-2.196765	1.106321	0.000871
5	6	0	-0.955080	1.278323	-0.660856
6	6	0	-0.363203	2.550354	-0.723534
7	1	0	-0.439201	4.605649	-0.107495
8	1	0	-2.570337	4.299552	1.151184
9	1	0	-3.686713	2.107238	1.179488
10	1	0	0.577431	2.662520	-1.265537
11	6	0	-2.992515	-0.140907	-0.056052
12	6	0	-4.371212	-0.052865	-0.292920
13	6	0	-2.426902	-1.417935	0.112130
14	6	0	-5.166147	-1.188688	-0.363059
15	1	0	-4.819526	0.926578	-0.455801
16	6	0	-3.229904	-2.552702	0.033232
17	1	0	0.269685	-1.862648	-1.471846
18	6	0	-4.595590	-2.446271	-0.198569
19	1	0	-6.232757	-1.090200	-0.556083
20	1	0	-2.772183	-3.532323	0.172290
21	1	0	-5.211433	-3.342248	-0.248204
22	49	0	2.070566	-0.284933	0.089157
23	17	0	3.157612	0.981088	-1.520287
24	17	0	1.477507	0.809827	2.036235
25	17	0	2.740332	-2.490072	0.304373
26	6	0	-0.241388	0.184887	-1.306252
27	6	0	-0.195760	-1.097066	-0.844756
28	1	0	0.312817	0.430726	-2.216953
29	6	0	-0.952790	-1.530947	0.382028
30	1	0	-0.676301	-2.555486	0.657642
31	1	0	-0.694908	-0.881567	1.235589

1b-AuPH$_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.825207	3.286337	-0.174643
2	6	0	4.664231	2.366605	-0.794170
3	6	0	4.361300	1.011178	-0.747271
4	6	0	3.227496	0.550777	-0.074485
5	6	0	2.376559	1.486644	0.535093
6	6	0	2.681405	2.844514	0.479983
7	1	0	4.054234	4.349173	-0.208031
8	1	0	5.557702	2.704052	-1.315009
9	1	0	5.021258	0.285125	-1.220947
10	1	0	2.013324	3.566993	0.949642
11	6	0	2.914318	-0.895641	-0.039888
12	6	0	2.757224	-1.571945	1.180542
13	6	0	2.749201	-1.611391	-1.232772
14	6	0	2.410691	-2.919871	1.207979
15	1	0	2.945275	-1.039756	2.113626
16	6	0	2.390610	-2.951884	-1.204812
17	1	0	2.878562	-1.095702	-2.184050
18	6	0	2.208989	-3.607579	0.016675
19	1	0	2.306347	-3.432732	2.162056
20	1	0	2.257743	-3.495617	-2.138446
21	1	0	1.937608	-4.661407	0.033107
22	6	0	1.115037	1.050888	1.260060
23	1	0	0.398810	1.889830	1.271999
24	1	0	1.303097	0.814722	2.319997
25	6	0	0.428058	-0.071320	0.646616
26	6	0	-0.318289	-0.930315	0.127197
27	1	0	-0.204203	-1.948258	-0.239871
28	15	0	-4.416112	0.832876	-0.294868
29	1	0	-4.580075	2.215263	-0.127459
30	1	0	-5.387581	0.325250	0.579416
31	1	0	-5.020938	0.626058	-1.542577
32	79	0	-2.227743	-0.023014	-0.039836

Ts1-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.910900	-3.212183	-0.127474

