Electronic Supplementary Material (ESI) for Dalton Transactions

Shedding light on the bonding, photophysical and magnetotropic properties of triangular Pt_3 complexes and their "open-face" $TlPt_3$ half-sandwiches

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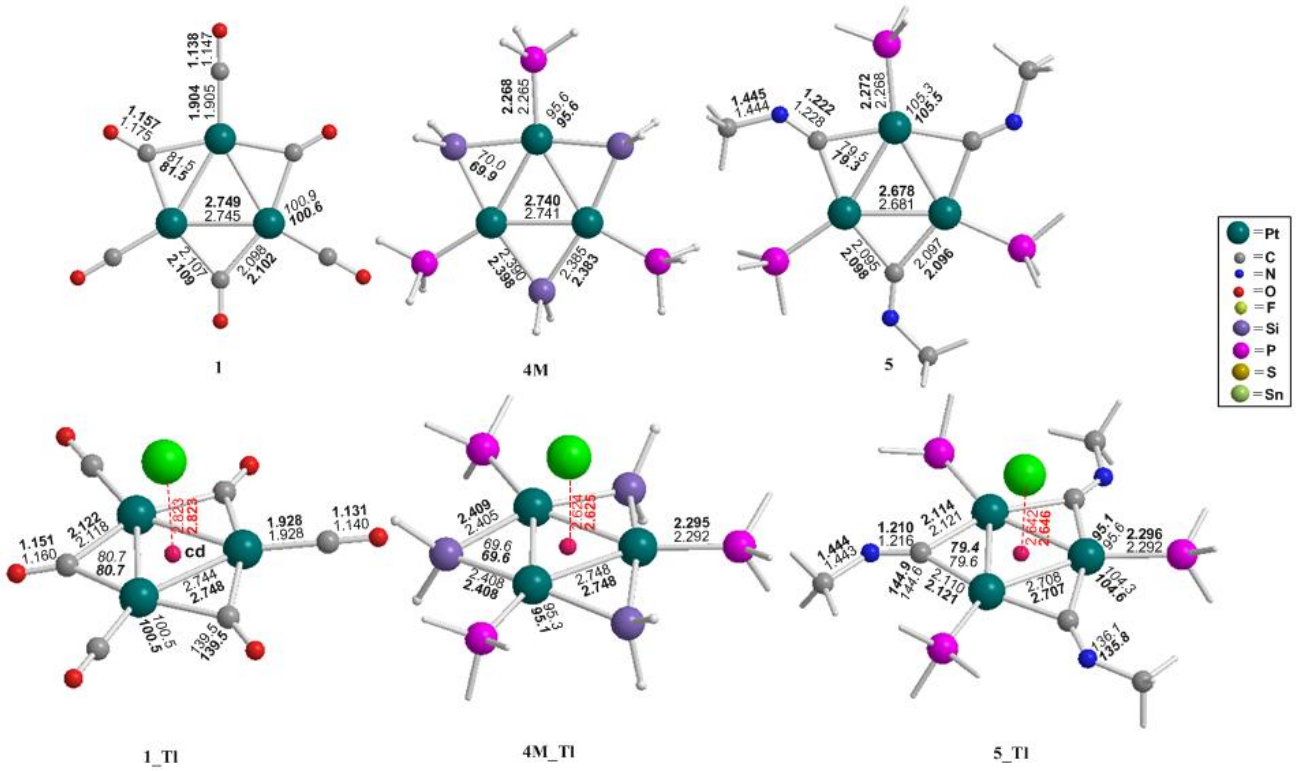
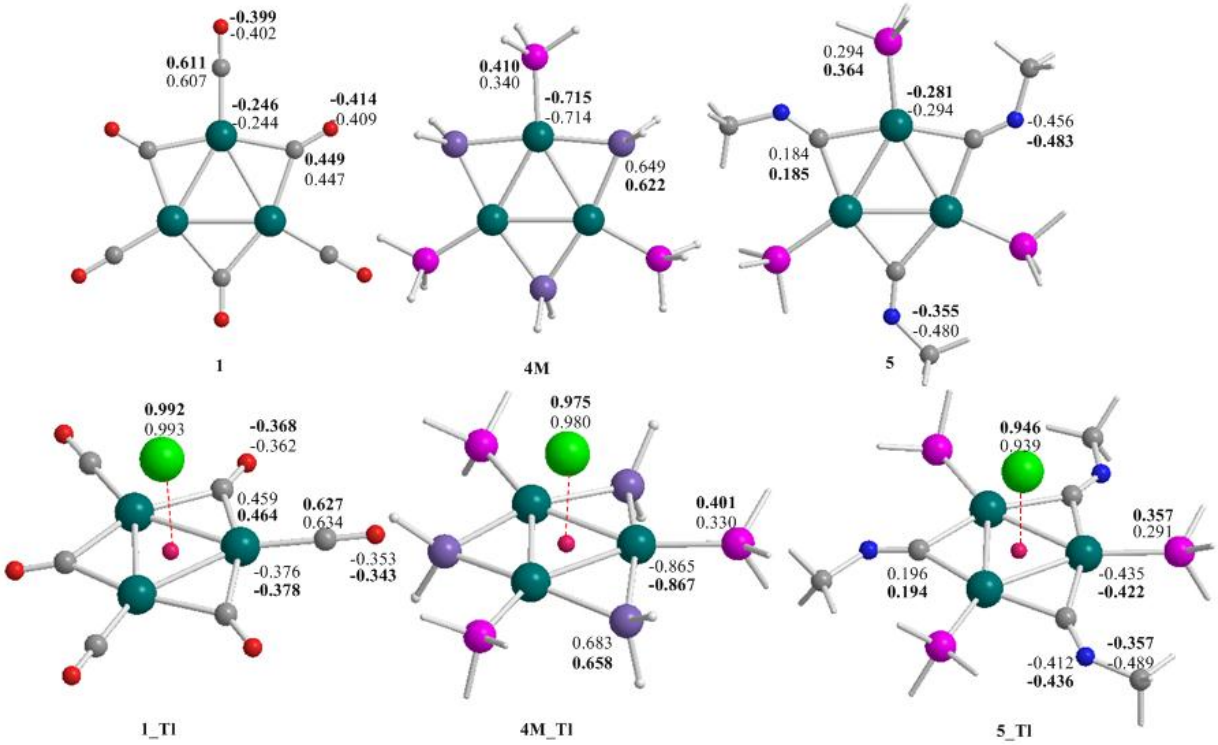
Table of Contents



(**a**)



(**b**)

Figure S1. Structural (**a**) and electronic (**b**) parameters of representaive $Pt_3(\mu_2\text{-}L)_3(L')_3]$ and $[Pt_3(\mu_2\text{-}L)_3(L')_3(\mu_3\text{-}Tl)]^+$ clusters calculated at the B3LYP/LANLTZ(f)(Pt) ∪ 6-311G(d,p)(E) ∪ SRLC(Tl) level

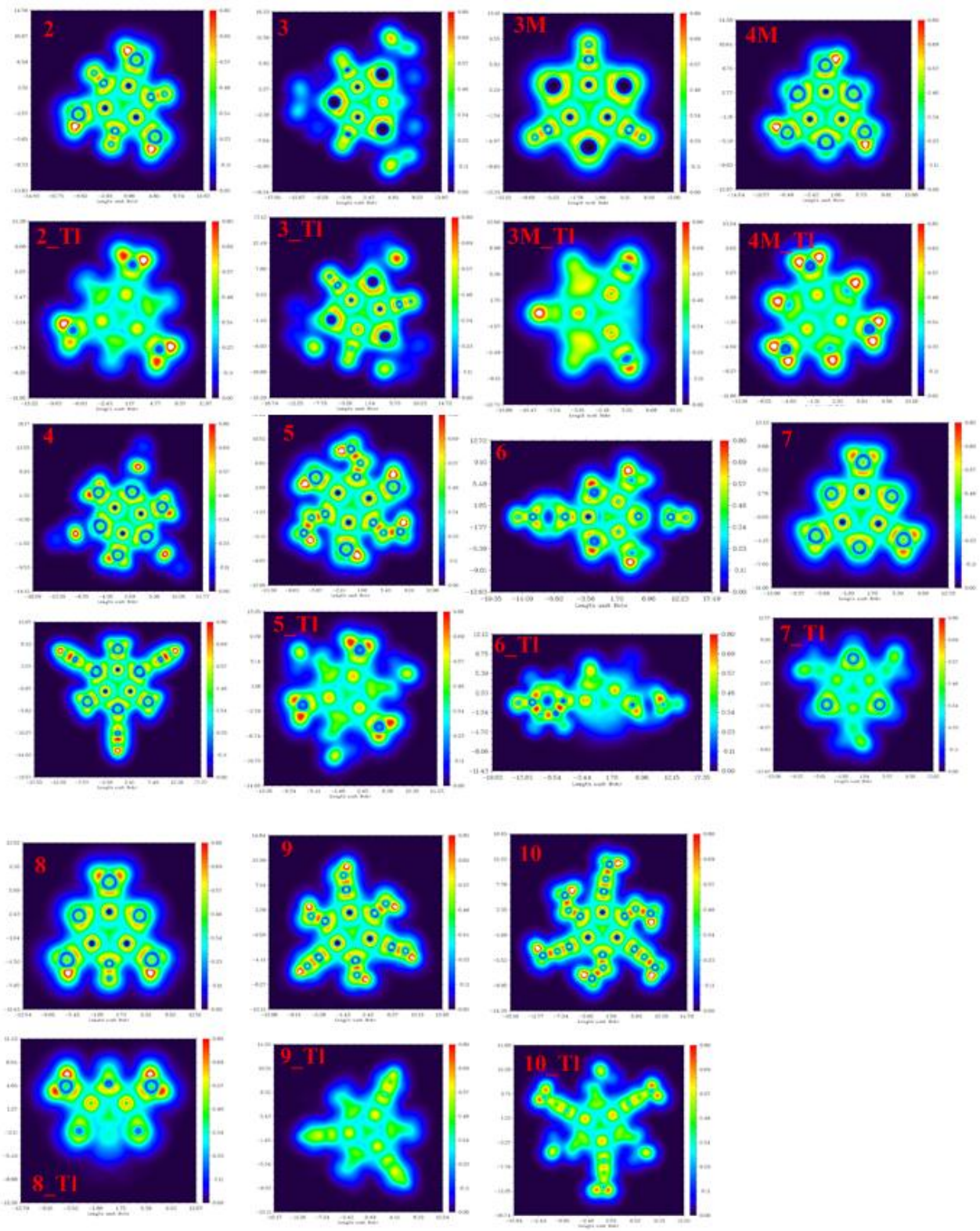
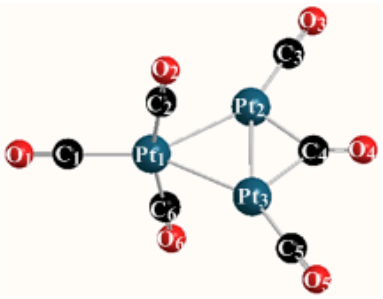
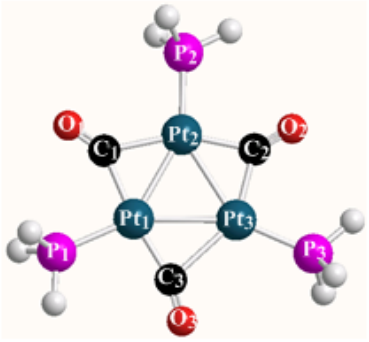


Figure S2. Cut-plane LOL profiles on the ring plane of the triangular platinum clusters and their $Pt_3Tl(I)$ "half-sandwich" complexes calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



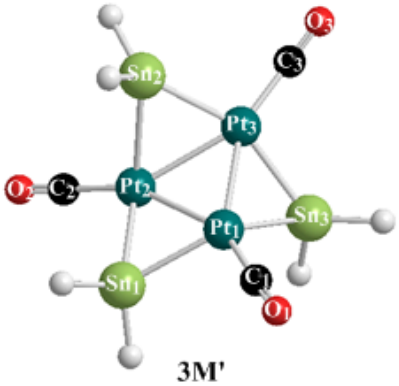
1'