2	6	0	-4.704898	-2.280364	-0.789544
3	6	0	-4.349309	-0.937970	-0.781765
4	6	0	-3.205750	-0.515176	-0.099337
5	6	0	-2.399931	-1.458625	0.556658
6	6	0	-2.759051	-2.801703	0.535864
7	1	0	-4.183117	-4.265343	-0.136361
8	1	0	-5.603387	-2.599511	-1.312806
9	1	0	-4.978839	-0.202045	-1.280814
10	1	0	-2.126050	-3.536878	1.032770
11	6	0	-2.814067	0.899646	-0.061823
12	6	0	-2.830760	1.704963	-1.211625
13	6	0	-2.353128	1.465569	1.156849
14	6	0	-2.416164	3.021014	-1.142332
15	1	0	-3.150727	1.274571	-2.158919
16	6	0	-1.998409	2.830005	1.221943
17	1	0	-2.540701	0.933878	2.089328
18	6	0	-1.993836	3.591287	0.076696
19	1	0	-2.423399	3.633185	-2.042481
20	1	0	-1.715391	3.262175	2.179314
21	1	0	-1.701856	4.638563	0.109255
22	6	0	-1.124448	-1.014643	1.235369
23	1	0	-0.326791	-1.751645	1.046690
24	1	0	-1.244431	-0.968885	2.329421
25	6	0	-0.619108	0.275991	0.728012
26	6	0	0.336553	0.936108	0.180036
27	1	0	0.255834	1.968191	-0.163184
28	79	0	2.187862	0.008859	-0.050630
29	15	0	4.334388	-0.963225	-0.350729
30	1	0	4.606248	-2.156851	0.335360
31	1	0	5.438431	-0.183500	0.026401
32	1	0	4.696524	-1.320891	-1.658400

Int1-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	3.328501	3.533490	-0.034329
2	6	0	4.363362	2.772880	-0.586678
3	6	0	4.265639	1.397949	-0.594445

4	6	0	3.140552	0.748456	-0.037063
5	6	0	2.099716	1.527419	0.530639
6	6	0	2.212940	2.913312	0.513917
7	1	0	3.396055	4.619506	-0.034440
8	1	0	5.240487	3.260721	-1.004353
9	1	0	5.087697	0.811840	-0.999074
10	1	0	1.407716	3.514710	0.934435
11	6	0	3.031622	-0.685781	-0.039209
12	6	0	3.808462	-1.509170	-0.865010
13	6	0	2.024266	-1.313440	0.856649
14	6	0	3.649844	-2.879242	-0.836386
15	1	0	4.512733	-1.076319	-1.570294
16	6	0	1.916885	-2.780771	0.806536
17	1	0	2.343989	-1.079194	1.897654
18	6	0	2.709415	-3.533436	0.008659
19	1	0	4.263234	-3.487783	-1.500275
20	1	0	1.172501	-3.237338	1.457949
21	1	0	2.634334	-4.617374	-0.007049
22	6	0	0.877144	0.881543	1.118055
23	1	0	-0.015315	1.475454	0.873637
24	1	0	0.972436	0.911002	2.221205
25	6	0	0.691480	-0.543073	0.682713
26	6	0	-0.419760	-1.083971	0.181655
27	1	0	-0.381538	-2.134378	-0.118304
28	79	0	-2.229324	-0.151016	-0.066979
29	15	0	-4.385073	0.859835	-0.379615
30	1	0	-5.444555	0.020248	-0.763467
31	1	0	-4.516056	1.866458	-1.351731
32	1	0	-4.981395	1.508228	0.715477

Ts2-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.263614	3.609769	-0.105619
2	6	0	-4.412879	2.904646	-0.450601
3	6	0	-4.414573	1.518878	-0.395950
4	6	0	-3.271464	0.819269	0.010271
5	6	0	-2.108311	1.535905	0.342975

6	6	0	-2.117161	2.923991	0.283660
7	1	0	-3.256446	4.696698	-0.147827
8	1	0	-5.306499	3.435455	-0.770566
9	1	0	-5.305787	0.973401	-0.701460
10	1	0	-1.216376	3.476061	0.550809
11	6	0	-3.251467	-0.643562	0.076329
12	6	0	-4.417460	-1.407140	0.184096
13	6	0	-2.014408	-1.348555	-0.007332
14	6	0	-4.374818	-2.792019	0.164263
15	1	0	-5.374817	-0.903359	0.296039
16	6	0	-1.982672	-2.763062	-0.026751
17	1	0	-1.375758	-0.772457	-0.968183
18	6	0	-3.157235	-3.476460	0.051763
19	1	0	-5.302050	-3.355025	0.248453
20	1	0	-1.026746	-3.280507	-0.064101
21	1	0	-3.135515	-4.563076	0.058081
22	6	0	-0.888660	0.789510	0.809570
23	1	0	-0.985880	0.562918	1.886225
24	1	0	0.008939	1.410941	0.695185
25	6	0	-0.680981	-0.514793	0.093619
26	6	0	0.510025	-1.010583	-0.343658
27	1	0	0.456908	-1.953331	-0.898921
28	15	0	4.561828	0.741964	0.165421
29	1	0	4.660784	2.139404	0.257749
30	1	0	5.499198	0.486595	-0.847685
31	1	0	5.296390	0.359636	1.299019
32	79	0	2.367219	-0.186299	-0.094860