Pt_1-Pt_2=Pt_3-Pt_1=2.745 Pt_1-Pt_2-Pt_3=59.3
Pt_2-Pt_3=2.811 Pt_3-Pt_1-Pt_2=61.4
Pt_1-C_1=1.976 C_1-Pt_1-C_2=98.2
Pt_1-C_2=Pt_1-C_6=1.924 C_2-Pt_1-Pt_2=83.3
Pt_2-C_3=Pt_3-C_5=1.881 C_3-Pt_2-C_4=105.0
Pt_2-C_4=Pt_3-C_4=2.028 Pt_2-C_4-O_4=136.5
C_1-O_1=1.148 Pt_2-C_4-Pt_3=87.6
C_2-O_2=C_6-O_6=1.152
C_3-O_3=C_5-O_5=1.151
C_4-O_4=1.173



2'

Pt_1-Pt_2=Pt_3-Pt_1=2.745 Pt_1-Pt_2-Pt_3=59.3
Pt_2-Pt_3=2.811 Pt_3-Pt_1-Pt_2=61.4
Pt_1-C_1=1.976 C_1-Pt_1-C_2=98.2
Pt_1-C_2=Pt_1-C_6=1.924 C_2-Pt_1-Pt_2=83.3
Pt_2-C_3=Pt_3-C_5=1.881 C_3-Pt_2-C_4=105.0
Pt_2-C_4=Pt_3-C_4=2.028 Pt_2-C_4-O_4=136.5
C_1-O_1=1.148 Pt_2-C_4-Pt_3=87.6
C_2-O_2=C_6-O_6=1.152
C_3-O_3=C_5-O_5=1.151
C_4-O_4=1.173



3M'

Pt_2-Pt_3=Pt_3-Pt_1=2.759 Pt_3-Pt_1-Pt_2=59.1
Pt_1-Pt_2=2.838 Pt_1-Pt_2-Pt_3=61.9
Pt_1-C_1=1.880 C_1-Pt_1-Sn_1=98.6
Pt_2-C_2=Pt_3-C_3=1.880 C_2-Pt_2-Sn_2=105.8
Pt_3-C_3=1.883 C_3-Pt_3-Sn_3=103.1
C_1-O_1=C_2-O_2=1.153 Pt_1-Sn_1-Pt_2=65.1
C_3-O_3=1.154 Pt_2-Sn_2-Pt_3=62.0
Pt_1-Sn_1=Pt_2-Sn_1=2.638 Pt_3-Sn_3-Pt_1=62.0
Pt_2-Sn_2=Pt_1-Sn_3=2.736 Pt_1-Pt_2-Sn_2-Pt_3=51.3
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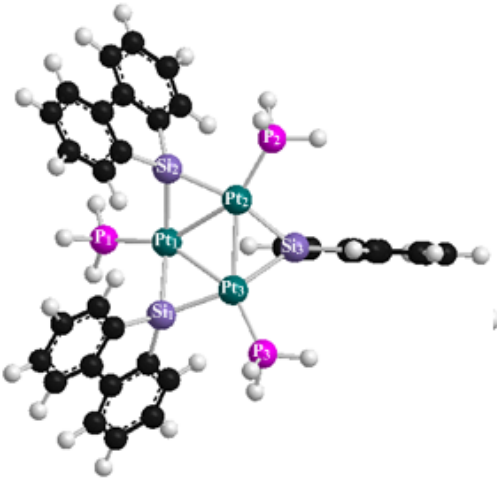

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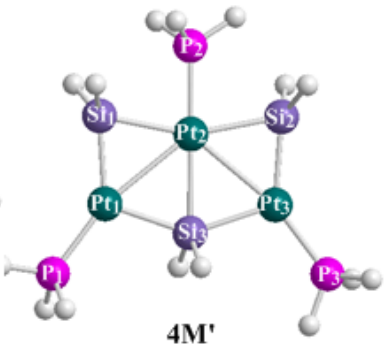
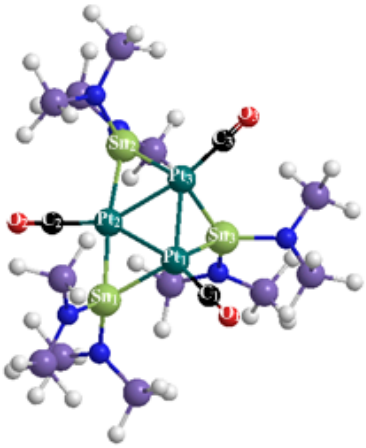
Pt_1-Pt_2=2.815 Pt_1-Pt_2-Pt_3=60.6
Pt_2-Pt_3=2.761 Pt_2-Pt_3-Pt_1=60.6
Pt_3-Pt_1=2.815 Pt_3-Pt_1-Pt_2=58.7
Pt_1-P_1=2.266 P_1-Pt_1-Si_1=P_1-Pt_1-Si_2=100.1
Pt_2-P_2=Pt_3-P_3=2.257 P_2-Pt_2-Si_2=98.2
Pt_1-Si_1=Pt_1-Si_2=2.422 P_2-Pt_2-Si_3=104.5
Pt_2-Si_2=Pt_3-Si_3=2.357 Pt_1-Si_2-Pt_2=72.2
Pt_2-Si_3=Pt_2-Si_3=2.432 Si_1-Pt_1-Si_2=135.3
Si_2-Pt_2-Si_3=Si_3-Pt_3-Si_1=147.7



4M'

Pt_1-Pt_2=2.926
Pt_2-Pt_3=2.912
Pt_3-Pt_1=4.545
Pt_1-Si_1=Pt_3-Si_2=2.300
Pt_1-Si_3=Pt_3-Si_3=2.392
Pt_2-Si_3=2.578
Pt_2-Si_1=2.484
Pt_2-Si_2=2.465
Pt_1-P_1=Pt_3-P_3=2.284
Pt_2-P_2=2.294

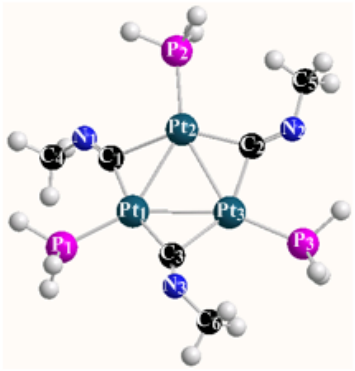
Pt_1-Pt_2-Pt_3=102.3
Pt_2-Pt_3-Pt_1=39.9
P_1-Pt_1-Si_1=138.9
P_2-Pt_2-Si_1=79.5
Pt_1-Si_1-Pt_2=75.3
Si_1-Pt_2-Si_2=158.5
Pt_1-Si_3-Pt_3=143.6
Si_1-Pt_1-Si_3=112.2



3'

Pt_1-Pt_2=2.831 Pt_3-Pt_1-Pt_2=59.4
Pt_2-Pt_3=2.768 Pt_1-Pt_2-Pt_3=59.0
Pt_3-Pt_1=2.758 C_1-Pt_1-Sn_1=107.7
Pt_1-C_1=1.885 C_2-Pt_2-Sn_2=93.4
Pt_2-C_2=1.888 C_3-Pt_3-Sn_3=105.1
Pt_3-C_3=1.893 Pt_1-Sn_1-Pt_2=64.7
C_1-O_1=1.154 Pt_2-Sn_2-Pt_3=63.1
C_2-O_2=1.154 Pt_3-Sn_3-Pt_1=56.8
C_3-O_3=1.153 Pt_1-Pt_2-Sn_1-Pt_3=179.0
Pt_1-Sn_1=2.634 Pt_1-Pt_2-Sn_2-Pt_3=174.9
Pt_2-Sn_1=2.658 Pt_1-Pt_2-Sn_3-Pt_3=57.7
Pt_2-Sn_2=2.674
Pt_3-Sn_2=2.619
Pt_3-Sn_3=2.730

Figure S3. T_1 optimized geometries of **1′**, **2′**, **3′**, **3M′**, **4′**, **4M′** clusters along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



5'

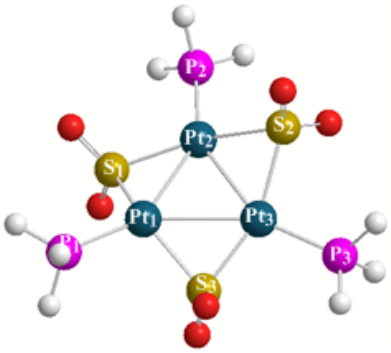
Pt_1-Pt_2=2.755, Pt_2-Pt_3=2.728
Pt_3-Pt_1=2.781
Pt_1-C_1=2.222, Pt_2-C_1=2.012
Pt_2-C_2=1.994, Pt_3-C_2=2.265
Pt_3-C_3=2.024, Pt_1-C_3=2.033
C_1-N_1=1.229, C_2-N_2=1.227
C_3-N_3=1.246
Pt_1-P_1=2.251, Pt_2-P_2=2.276
Pt_3-P_3=2.258
N_1-C_4=1.452, N_2-C_5=1.441
N_3-C_6=1.447

Pt_1-Pt_2-Pt_3=60.9
Pt_2-Pt_3-Pt_1=59.0
Pt_1-C_1-Pt_2=81.0
Pt_2-C_2-Pt_3=79.4
Pt_3-C_3-Pt_1=86.6
P_1-Pt_1-C_1=103.9
P_2-Pt_2-C_2=96.6
P_3-Pt_3-C_3=95.6
Pt_1-C_1-N_1=122.9
Pt_2-C_2-N_2=149.8
Pt_3-C_3-N_3=131.0
C_1-N_1-C_4=131.1
Pt_1-Pt_2-Pt_3-C_1=22.0
Pt_1-Pt_2-Pt_3-C_2=24.0
Pt_1-Pt_2-Pt_3-C_3=1.3

6'

Pt_1-Pt_2=2.689
Pt_2-Pt_3=2.780
Pt_3-Pt_1=2.781
Pt_1-P_1=2.335
Pt_1-P_4=2.374
Pt_1-C_1=2.136
Pt_2-P_2=2.335
Pt_2-P_3=2.374
Pt_2-C_1=2.135
Pt_3-P_3=2.307
Pt_3-P_4=2.307
Pt_3-C_3=2.054
Pt_1-Pt_2-Pt_3=61.1
Pt_2-Pt_3-Pt_1=57.8
Pt_1-C_1-Pt_2=78.0

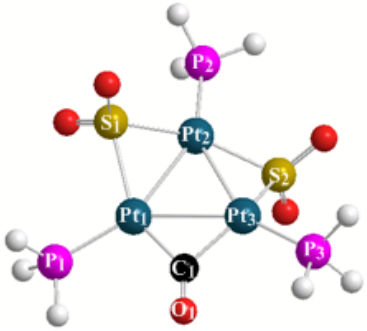
P_1-Pt_1-C_1=97.6
P_2-Pt_2-C_1=97.5
P_2-Pt_2-P_3=98.1
Pt_2-P_3-Pt_3=72.8
P_3-Pt_3-P_4=166.7
Pt_3-P_4-Pt_1=72.9
P_4-Pt_1-P_1=98.1
Pt_1-C_1-C_2=115.9
Pt_3-C_3-C_4=121.8
Pt_1-Pt_2-C_1-C_2=113.1
Pt_1-Pt_3-C_3-C_4=107.2



7'

Pt_1-Pt_2=2.870
Pt_2-Pt_3=2.876
Pt_3-Pt_1=2.862
Pt_1-P_1=2.300
Pt_2-P_2=2.285
Pt_3-P_3=2.287
Pt_1-S_1=2.350, Pt_2-S_1=2.286
Pt_2-S_2=2.379, Pt_3-S_2=2.371
Pt_1-S_3=2.354, Pt_3-S_3=2.289

Pt_1-Pt_2-Pt_3=60.0
Pt_2-Pt_3-Pt_1=60.2
P_1-Pt_1-S_1=101.6
Pt_1-S_1-Pt_2=76.5
P_2-Pt_2-S_1=98.6
P_2-Pt_2-S_2=102.4
Pt_2-S_2-Pt_3=74.5
P_3-Pt_3-S_2=101.1
P_3-Pt_3-S_3=99.4
S_3-Pt_1-P_1=102.1
Pt_1-Pt_2-Pt_3-S_1=21.4
Pt_1-Pt_2-Pt_3-S_2=31.0
Pt_1-Pt_2-Pt_3-S_3=21.3

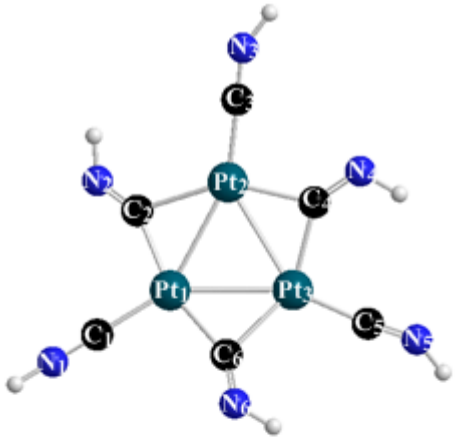


8'

Pt_1-Pt_2=2.872
Pt_2-Pt_3=2.856
Pt_1-Pt_3=2.761
Pt_1-P_1=2.287
Pt_2-P_2=2.280
Pt_3-P_3=2.294
Pt_1-S_1=2.447
Pt_2-S_1=2.349
Pt_2-S_2=2.315
Pt_3-S_2=2.419
Pt_1-C_1=1.986
Pt_3-C_1=2.020
C_1-O_1=1.186

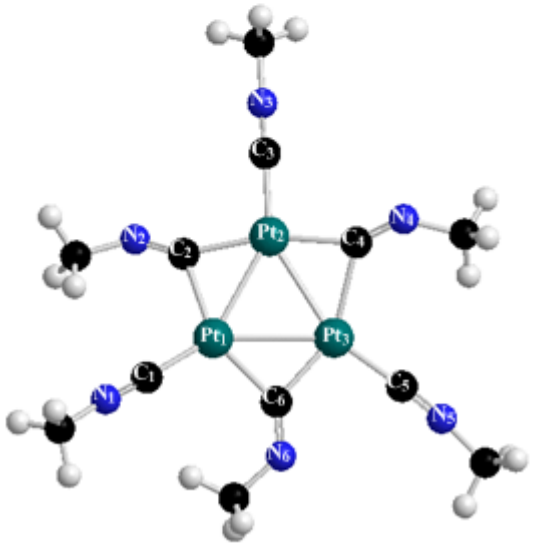
Pt_1-Pt_2-Pt_3=57.6
Pt_2-Pt_3-Pt_1=61.1
P_1-Pt_1-S_1=107.3
S_1-Pt_2-P_2=101.1
Pt_1-S_1-Pt_2=73.6
P_2-Pt_2-S_2=100.4
Pt_2-S_2-Pt_3=74.2
P_3-Pt_3-S_2=107.1
P_3-Pt_3-C_1=101.0
P_1-Pt_1-C_1=100.3
Pt_1-Pt_2-Pt_3-S_1=33.0
Pt_1-Pt_2-Pt_3-S_1=33.0
Pt_1-Pt_2-Pt_3-S_2=30.5
Pt_1-Pt_2-Pt_3-C_1=7.8

Figure S4. T_1 optimized geometries of **5′**, **6′**, **7′**, **8′** clusters along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



9'

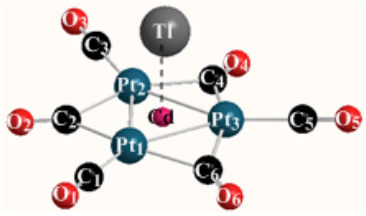
Pt_1-Pt_2=2.814 C_1-Pt_1-C_2=96.8
Pt_2-Pt_3=2.762 Pt_1-C_2-Pt_2=89.3
Pt_1-Pt_3=2.748 C_2-Pt_2-C_3=100.9
Pt_1-C_1=1.915 C_3-Pt_2-C_4=113.5
C_1-N_1=1.177 Pt_2-C_4-Pt_3=82.5
Pt_1-C_2=2.009 C_4-Pt_3-C_5=98.9
C_2-N_2=1.245 C_5-Pt_3-C_6=99.2
Pt_2-C_2=2.054 Pt_3-C_6-Pt_1=81.6
Pt_2-C_3=1.908 C_6-Pt_1-C_1=115.0
C_3-N_3=1.181 Pt_1-Pt_2-Pt_3-C_2=-1.8
Pt_2-C_4=2.228
C_4-N_4=1.227
Pt_3-C_4=1.997
Pt_3-C_5=1.936
C_5-N_5=1.174
Pt_3-C_6=2.006
C_6-N_6=1.227
Pt_1-C_6=2.236



10'

Pt_1-Pt_2=2.847 C_1-Pt_1-C_2=97.2
Pt_2-Pt_3=2.775 Pt_1-C_2-Pt_2=87.7
Pt_1-Pt_3=2.763 C_2-Pt_2-C_3=104.7
Pt_1-C_1=1.897 C_3-Pt_2-C_4=108.9
C_1-N_1=1.185 Pt_2-C_4-Pt_3=81.4
Pt_1-C_2=2.008 C_4-Pt_3-C_5=97.6
C_2-N_2=1.250 C_5-Pt_3-C_6=98.2
Pt_2-C_2=2.043 Pt_3-C_6-Pt_1=80.6
Pt_2-C_3=1.890 C_6-Pt_1-C_1=112.2
C_3-N_3=1.191 Pt_1-Pt_2-Pt_3-C_2=173.8
Pt_2-C_4=2.207 Pt_1-Pt_2-Pt_3-C_4=161.2
C_4-N_4=1.234 Pt_1-Pt_2-Pt_3-C_6=157.7
Pt_3-C_4=1.997
Pt_3-C_5=1.926
C_5-N_5=1.174
Pt_3-C_6=2.004
C_6-N_6=1.233
Pt_1-C_6=2.218

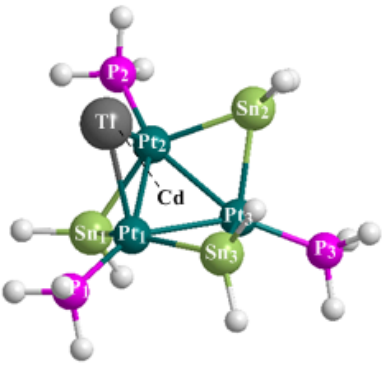
Figure S5. T_1 optimized geometries of **9′**, **10′** clusters along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



1'_Tl

Pt_1-Pt_2=2.753
Pt_1-C_1=1.930
Pt_1-C_2=2.118
C_1-O_1=1.141
C_2-O_2=1.161
Tl-Cd=2.551

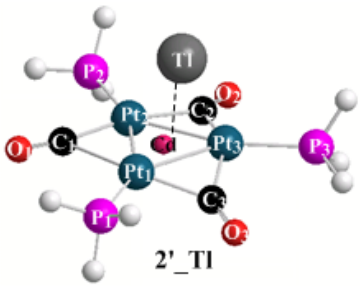
Pt_1-Pt_2-Pt_3=60.0
Pt_1-C_2-Pt_2=80.5
C_1-Pt_1-C_2=100.6
Pt_1-C_2-O_2=139.7
Tl-Cd-Pt_1=90.0



3M'_Tl

Pt_1-Pt_2=2.828
Pt_1-Pt_3=2.807
Pt_1-P_1=2.289
Pt_3-P_3=2.271
Pt_1-Sn_1=2.685
Pt_2-Sn_2=2.620
Pt_3-Sn_2=2.661
Tl-Cd=3.049
Pt_1-Tl=2.892
Pt_3-Tl=4.369

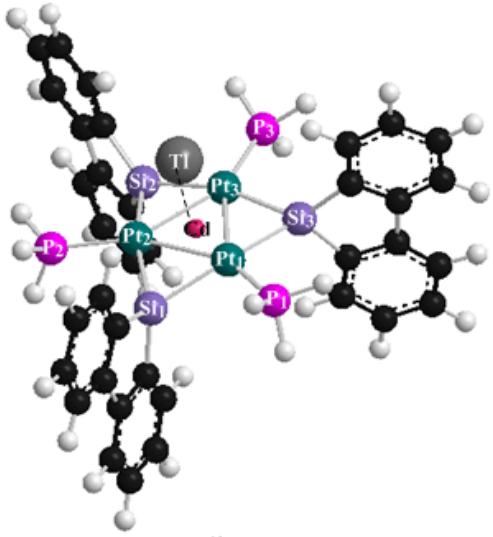
Pt_1-Pt_2-Pt_3=60.5
Pt_2-Pt_3-Pt_1=59.7
Pt_1-Sn_1-Pt_2=63.6
Pt_2-Sn_2-Pt_3=64.2
P_1-Pt_1-Sn_1=103.1
P_2-Pt_2-Sn_2=100.0
P_3-Pt_3-Sn_3=101.4
Tl-Cd-Pt_1=68.8
Pt_1-Pt_2-Pt_3-Sn_1=53.5
Pt_1-Pt_2-Pt_3-Sn_2=32.6
Pt_1-Pt_2-Pt_3-Sn_3=142.6



2'_Tl

Pt_1-Pt_2=2.725
Pt_2-Pt_3=2.814
Pt_3-Pt_1=2.728
Pt_1-P_1=2.297
Pt_2-P_2=2.296
Pt_3-P_3=2.337
Pt_1-C_1=2.036
Pt_2-C_1=2.027
Pt_2-C_2=2.622
Pt_3-C_2=1.932
Pt_3-C_3=2.031
Pt_1-C_3=2.153
C_1-O_1=1.176
C_2-O_2=1.159
C_3-O_3=1.177
Tl-Cd=2.911

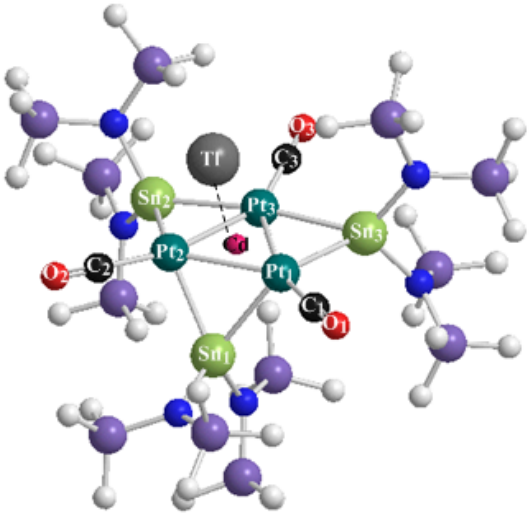
Pt_1-Pt_2-Pt_3=58.9
Pt_2-Pt_3-Pt_1=62.1
Pt_1-C_1-Pt_2=47.7
Pt_2-C_2-Pt_3=74.6
Pt_3-C_3-Pt_1=81.3
P_1-Pt_1-C_1=100.1
P_2-Pt_2-C_2=111.7
P_3-Pt_3-C_3=91.1
Tl-Cd-Pt_1=82.3
Pt_1-Pt_2-Pt_3-C_1=157.8
Pt_1-Pt_2-Pt_3-C_2=174.5
Pt_1-Pt_2-Pt_3-C_3=174.0



4'_Tl

Pt_1-Pt_2=Pt_2-Pt_3=2.814
Pt_3-Pt_1=2.800
Pt_1-P_1=Pt_2-P_2=Pt_3-P_3=2.278
Pt_1-Si_1=Pt_2-Si_1=Pt_2-Si_2=
Pt_3-Si_2=2.408
Pt_1-Si_3=Pt_3-Si_3=2.446
Tl-Cd=2.521