Int2-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.699024	-2.563623	0.288865
2	6	0	5.346202	-1.363350	0.575724
3	6	0	4.647168	-0.169175	0.525651
4	6	0	3.283699	-0.142797	0.193572
5	6	0	2.648510	-1.355761	-0.110132
6	6	0	3.354206	-2.553444	-0.053570
7	1	0	5.246723	-3.502976	0.318487

8	1	0	6.403317	-1.358918	0.831201
9	1	0	5.183217	0.754458	0.729158
10	1	0	2.843687	-3.486522	-0.293225
11	6	0	2.513072	1.102204	0.127205
12	6	0	3.053549	2.316331	0.574022
13	6	0	1.202421	1.130331	-0.436730
14	6	0	2.360533	3.506916	0.455885
15	1	0	4.036433	2.333402	1.036011
16	6	0	0.522254	2.364399	-0.559148
17	1	0	-0.735864	-1.058579	-2.237312
18	6	0	1.084187	3.539581	-0.120288
19	1	0	2.813395	4.427158	0.819728
20	1	0	-0.483007	2.381143	-0.975785
21	1	0	0.542036	4.477851	-0.206583
22	6	0	1.192601	-1.379912	-0.456094
23	1	0	0.636803	-1.690012	0.448820
24	1	0	0.976796	-2.162543	-1.196889
25	6	0	0.583202	-0.085151	-0.885630
26	6	0	-0.592537	-0.131574	-1.673630
27	1	0	-0.850712	0.759051	-2.251034
28	15	0	-3.936584	-0.396117	1.380564
29	1	0	-3.796337	-1.322704	2.425038
30	1	0	-5.186405	-0.763774	0.860094
31	1	0	-4.268455	0.766262	2.092604
32	79	0	-2.148119	-0.251916	-0.174468

Ts3-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	4.669815	-2.465118	0.494339
2	6	0	5.138578	-1.260706	1.041507
3	6	0	4.427124	-0.081402	0.911688
4	6	0	3.199967	-0.048532	0.232342
5	6	0	2.733594	-1.274769	-0.321436
6	6	0	3.478750	-2.467562	-0.190928
7	1	0	5.246540	-3.379487	0.606814
8	1	0	6.084493	-1.250726	1.579362
9	1	0	4.839733	0.823079	1.349447

10	1	0	3.089252	-3.383957	-0.633030
11	6	0	2.408503	1.162717	0.061040
12	6	0	2.831809	2.395355	0.590066
13	6	0	1.173237	1.123088	-0.637368
14	6	0	2.071331	3.537615	0.443529
15	1	0	3.773548	2.464011	1.127685
16	6	0	0.413323	2.291136	-0.773639
17	1	0	-0.809795	-1.259191	-2.254399
18	6	0	0.852297	3.487187	-0.238605
19	1	0	2.424931	4.477815	0.860771
20	1	0	-0.535978	2.256348	-1.302539
21	1	0	0.250227	4.386020	-0.349766
22	6	0	1.493112	-1.302196	-0.993344
23	1	0	1.130266	-2.245234	-1.409519
24	1	0	1.442389	-0.358669	-2.166063
25	6	0	0.693215	-0.141606	-1.230717
26	6	0	-0.709212	-0.306907	-1.717634
27	1	0	-0.991716	0.490956	-2.413416
28	79	0	-2.103384	-0.312382	-0.139820
29	15	0	-3.758635	-0.344721	1.589955
30	1	0	-4.214900	-1.596814	2.034901
31	1	0	-4.986943	0.281065	1.318601
32	1	0	-3.447823	0.254005	2.822595