Pt_1-Pt_2-Pt_3=60.2
Pt_1-Si_1-Pt_2=82.4
P_1-Pt_1-Si_1=P_2-Pt_2-Si_3=69.8
Tl-Cd-Pt_1=90.1
Pt_1-Pt_2-Pt_3-Si_1=173.0
Pt_1-Pt_2-Pt_3-Si_2=173.0
Pt_1-Pt_2-Pt_3-Si_3=170.4
Pt_1-Pt_2-Pt_3-P_1=175.8
Pt_1-Pt_2-Pt_3-P_2=178.0
Pt_1-Pt_2-Pt_3-P_3=175.8



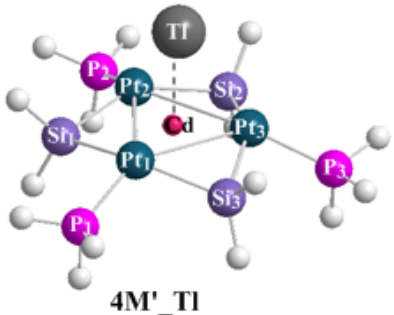
3'_Tl

Pt_1-Pt_2=2.802
Pt_3-Pt_1=2.789
Pt_2-Pt_3=2.769
Pt_1-C_1=1.895
Pt_2-C_2=1.901
Pt_3-C_3=1.897
Pt_1-Sn_1=2.716
Pt_2-Sn_1=2.652
Pt_2-Sn_2=2.647
Pt_3-Sn_2=2.682
Pt_3-Sn_3=2.679
Pt_1-Sn_3=2.663
Tl-Cd=2.944

Pt_1-Pt_2-Pt_3=60.1
Pt_2-Pt_3-Pt_1=60.6
Pt_3-Pt_1-Pt_2=59.4
Pt_1-Sn_1-Pt_2=62.9
Pt_3-Sn_3-Pt_1=62.9
Pt_2-Sn_2-Pt_3=62.6
C_1-Pt_1-Sn_1=103.4
C_2-Pt_2-Sn_2=108.6
C_3-Pt_3-Sn_3=92.0
Tl-Cd-Pt_1=87.4

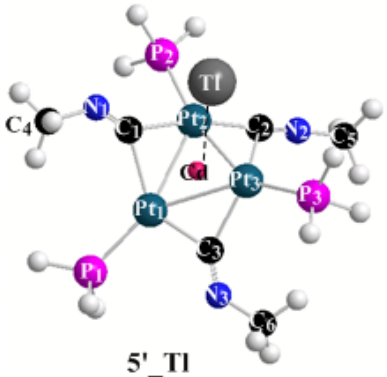
Pt_1-Pt_2-Pt_3-Sn_1=126.7
Pt_1-Pt_2-Pt_3-Sn_2=174.0
Pt_1-Pt_2-Pt_3-Sn_3=176.9
Pt_1-Pt_2-Pt_3-C_1=162.0
Pt_1-Pt_2-Pt_3-C_2=154.4
Pt_1-Pt_2-Pt_3-C_3=169.7

Figure S6. T_1 optimized geometries of **1_Tl′**, **2_Tl′**, **3_Tl′**, **3M_Tl′**, **4_Tl′** open face adducts along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



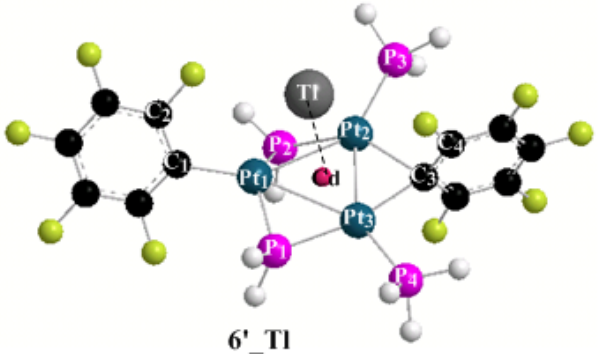
4M'_Tl

Pt_1-Pt_2=3.123	Pt_1-Pt_2-Pt_3=60.0	Pt_1-Pt_2-Pt_3-Si_1=15.5
Pt_1-P_1=2.234	Pt_1-Si_1-Pt_2=82.4	Pt_1-Pt_2-Pt_3-Si_1=21.0
Pt_1-Si_1=2.400	P_1-Pt_1-Si_1=90.1	Pt_1-Pt_2-Pt_3-Si_1=14.0
Pt_2-Si_1=2.342	P_2-Pt_2-Si_1=102.9	Pt_1-Pt_2-Pt_3-P_1=48.4
Tl-Cd=2.644	Tl-Cd-Pt_1=90.0	Pt_1-Pt_2-Pt_3-P_2=10.3
		Pt_1-Pt_2-Pt_3-P_3=48.4



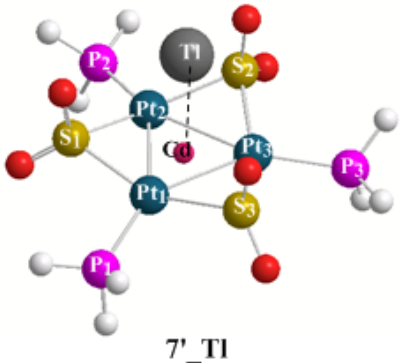
5'_Tl

Pt_1-Pt_2=2.792	C_1-N_1=1.229	Pt_1-Pt_2-Pt_3=60.7
Pt_2-Pt_3=2.750	C_2-N_2=1.171	Pt_2-Pt_3-Pt_1=59.2
Pt_3-Pt_1=2.777	C_3-N_3=1.227	Pt_3-Pt_1-Pt_2=60.1
Pt_1-C_1=2.202	N_1-C_4=1.450	Pt_1-C_1-Pt_2=83.0
Pt_2-C_1=2.006	N_2-C_5=1.421	Pt_2-C_2-Pt_3=61.3
Pt_2-C_2=1.980	N_3-C_6=1.227	Pt_1-C_1-Pt_2=85.5
Pt_3-C_2=3.082	Tl-Cd=3.117	P_1-Pt_1-C_1=121.1
Pt_3-C_3=2.078		P_2-Pt_2-C_1=93.6
Pt_1-C_3=2.013		P_2-Pt_2-C_2=96.6
P_1-Pt_1=2.273		P_3-Pt_3-C_2=121.8
P_2-Pt_2=2.348		P_3-Pt_3-C_3=104.3
P_3-Pt_3=2.271		P_1-Pt_1-C_3=99.5
		Tl-Cd-Pt_1=125.2
		Pt_1-Pt_2-Pt_3-C_1=42.3
		Pt_1-Pt_2-Pt_3-C_2=51.7
		Pt_1-Pt_2-Pt_3-C_3=18.8



6'_Tl

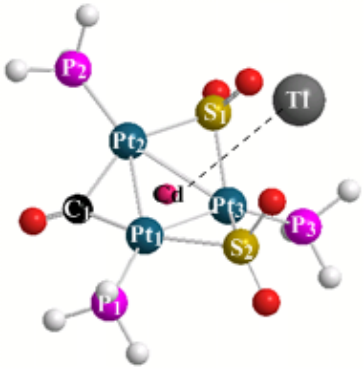
Pt_1-Pt_2=2.920	Pt_1-Pt_2-Pt_3=62.9	
Pt_2-Pt_3=2.785	Pt_2-Pt_3-Pt_1=56.3	
Pt_3-Pt_1=2.979	Pt_3-Pt_1-Pt_2=62.9	
Pt_1-P_1=2.290	P_1-Pt_1-C_1=107.6	
Pt_1-P_2=2.364	C_1-Pt_1-P_2=107.0	
Pt_2-P_2=2.333	Pt_1-P_2-Pt_2=52.0	
Pt_2-P_3=2.325	P_2-Pt_2-P_3=105.8	
Pt_3-P_4=2.303	P_3-Pt_2-C_3=103.2	
Pt_3-P_1=2.300	Pt_2-C_3-Pt_3=77.2	
Pt_1-C_1=2.019	C_3-Pt_3-P_4=94.2	
Pt_2-C_3=2.341	P_4-Pt_3-P_1=100.9	
Pt_3-C_3=2.115	Pt_3-P_1-Pt_1=80.9	
Tl-Cd=2.752	Tl-Cd-Pt_1=82.3	



7'_Tl

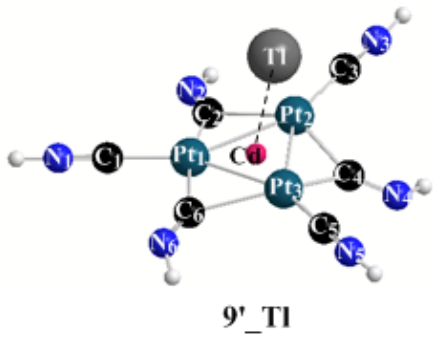
Pt_1-Pt_2=2.838	Pt_1-Pt_2-Pt_3=59.6	Pt_1-Pt_2-Pt_3-S_1=146.6
Pt_2-Pt_3=2.871	Pt_2-Pt_3-Pt_1=60.8	Pt_1-Pt_2-Pt_3-S_2=123.6
Pt_3-Pt_1=2.835	Pt_1-S_1-Pt_2=53.5	Pt_1-Pt_2-Pt_3-S_3=146.8
Pt_1-P_1=2.318	Pt_2-S_2-Pt_3=52.7	Pt_1-Pt_2-Pt_3-P_1=152.1
Pt_2-P_2=2.305	Pt_3-S_3-Pt_1=51.2	Pt_1-Pt_2-Pt_3-P_2=173.7
Pt_3-P_3=2.304	P_1-Pt_1-S_1=106.0	Pt_1-Pt_2-Pt_3-P_3=178.3
Pt_1-S_1=2.356	P_2-Pt_2-S_1=100.8	
Pt_2-S_1=2.284	P_2-Pt_2-S_2=102.9	
Pt_2-S_2=2.368	P_3-Pt_3-S_2=102.3	
Pt_3-S_2=2.366	P_3-Pt_3-S_3=101.1	
Pt_3-S_3=2.286	P_1-Pt_1-S_3=105.4	
Pt_1-S_3=2.358	Tl-Cd-Pt_1=75.9	
Tl-Cd=4.447		

Figure S7 T_1 optimized geometries of **4M_Tl′**, **5_Tl′**, **6_Tl′**, **7_Tl′** open face adducts along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.



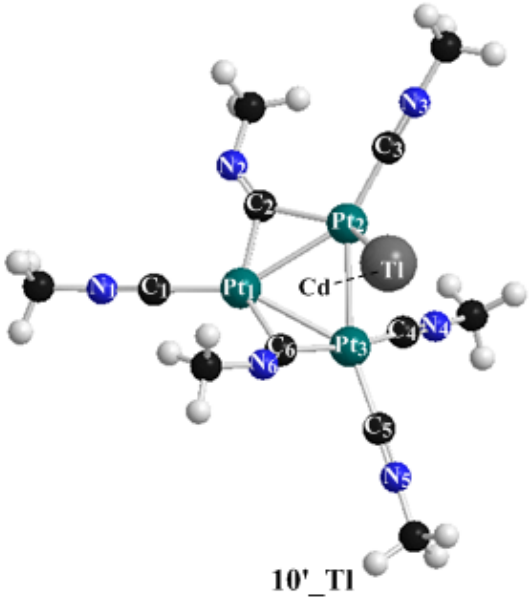
8'_Tl

Pt_1-Pt_2=2.741 Pt_1-Pt_2-Pt_3=57.4 Pt_1-Pt_2-Pt_3-C_1=38.4
Pt_2-Pt_3=2.903 Pt_3-Pt_1-Pt_2=59.4 Pt_1-Pt_2-Pt_3-S_1=157.6
Pt_3-Pt_1=2.802 Pt_1-S_2-Pt_3=71.9 Pt_1-Pt_2-Pt_3-S_2=31.7
Pt_1-P_1=2.315 Pt_2-S_1-Pt_3=77.0
Pt_3-P_3=2.301 Pt_1-C_1-Pt_2=84.1
Pt_1-C_1=1.989 P_1-Pt_1-C_1=102.8
Pt_2-C_1=2.103 P_2-Pt_2-C_1=109.6
Pt_1-S_2=2.360 P_3-Pt_3-S_1=102.8
Pt_2-S_1=2.329 P_3-Pt_3-S_2=109.0
Pt_3-S_1=2.333 P_1-Pt_1-S_2=101.0
Pt_3-S_2=2.413 Tl-Cd-Pt_1=104.8
Tl-Cd=4.437



9'_Tl

Pt_1-Pt_2=2.732 Pt_1-Pt_2-Pt_3=60.0 Pt_1-Pt_2-Pt_3-C_2=8.2
Pt_2-Pt_3=2.745 C_1-Pt_1-C_2=95.2 Pt_1-Pt_2-Pt_3-C_4=150.5
Pt_3-Pt_1=2.720 Pt_1-C_2-Pt_2=79.9 Pt_1-Pt_2-Pt_3-C_6=177.6
Pt_1-C_1=1.951 C_2-Pt_2-C_3=108.0
Pt_2-C_3=1.924 C_3-Pt_2-C_4=103.1
Pt_3-C_5=1.930 Pt_2-C_4-Pt_3=84.2
Pt_1-C_2=2.000 C_4-Pt_3-C_5=99.7
Pt_2-C_2=2.243 C_5-Pt_3-C_6=108.9
Pt_2-C_4=2.069 Pt_3-C_6-Pt_1=78.5
Pt_3-C_4=2.023 C_6-Pt_1-C_1=95.8
Pt_3-C_6=2.284 Tl-Cd-Pt_1=106.2
Pt_1-C_6=2.001
Tl-Cd=2.942



10'_Tl

Pt_1-Pt_2=2.776 Pt_1-Pt_2-Pt_3=60.2 Pt_1-Pt_2-Pt_3-C_2=159.8
Pt_2-Pt_3=2.764 C_1-Pt_1-C_2=102.2 Pt_1-Pt_2-Pt_3-C_4=126.3
Pt_3-Pt_1=2.772 Pt_1-C_2-Pt_2=85.6 Pt_1-Pt_2-Pt_3-C_6=159.0
Pt_1-C_1=1.932 C_2-Pt_2-C_3=105.5
Pt_2-C_3=1.927 C_3-Pt_2-C_4=119.5
Pt_3-C_5=1.983 Pt_2-C_4-Pt_3=63.4
Pt_1-C_2=2.013 C_4-Pt_3-C_5=96.1
Pt_2-C_2=2.073 C_5-Pt_3-C_6=95.6
Pt_2-C_4=3.008 Pt_3-C_6-Pt_1=82.0
Pt_3-C_4=1.986 C_6-Pt_1-C_1=115.5
Pt_3-C_6=1.999 Tl-Cd-Pt_1=125.1
Pt_1-C_6=2.219
Tl-Cd=3.110

Figure S8. T_1 optimized geometries of **8_Tl′**, **9_Tl′**, **10_Tl′** open face adducts along with selected structural parameters (bond lengths in Å, bond angles in degrees) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

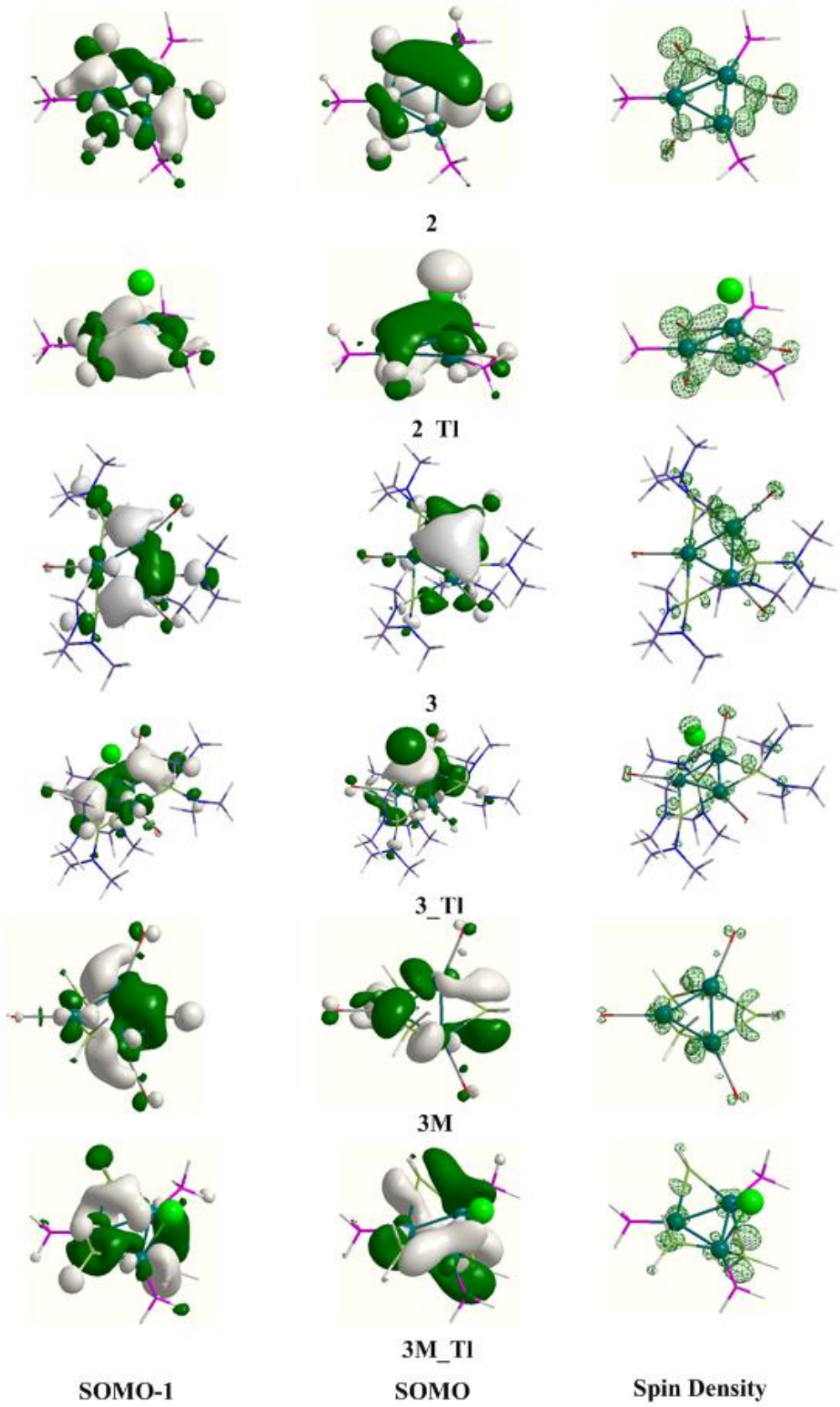


Figure S9. 3D contour plots of SOMO-1 and SOMO along with spin density isosurface (0.005 au) of **2**, **2_Tl′**, **3**, **3_Tl′**, **3M**, **3M_Tl′** computed at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p) level.

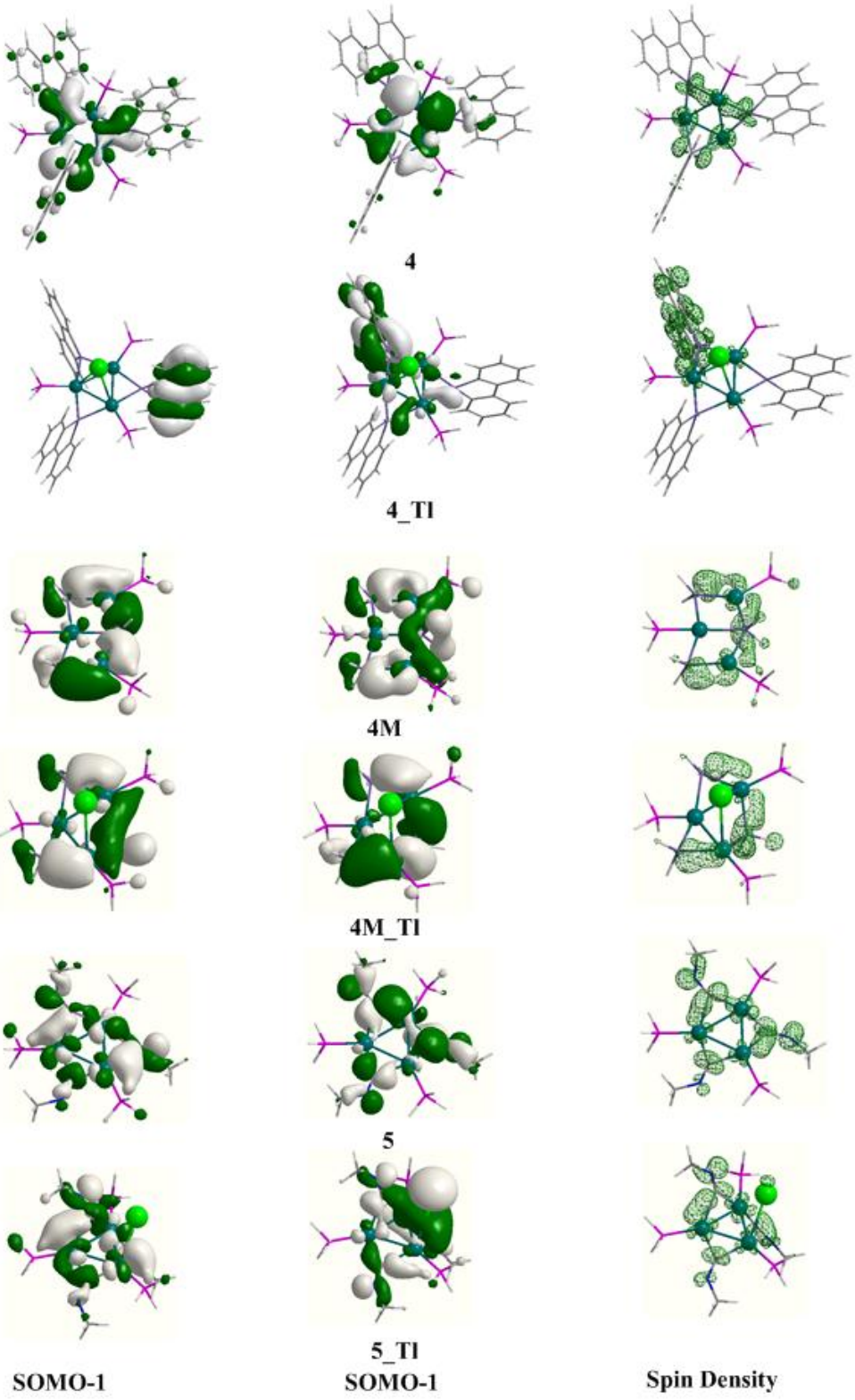


Figure S10. 3D contour plots of SOMO-1 and SOMO along with spin density isosurface (0.005 au) of **4**, **4_Tl′**, **4M**, **4M_Tl′**, **5**, **5_Tl′** computed at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p) level.