Int3-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	1.907787	3.741395	0.306652
2	6	0	2.619361	3.228097	-0.798626
3	6	0	2.752659	1.870281	-1.024729
4	6	0	2.181836	0.931797	-0.152497
5	6	0	1.459338	1.454905	0.978389
6	6	0	1.332664	2.862043	1.180146
7	1	0	1.825407	4.814947	0.453037
8	1	0	3.079645	3.923305	-1.498816
9	1	0	3.315084	1.544717	-1.894826
10	1	0	0.773681	3.210669	2.047637
11	6	0	2.294305	-0.501855	-0.339228

12	6	0	3.007735	-1.054650	-1.422885
13	6	0	1.702964	-1.378256	0.600082
14	6	0	3.137671	-2.420189	-1.564919
15	1	0	3.471433	-0.408259	-2.163479
16	6	0	1.854498	-2.755946	0.447611
17	1	0	-1.095518	-1.030106	2.595712
18	6	0	2.562810	-3.278188	-0.621608
19	1	0	3.692155	-2.827448	-2.406978
20	1	0	1.415194	-3.424936	1.187624
21	1	0	2.674486	-4.355248	-0.725607
22	6	0	0.894256	0.584602	1.888980
23	1	0	0.359507	0.996364	2.748615
24	1	0	1.283234	-1.316176	2.696301
25	6	0	0.913654	-0.865250	1.756974
26	6	0	-0.613817	-1.224784	1.629123
27	1	0	-0.674455	-2.302327	1.429418
28	79	0	-1.675960	-0.256579	0.110168
29	15	0	-3.034012	0.749156	-1.607959
30	1	0	-4.169067	1.473056	-1.203465
31	1	0	-3.625570	-0.116265	-2.544298
32	1	0	-2.460523	1.686101	-2.485518

Ts4-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.806416	-2.247497	0.568180
2	6	0	5.205541	-0.993383	1.056144
3	6	0	4.410161	0.122277	0.884733
4	6	0	3.174911	0.039443	0.218235
5	6	0	2.779317	-1.233733	-0.276708
6	6	0	3.606631	-2.362254	-0.092760
7	1	0	5.443893	-3.116842	0.709838
8	1	0	6.156790	-0.895306	1.575141
9	1	0	4.763166	1.072802	1.275941
10	1	0	3.276538	-3.323567	-0.485557
11	6	0	2.303053	1.184039	0.010066
12	6	0	2.632220	2.467657	0.485002
13	6	0	1.068294	1.030699	-0.678671

14	6	0	1.795194	3.547485	0.295772
15	1	0	3.566599	2.623983	1.017173
16	6	0	0.222693	2.141453	-0.854461
17	1	0	-0.877447	-1.579460	-2.151248
18	6	0	0.579425	3.386312	-0.376686
19	1	0	2.083999	4.526034	0.672746
20	1	0	-0.720100	2.030650	-1.387544
21	1	0	-0.081933	4.236616	-0.526991
22	6	0	1.555020	-1.360268	-0.978148
23	1	0	1.281977	-2.336362	-1.383160
24	1	0	0.361491	-0.409792	-2.414414
25	6	0	0.719132	-0.285876	-1.163617
26	6	0	-0.721351	-0.548288	-1.815266
27	1	0	-1.156783	0.201405	-2.488147
28	79	0	-2.070262	-0.356492	-0.126537
29	15	0	-3.564339	-0.237926	1.691037
30	1	0	-3.411251	-1.201734	2.698780
31	1	0	-4.926600	-0.371980	1.385514
32	1	0	-3.564502	0.946944	2.441880

Int4-6Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.146620	3.818741	0.350116
2	6	0	2.160102	3.499271	-0.564568
3	6	0	2.518947	2.185301	-0.786270
4	6	0	1.881064	1.130797	-0.105263
5	6	0	0.854196	1.465324	0.811596
6	6	0	0.498500	2.808637	1.027251
7	1	0	0.878686	4.857772	0.527863
8	1	0	2.675364	4.294027	-1.099577
9	1	0	3.316500	1.978163	-1.494886
10	1	0	-0.289968	3.036097	1.745302
11	6	0	2.240622	-0.267233	-0.286948
12	6	0	3.243641	-0.662046	-1.190500
13	6	0	1.586491	-1.287456	0.466104
14	6	0	3.598417	-1.986740	-1.340791
15	1	0	3.762971	0.084240	-1.785380

16	6	0	1.971361	-2.634990	0.298376
17	1	0	-0.800510	-1.521949	2.976471
18	6	0	2.962876	-2.984517	-0.589436
19	1	0	4.382481	-2.255429	-2.045564
20	1	0	1.479698	-3.411026	0.880494
21	1	0	3.251670	-4.026324	-0.706168
22	6	0	0.171709	0.407558	1.533954
23	1	0	-0.434223	0.696093	2.399258
24	1	0	0.772312	-2.340771	3.013416
25	6	0	0.558429	-0.936416	1.414195
26	6	0	-0.014970	-1.957615	2.349321
27	1	0	-0.439723	-2.821033	1.822857
28	79	0	-1.424946	-0.103052	0.030654
29	15	0	-3.159408	-0.324929	-1.540366
30	1	0	-3.841490	0.850766	-1.884754
31	1	0	-4.218779	-1.172670	-1.187709
32	1	0	-2.801175	-0.824608	-2.800610

Ts1-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.306520	-3.464752	-0.173664
2	6	0	-4.222561	-2.590536	-0.746385
3	6	0	-3.991900	-1.224853	-0.687057
4	6	0	-2.861736	-0.694702	-0.048583
5	6	0	-1.933107	-1.583933	0.531032
6	6	0	-2.172958	-2.956879	0.445440
7	1	0	-3.468738	-4.539632	-0.212877
8	1	0	-5.117731	-2.968925	-1.234767
9	1	0	-4.724382	-0.540178	-1.112786
10	1	0	-1.447064	-3.645472	0.878251
11	6	0	-2.739242	0.780833	-0.024842
12	6	0	-3.044958	1.535409	-1.177023
13	6	0	-2.416223	1.489880	1.155503
14	6	0	-3.044984	2.917736	-1.141963
15	1	0	-3.266977	1.012918	-2.105850
16	6	0	-2.461757	2.892240	1.194248
17	1	0	-2.251776	0.937742	2.080100

18	6	0	-2.761641	3.604841	0.048269
19	1	0	-3.277234	3.477751	-2.045729
20	1	0	-2.251759	3.407382	2.129027
21	1	0	-2.788542	4.691960	0.068498
22	6	0	-0.654893	-1.157662	1.217933
23	1	0	0.010519	-2.023903	1.305217
24	1	0	-0.843665	-0.831880	2.254456
25	6	0	0.040391	-0.016613	0.538913
26	6	0	-0.387658	1.120646	0.166188
27	1	0	-0.337330	2.084601	-0.317619
28	79	0	2.083715	-0.025428	0.005801
29	15	0	4.392339	-0.157886	-0.528510
30	1	0	4.922711	-1.446736	-0.686987
31	1	0	5.288996	0.393408	0.398935
32	1	0	4.812879	0.458119	-1.716576

Int1-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-3.642831	-3.270268	-0.100222
2	6	0	-4.427016	-2.289992	-0.699692
3	6	0	-3.987019	-0.973553	-0.727996
4	6	0	-2.761164	-0.622578	-0.155596
5	6	0	-1.975490	-1.606927	0.451120
6	6	0	-2.422409	-2.926021	0.467236
7	1	0	-3.978139	-4.304831	-0.079901
8	1	0	-5.385598	-2.548289	-1.143926
9	1	0	-4.616300	-0.204611	-1.174527
10	1	0	-1.797486	-3.693096	0.924690
11	6	0	-2.353604	0.807883	-0.144600
12	6	0	-2.788869	1.692149	-1.209633
13	6	0	-1.987158	1.438939	1.126182
14	6	0	-2.840710	3.037660	-1.031181
15	1	0	-3.065301	1.241831	-2.161146
16	6	0	-2.170380	2.865558	1.292345
17	1	0	-2.001658	0.815101	2.020038
18	6	0	-2.546342	3.633342	0.238602
19	1	0	-3.154217	3.677229	-1.853604