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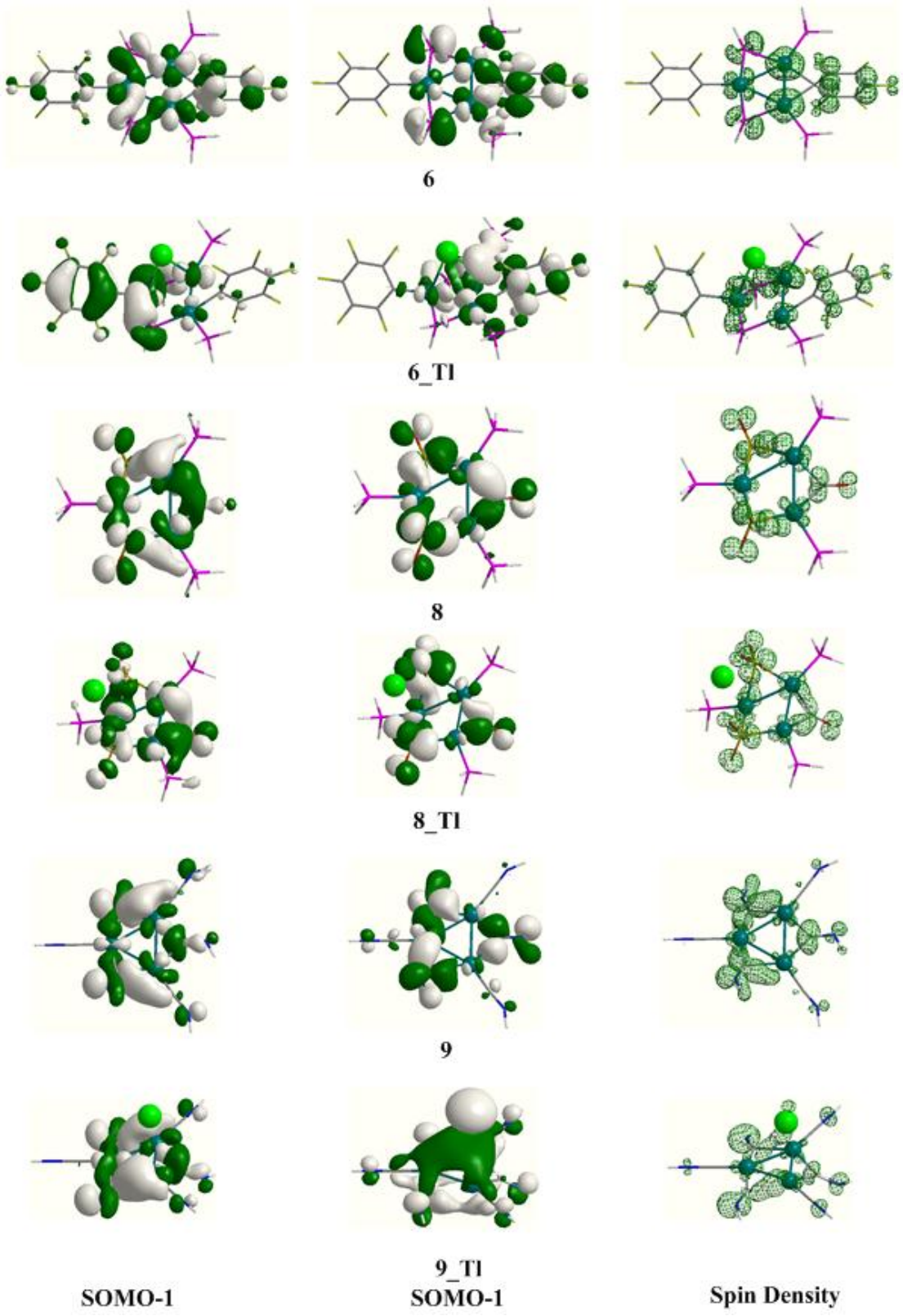

Figure S11 3D contour plots of SOMO-1 and SOMO along with spin density isosurface (0.005 au) of **6′**, **6_Tl′**, **8′**, **8_Tl′**, **9′**, **9_Tl′** computed at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p) level.

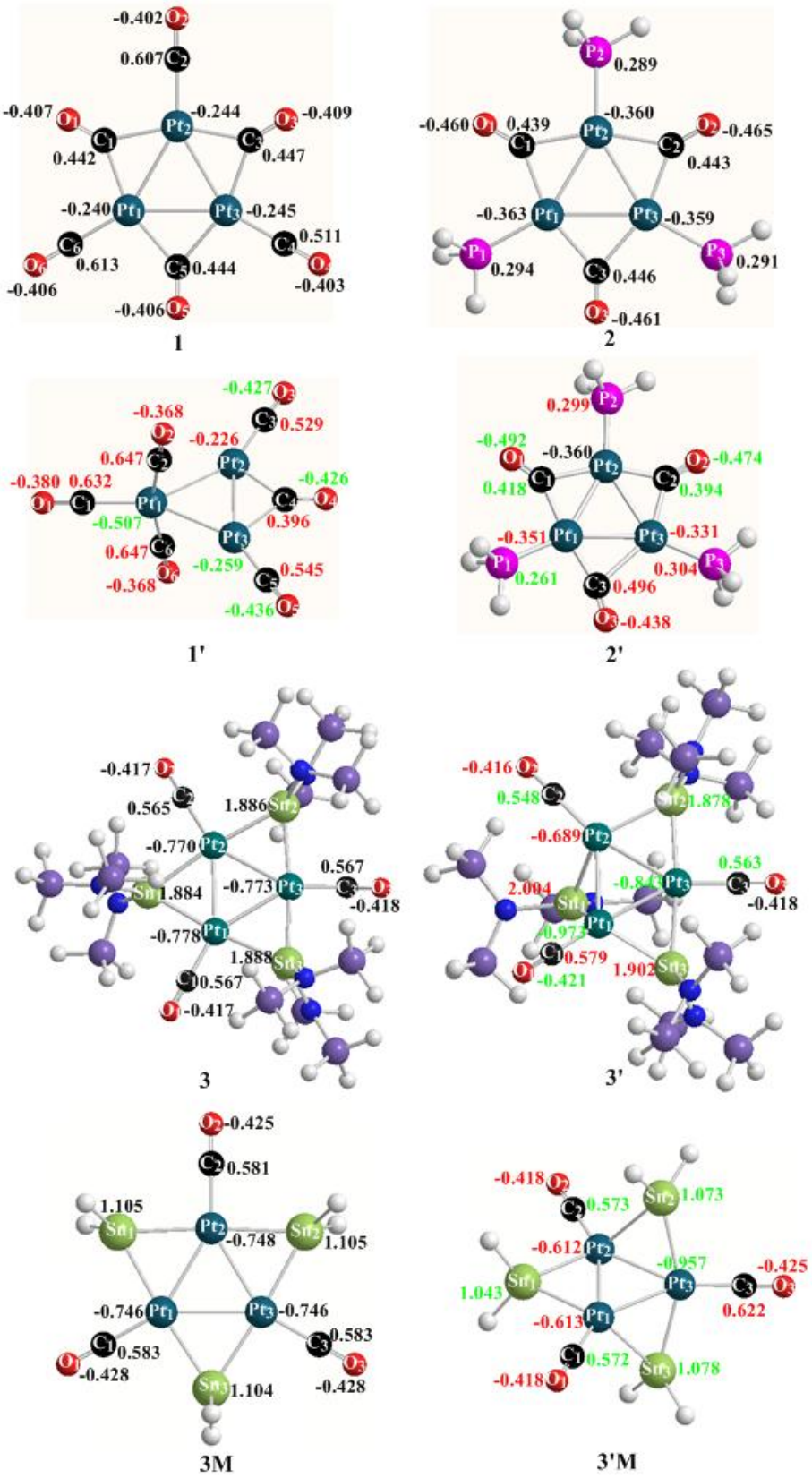

Figure S12 NBO charges of the S_0 **1**, **2**, **3**, **3M** and T_1 **1′**, **2′**, **3′**, **3M′** clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

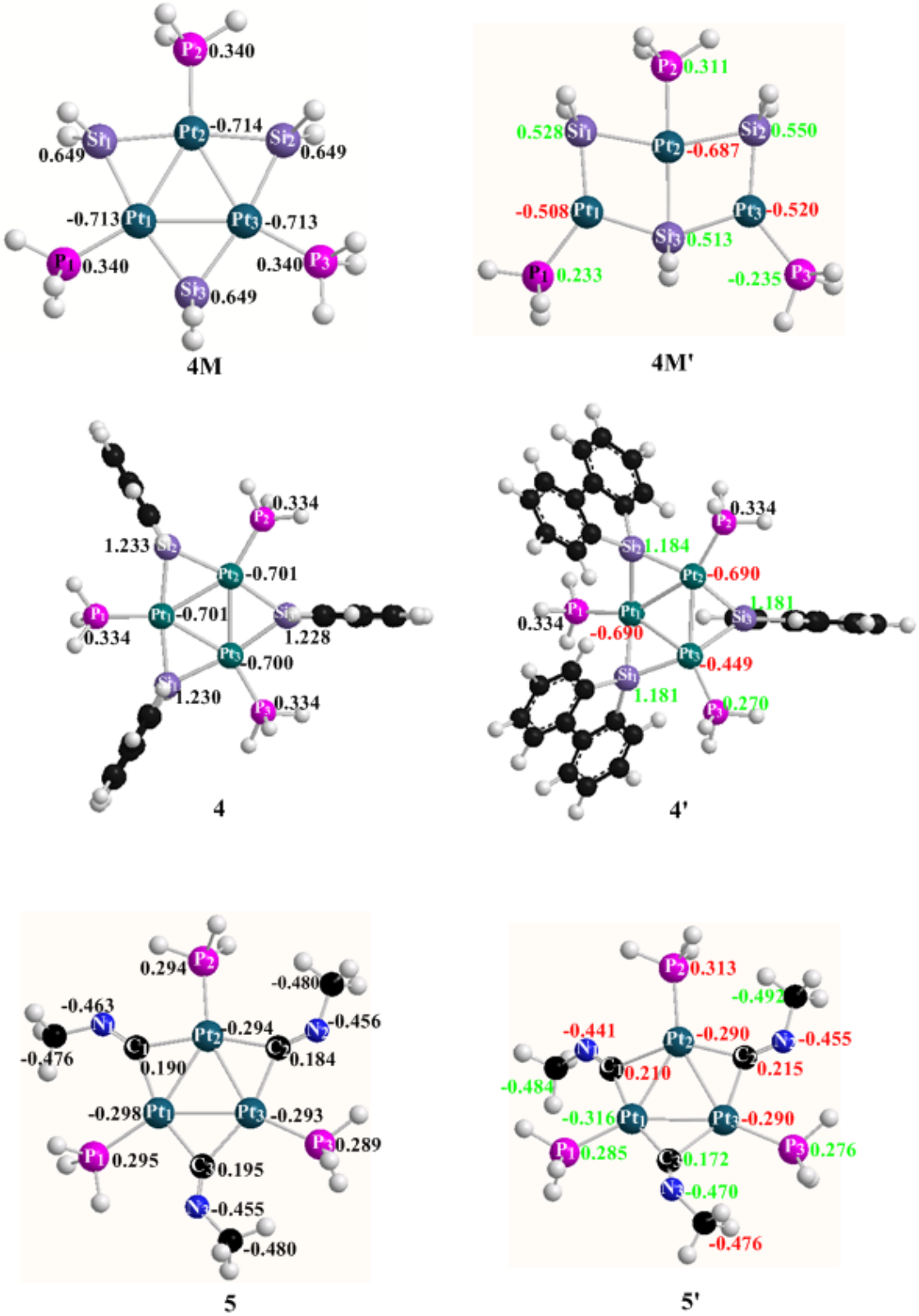

Figure S13 NBO charges of the S_0 **4M**, **4**, **5** and T_1 **4M′**, **4′**, **5′** clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