20	1	0	-2.005614	3.297567	2.276668
21	1	0	-2.668921	4.707195	0.360407
22	6	0	-0.633470	-1.264614	1.054221
23	1	0	0.024996	-2.141597	1.026800
24	1	0	-0.752413	-1.041259	2.134639
25	6	0	0.023478	-0.072405	0.451601
26	6	0	-0.729109	1.042423	0.181078
27	1	0	-0.318999	1.911833	-0.329355
28	79	0	2.031558	-0.099194	0.003705
29	15	0	4.377211	-0.154828	-0.502808
30	1	0	4.965997	-1.414760	-0.693457
31	1	0	5.252472	0.397759	0.445611
32	1	0	4.802521	0.509117	-1.664278

Ts2-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.268210	-3.462775	-0.087686
2	6	0	-4.116591	-2.608501	-0.785142
3	6	0	-3.846852	-1.250336	-0.814457
4	6	0	-2.740735	-0.716294	-0.131610
5	6	0	-1.876047	-1.584728	0.566175
6	6	0	-2.157235	-2.948912	0.569109
7	1	0	-3.463621	-4.532688	-0.066260
8	1	0	-4.989610	-2.998600	-1.302915
9	1	0	-4.534883	-0.582310	-1.329595
10	1	0	-1.476739	-3.623721	1.087896
11	6	0	-2.589819	0.739184	-0.121949
12	6	0	-3.030061	1.535005	-1.216158
13	6	0	-2.072321	1.433113	1.049901
14	6	0	-3.133864	2.894426	-1.092089
15	1	0	-3.293559	1.047129	-2.151560
16	6	0	-2.347453	2.863508	1.179483
17	1	0	-2.108689	0.872659	1.987986
18	6	0	-2.827037	3.570393	0.129346
19	1	0	-3.479628	3.478872	-1.943123
20	1	0	-2.102534	3.346237	2.123200
21	1	0	-2.993602	4.641917	0.205061

22	6	0	-0.614966	-1.104380	1.239043
23	1	0	0.074984	-1.949617	1.346005
24	1	0	-0.845510	-0.796418	2.278858
25	6	0	0.051111	0.065324	0.574382
26	6	0	-0.642254	1.194120	0.365947
27	1	0	-0.311403	2.044933	-0.227138
28	79	0	2.034832	-0.023674	0.013470
29	15	0	4.342579	-0.149194	-0.617472
30	1	0	4.668139	-0.909262	-1.752475
31	1	0	5.235924	-0.697542	0.317225
32	1	0	5.004296	1.051708	-0.920964

Int2-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.022909	3.570540	-0.063976
2	6	0	3.955685	2.797008	-0.750066
3	6	0	3.809635	1.423433	-0.775734
4	6	0	2.750993	0.781311	-0.100009
5	6	0	1.802491	1.572996	0.597742
6	6	0	1.961366	2.957518	0.588838
7	1	0	3.117844	4.654082	-0.043288
8	1	0	4.795117	3.264924	-1.258617
9	1	0	4.566051	0.824635	-1.278323
10	1	0	1.222430	3.571051	1.103134
11	6	0	2.731557	-0.672050	-0.111660
12	6	0	3.313106	-1.410098	-1.165916
13	6	0	2.088601	-1.427111	0.967390
14	6	0	3.452343	-2.774944	-1.073323
15	1	0	3.654346	-0.896747	-2.061039
16	6	0	2.402620	-2.855389	1.075493
17	1	0	2.107373	-0.917308	1.938028
18	6	0	3.033591	-3.511129	0.072709
19	1	0	3.910919	-3.311949	-1.902573
20	1	0	2.035610	-3.383091	1.954044
21	1	0	3.220088	-4.580484	0.125215
22	6	0	0.590628	1.009228	1.292762
23	1	0	-0.117260	1.825750	1.476793

24	1	0	0.882399	0.658991	2.303509
25	6	0	-0.077778	-0.149052	0.599454
26	6	0	0.606902	-1.273002	0.388731
27	1	0	0.276182	-2.125809	-0.201287
28	79	0	-2.053437	-0.028943	0.012864
29	15	0	-4.346898	0.129616	-0.659921
30	1	0	-5.243417	-0.827061	-0.155927
31	1	0	-4.632905	0.039890	-2.032222
32	1	0	-5.037633	1.309866	-0.339522

Ts3-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	1.401789	3.713628	-0.140052
2	6	0	2.589077	3.397508	-0.801283
3	6	0	3.115198	2.123170	-0.704431
4	6	0	2.475508	1.118735	0.050535
5	6	0	1.282017	1.457114	0.725584
6	6	0	0.754855	2.743713	0.608442
7	1	0	0.986427	4.716747	-0.209134
8	1	0	3.095394	4.145824	-1.406564
9	1	0	4.009522	1.878944	-1.273515
10	1	0	-0.166039	2.982683	1.140598
11	6	0	3.064887	-0.220053	0.064845
12	6	0	4.456306	-0.355706	-0.067513
13	6	0	2.303075	-1.444794	0.064898
14	6	0	5.072315	-1.580082	-0.258534
15	1	0	5.072391	0.538681	-0.012258
16	6	0	2.962344	-2.691115	-0.180398
17	1	0	1.615868	-1.751687	1.015265
18	6	0	4.321037	-2.760416	-0.345183
19	1	0	6.156109	-1.622571	-0.343817
20	1	0	2.353440	-3.595084	-0.193364
21	1	0	4.807920	-3.717298	-0.514074
22	6	0	0.573457	0.428856	1.551268
23	1	0	-0.179830	0.898243	2.192450
24	1	0	1.281499	-0.091795	2.220130
25	6	0	-0.048082	-0.518194	0.561935

26	6	0	0.751633	-1.437819	-0.039863
27	1	0	0.371986	-2.270571	-0.630327
28	79	0	-2.026280	-0.316945	0.031976
29	15	0	-4.328517	-0.062083	-0.586044
30	1	0	-4.972245	1.135608	-0.235822
31	1	0	-5.240108	-0.998660	-0.072936
32	1	0	-4.640937	-0.126425	-1.953536

Int3-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.554399	3.446851	-0.014328
2	6	0	1.811833	3.468234	-0.642464
3	6	0	2.626685	2.348614	-0.665976
4	6	0	2.226193	1.153579	-0.057436
5	6	0	0.950515	1.124603	0.588011
6	6	0	0.132555	2.288835	0.586506
7	1	0	-0.070115	4.336298	-0.007372
8	1	0	2.147861	4.379694	-1.133777
9	1	0	3.577744	2.382834	-1.193389
10	1	0	-0.831539	2.242503	1.093976
11	6	0	3.065426	-0.036887	-0.096452
12	6	0	4.464631	0.055331	-0.055467
13	6	0	2.454786	-1.302857	-0.183643
14	6	0	5.245001	-1.088787	-0.091739
15	1	0	4.937448	1.030833	0.050925
16	6	0	3.251997	-2.442488	-0.224239
17	1	0	0.611792	-2.384273	-0.018510
18	6	0	4.637531	-2.340301	-0.180233
19	1	0	6.328340	-1.008003	-0.042304
20	1	0	2.780650	-3.421920	-0.301933
21	1	0	5.247831	-3.240426	-0.210644
22	6	0	0.700872	0.068999	1.718722
23	1	0	0.034555	0.452991	2.490695
24	1	0	1.639031	-0.348567	2.095493
25	6	0	0.151398	-0.407202	0.482079
26	6	0	0.963719	-1.386119	-0.328450
27	1	0	0.690673	-1.305825	-1.392234