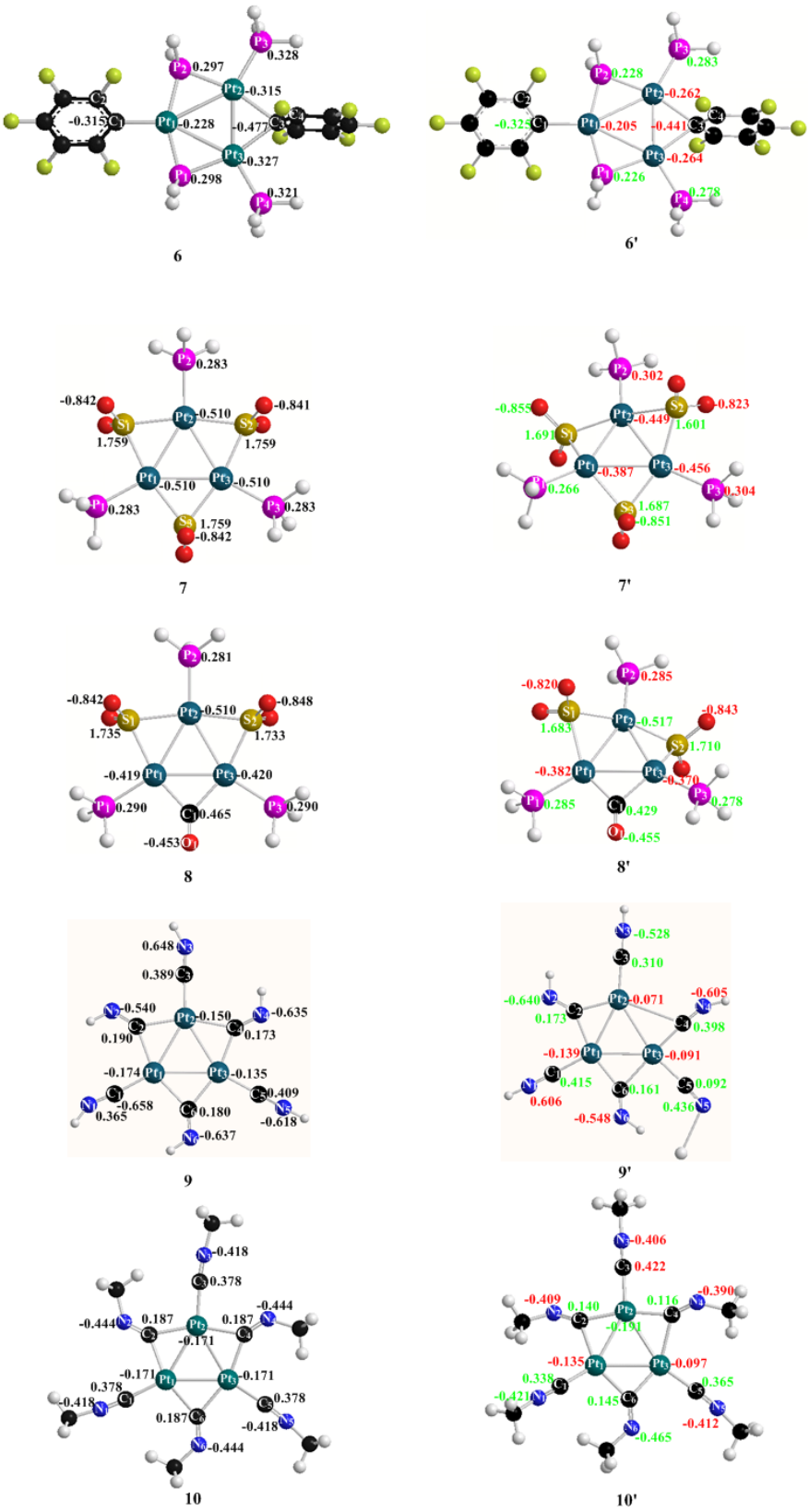

Figure S14. NBO charges of the S_0 **6**, **7**, **8**, **9**, **10** and T_1 **6′**, **7′**, **8′**, **9′**, **10′** clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

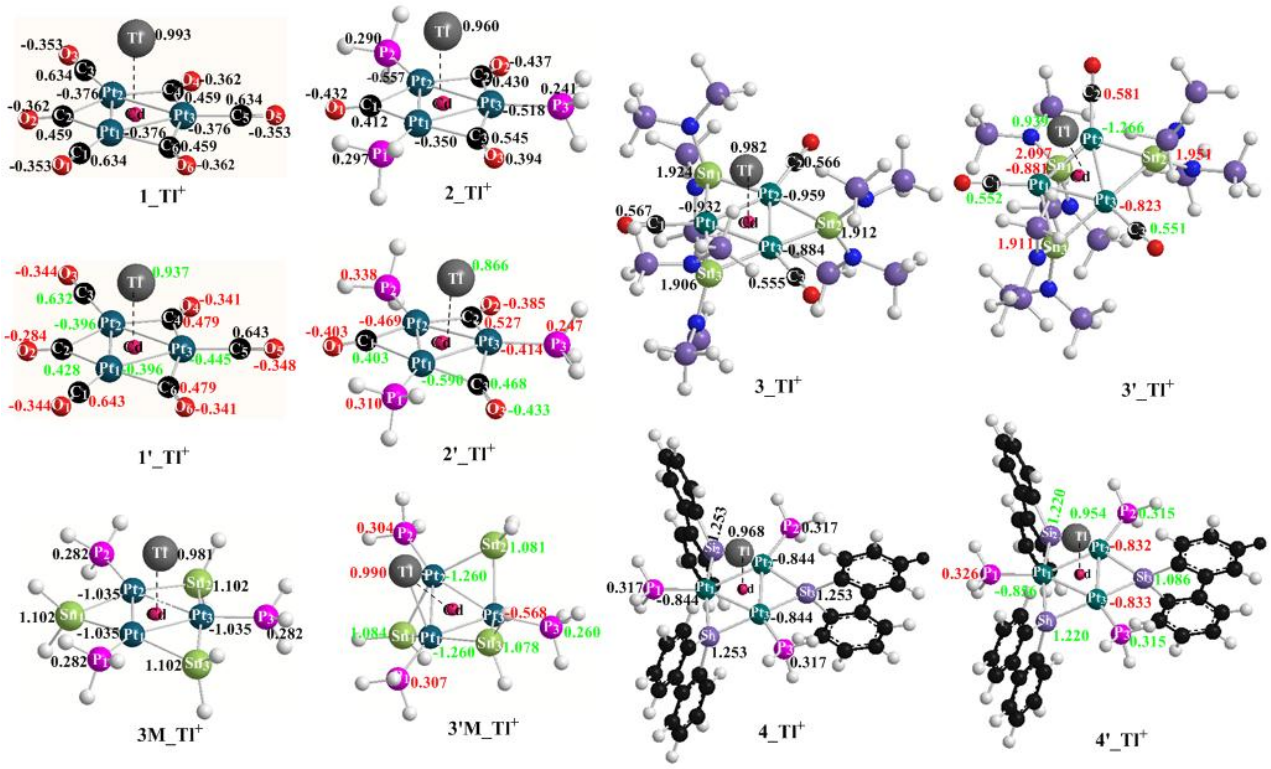

Figure S15. NBO charges of the S_0 **1_Tl**, **2_Tl**, **3_Tl**, **3M_Tl**, **4_Tl** and T_1 **1′_Tl**, **2′_Tl**, **3′_Tl**, **3M′_Tl**, **4′_Tl** clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

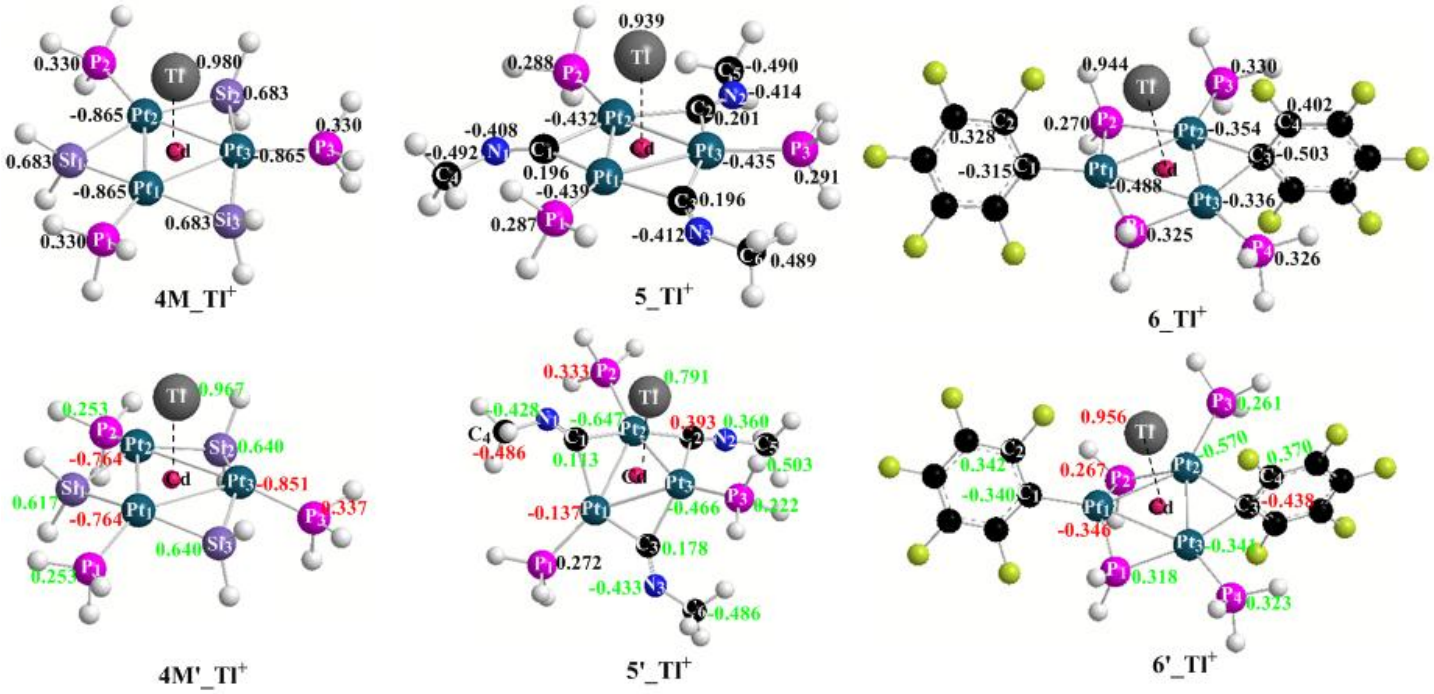

Figure S16. NBO charges of the S_0 **4M_Tl**, **5_Tl**, **6_Tl** and T_1 **4M′_Tl**, **5′_Tl**, **6′_Tl** clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

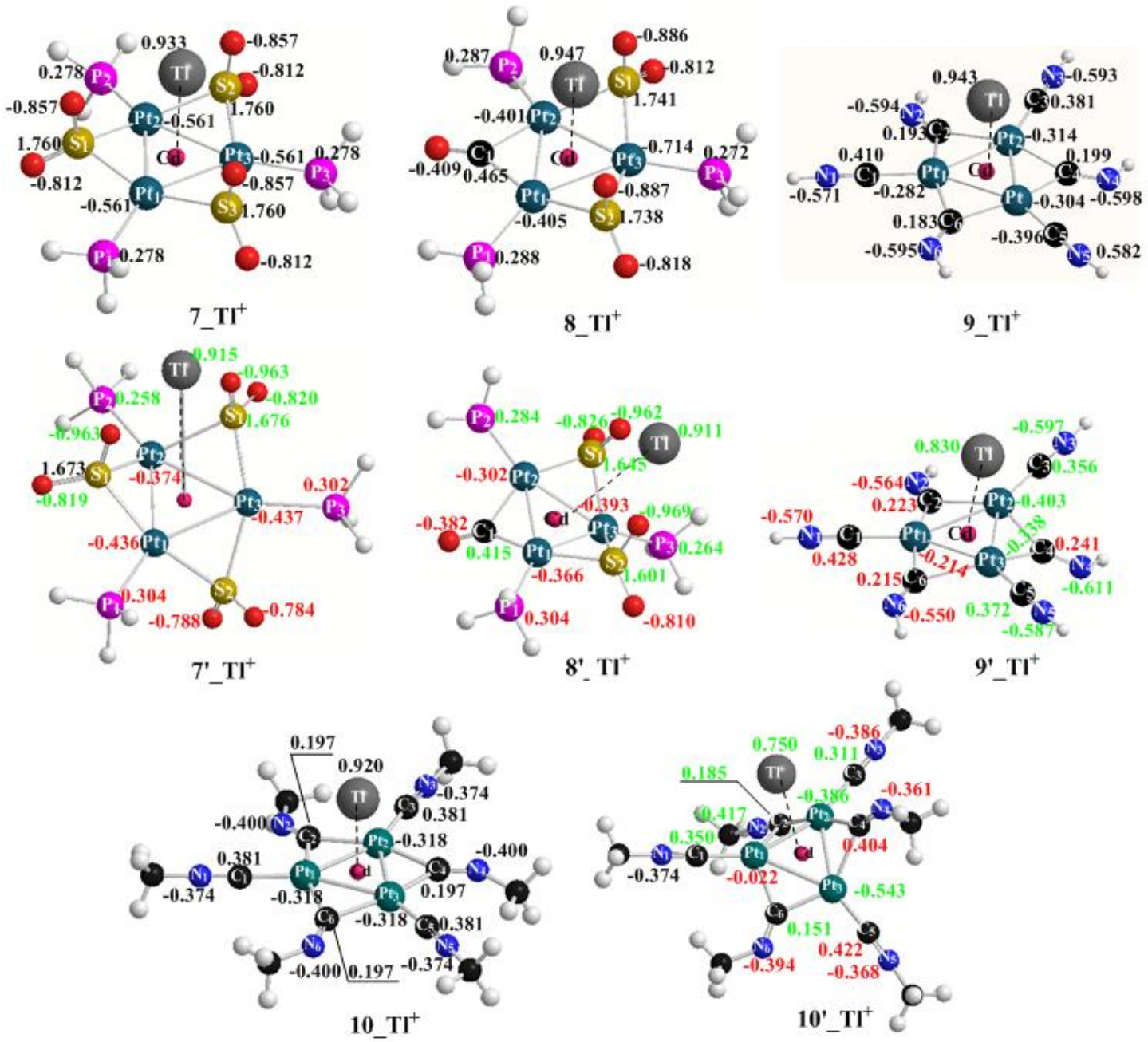

Figure S17. NBO charges of the S_0 **7_Tl**, **8_Tl**, **9_Tl**, **10_Tl** and T_1 **7′_Tl**, **8′_Tl**, **9′_Tl**, **10′_Tl** and clusters (green and red colors indicate an increase and a decrease of charge respectively) calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E) level.