28	79	0	-1.882121	-0.327617	0.033179
29	15	0	-4.218748	-0.381132	-0.480173
30	1	0	-5.046123	0.603932	0.082474
31	1	0	-4.917194	-1.541430	-0.109830
32	1	0	-4.587424	-0.282350	-1.831484

Ts4-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.215925	3.704692	-0.035763
2	6	0	2.360623	3.458195	-0.789003
3	6	0	2.942581	2.198383	-0.781324
4	6	0	2.397021	1.153103	-0.023655
5	6	0	1.244090	1.416359	0.740452
6	6	0	0.658236	2.680689	0.718110
7	1	0	0.761923	4.693214	-0.034405
8	1	0	2.799344	4.250212	-1.391983
9	1	0	3.818713	2.007987	-1.399128
10	1	0	-0.231307	2.862971	1.322265
11	6	0	3.053182	-0.169784	-0.029818
12	6	0	4.453433	-0.233375	-0.040346
13	6	0	2.347087	-1.396704	-0.113426
14	6	0	5.127957	-1.441806	-0.122968
15	1	0	5.019540	0.692221	0.046107
16	6	0	3.041523	-2.609288	-0.244495
17	1	0	0.239602	-1.873568	0.850564
18	6	0	4.422930	-2.641194	-0.231808
19	1	0	6.215723	-1.450788	-0.107312
20	1	0	2.474345	-3.534916	-0.345435
21	1	0	4.951380	-3.588071	-0.310846
22	6	0	0.638056	0.302592	1.549169
23	1	0	-0.101043	0.685218	2.261124
24	1	0	1.416661	-0.231695	2.118148
25	6	0	0.007023	-0.597947	0.525895
26	6	0	0.886441	-1.436346	-0.187932
27	1	0	0.449942	-2.104593	-0.938957
28	79	0	-1.995838	-0.369881	0.033968
29	15	0	-4.282862	0.009295	-0.548750

30	1	0	-4.935355	1.069175	0.099339
31	1	0	-5.191791	-1.036700	-0.328345
32	1	0	-4.550166	0.315061	-1.891892

Int4-7Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z --------
1	6	0	-1.085107	3.282282	0.309555
2	6	0	-0.341790	3.235332	-0.866461
3	6	0	0.704275	2.329875	-0.990120
4	6	0	1.037874	1.450215	0.051949
5	6	0	0.271757	1.497677	1.236449
6	6	0	-0.777159	2.413961	1.350157
7	1	0	-1.894739	4.000554	0.421707
8	1	0	-0.572921	3.908695	-1.689467
9	1	0	1.272083	2.288380	-1.918761
10	1	0	-1.347705	2.449802	2.278418
11	6	0	2.165880	0.511020	-0.140680
12	6	0	3.317499	0.975895	-0.786734
13	6	0	2.102261	-0.869265	0.186168
14	6	0	4.367612	0.128900	-1.111258
15	1	0	3.393292	2.036670	-1.020035
16	6	0	3.150367	-1.721331	-0.199163
17	1	0	-0.352991	-1.512522	2.557958
18	6	0	4.281949	-1.232172	-0.827543
19	1	0	5.254923	0.532284	-1.594465
20	1	0	3.074694	-2.784122	0.030227
21	1	0	5.094202	-1.904414	-1.093134
22	6	0	0.555678	0.530999	2.355585
23	1	0	-0.045045	0.783795	3.236256
24	1	0	1.615705	0.587633	2.656971
25	6	0	0.268040	-0.879700	1.918990
26	6	0	1.013817	-1.491115	0.929865
27	1	0	0.907317	-2.573502	0.813329
28	79	0	-1.134762	-0.774092	0.044439
29	15	0	-2.865297	-0.441204	-1.525028
30	1	0	-2.791071	0.752733	-2.258030
31	1	0	-4.168943	-0.376789	-1.012953

32	1	0	-3.010853	-1.393305	-2.543788