Table S1. Selected electronic parameters of the [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3$] and [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3(\mu_3\text{-}Tl)]^+$ clusters calculated at the B3LYP/LANLTZ(f)(Pt)∪6-31G(d,p)(E).

Cluster	$Q(Pt_3)$	I_{PtPtPt}[a]	WBO(Pt-Pt)	Cluster	$Q(Pt_3)$	Q_{Tl}	I_{PtPtPt}	WBO(Pt-Pt)	WBO(Pt_3···Tl)
1	-0.729 (0.867)[b]	0.080	0.310	**1_Tl**	-1.122 (0.615)	0.990 (0.755)	0.068	0.329	0.384
2	-1.083 (0.096)	0.083	0.321	**2_Tl**	-1.473 (-0.271)	0.961 (0.662)	0.062	0.329	0.524
3	-2.313(-1.575)	0.117	0.359	**3_Tl**	-2.775 (-1.969)	0.982 (0.665)	0.121	0.373, 0.376, 0.388	0.606
3M	-2.238 (-0.960)	0.143	0.402	**3M_Tl**	-2.805 (-1.923)	1.003 (0.618)	0.120	0.423	0.553
4	-2.101 (-2.178)	0.062	0.335	**4_Tl**	-2.595 (-2.625)	0.980 (0.603)	0.040	0.370	0.563
4M	-2.140 (-1.299)	0.081	0.362	**4M_Tl**	-2.532 (-1.944)	0.968 (0.657)	0.061	0.337	0.694
5	-0.879 (0.381)	0.092	0.323	**5_Tl**	-1.299 (-0.042)	0.939 (0.625)	0.067	0.322	0.572
6	-0.907 (-0.134)	0.074	0.254, 0.254, 0.374	**6_Tl**	-1.218 (-0.530)	0.944 (0.653)	0.080	0.273, 0.336, 0.276	0.415
7	-1.530 (-1.098)	0.156	0.334	**7_Tl**	-1.683 (-1.506)	0.933 (0.736)	0.138	0.335	0.190
8	-1.348 (-0.687)	0.128	0.325, 0.325, 0.341	**8_Tl**	-1.525 (-1.003)	0.948 (0.715)	0.115	0.342, 0.342, 0.312	0.214
9	-0.459 (1.016)	0.079	0.315, 0.321, 0.321	**9_Tl**	-0.900(0.689)	0.943 (0.684)	0.059	0.330, 0.330, 0.334	0.493
10	-0.513 (0.888)	0.059	0.321	**10_Tl**	-0.954 (0.552)	0.920 (0.649)	0.049	0.327	0.554

[a] Three-center bond Index (I_{PtPtPt}). [b] Figures in parentheses are the Mulliken net atomic charges.

Table S2. Structural changes of selected structural parameters of the [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3$] clusters, upon $S_0 \rightarrow T_1$ excitation, calculated at the B3LYP/LANL2TZ(f)(Pt) ∪ 6-31G(d,p)(E) level.[a]

Parameter	**1**	**2**	**3**	**3M**	**4**	**4M**	**5**	**6**	**7**	**8**	**9**	**10**
Pt_1-Pt_2	0.009	0.028	-0.090	-0.025	0.064	0.185	0.075	-0.025	0.086	0.088	0.082	0.044
Pt_2-Pt_3	0.009	-0.012	-0.045	-0.031	0.012	0.172	0.047	-0.201	0.078	0.072	0.123	0.058
Pt_3-Pt_1	0.066	0.079	-0.118	-0.051	0.067	1.804	0.100	-0.203	0.092	0.067	0.059	0.110
Pt-L_1	0.071	-0.014	0.009	-0.012	-0.001	0.030	0.008	0.069	-0.002	-0.014	-0.016	-0.013
Pt-L_2	-0.024	0.039	0.004	-0.008	-0.010	0.019	-0.010	0.017	-0.016	0.000	-0.002	0.008
Pt-L_3	-0.023	-0.013	0.001	-0.003	-0.010	0.021	-0.017	0.069	-0.017	-0.007	-0.004	-0.020
Pt_1-X_1	1.054	-0.067	-0.018	0.045	0.128	-0.090	0.127	-0.095	-0.059	0.080	-0.069	0.136
Pt_2-X_1	-0.183	-0.090	0.039	-0.005	0.063	0.099	-0.084	-0.110	0.004	-0.014	0.079	-0.080
Pt_2-X_2	-0.174	0.076	0.023	0.059	0.138	0.075	-0.102	0.093	0.010	-0.048	-0.017	-0.103
Pt_3-X_2	1.063	-0.076	-0.002	0.038	0.138	-0.093	0.171	0.042	-0.056	0.052	-0.109	0.142
Pt_3-X_3	-0.070	-0.166	-0.025	-0.025	0.063	0.006	-0.073	0.041	0.026	-0.031	0.088	-0.091
Pt_1-X_3	-0.075	0.362	0.096	0.084	0.128	-0.003	-0.062	0.090	0.033	-0.065	-0.052	-0.032
Cd-Tl	1.4	1.7	-1.0	-0.5	0.6	42.3	0.9	-1.9	0.2	-0.3	-1.0	1.4
<Pt_1-Pt_2-Pt_3	-0.7	-0.2	-0.6	0.4	0.6	-21.0	0.0	3.7	0.0	0.4	-0.2	-1.0
<Pt_2-Pt_3-Pt_1	-0.7	-1.6	1.6	0.2	-1.3	-21.2	-1.0	-1.8	-0.3	-0.2	1.3	-0.5
<Pt_2-Pt_1-Pt_3	-21.4	4.9	-3.0	-1.2	2.2	5.2	1.5	3.4	3.7	1.5	2.6	2.5
<Pt-X_1-Pt	5.1	-2.6	0.0	-36.0	-22.2	-9.3	3.5	0.2	-29.8	-7.3	-17.6	-9.5
<X_1-Pt-X_2	-2.7	-1.9	20.2	9.2	3.2	-16.9	5.2	-0.4	5.3	4.0	12.5	1.8
<X_1-Pt-L_1	0.009	0.028	-0.090	-0.025	0.064	0.185	0.075	-0.025	0.086	0.088	0.082	0.044
<Tl-Cd-Pt_1	0.009	-0.012	-0.045	-0.031	0.012	0.172	0.047	-0.201	0.078	0.072	0.123	0.058

[a] Positive sign means increase while negative sign means decrease of the structural parameter.

Table S3. Structural changes of selected structural parameters of the [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3(\mu_3\text{-}Tl)]^+$ open face adducts, upon $S_0 \rightarrow T_1$ excitation, calculated at the B3LYP/LANL2TZ(f)(Pt) ∪ 6-31G(d,p)(E) level.[a]

Parameter	**1_Tl**	**2_Tl**	**3_Tl**	**3M_Tl**	**4_Tl**	**4M_Tl**	**5_Tl**	**6_Tl**	**7_Tl**	**8_Tl**	**9_Tl**	**10_Tl**
Pt_1-Pt_2	0.009	0.006	-0.052	-0.020	0.049	0.057	0.084	0.018	0.077	0.007	0.032	0.053
Pt_2-Pt_3	0.009	0.002	-0.060	0.001	0.035	0.057	0.042	0.009	0.044	0.108	0.017	0.050
Pt_3-Pt_1	0.009	0.092	-0.086	-0.020	0.049	0.975	0.069	-0.049	0.041	0.038	0.013	0.042
Pt-L_1	0.002	-0.010	-0.002	-0.002	-0.009	0.000	0.056	0.019	-0.016	-0.013	-0.019	-0.023
Pt-L_2	0.002	-0.011	0.005	-0.002	-0.008	0.019	-0.021	-0.020	-0.003	-0.015	0.011	-0.018
Pt-L_3	0.002	0.031	0.000	-0.020	-0.008	0.019	-0.019	0.042	-0.017	-0.001	-0.008	0.033
Pt_1-X_1	0.012	-0.082	0.051	0.025	-0.008	-0.049	0.092	0.061	0.026	0.011	-0.073	-0.050
Pt_2-X_1	0.012	0.045	-0.015	-0.016	-0.010	0.012	-0.115	-0.056	0.026	0.051	-0.058	-0.089
Pt_2-X_2	0.012	-0.075	-0.016	0.049	0.029	0.014	-0.130	0.019	-0.056	-0.029	0.194	0.117
Pt_3-X_2	0.012	-0.082	0.018	0.049	0.029	-0.052	0.961	0.002	0.014	-0.020	-0.130	-0.124
Pt_3-X_3	0.012	0.512	0.007	-0.016	-0.010	-0.011	-0.032	0.071	0.018	0.045	0.154	-0.116
Pt_1-X_3	0.012	-0.178	0.000	0.025	-0.008	-0.014	-0.108	0.031	-0.056	-0.070	-0.128	0.884
Cd-Tl	-0.272	0.231	0.214	0.500	-0.031	-0.086	0.475	-0.110	1.271	1.202	0.252	0.471
<Pt_1-Pt_2-Pt_3	0.00	2.10	0.00	-0.30	0.20	23.10	0.10	-1.50	-0.40	-0.40	-0.30	0.20
<Pt_2-Pt_3-Pt_1	0.00	-1.00	0.50	-0.30	0.20	-11.60	0.70	-5.90	0.80	-1.70	0.50	0.20
<Pt_2-Pt_1-Pt_3	0.00	-1.10	-0.40	0.50	-0.40	-11.60	-0.80	7.40	-0.40	2.10	-0.10	-0.20
<Pt-X_1-Pt	-0.20	1.00	-1.80	-0.60	0.00	2.30	3.40	0.30	-13.70	-0.90	4.30	3.80
<X_1-Pt-X_2	-0.90	-11.30	-52.50	-21.80	-0.70	-5.50	8.60	3.70	0.60	-25.00	-17.50	-22.80
<X_1-Pt-L_1	0.10	3.00	15.10	6.70	0.70	-7.60	-10.70	-6.10	4.00	8.40	0.40	1.00
<Tl-Cd-Pt_1	0.00	15.50	-3.20	46.70	0.10	-6.80	35.20	-12.10	6.80	10.50	-9.40	-20.10

[a] Positive sign means increase while negative sign means decrease of the structural parameter.

Table S9. Cartesian coordinates and energetic results of the [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3$] and [*cyclo*-$Pt_3(\mu_2\text{-}L)_3(L')_3(\mu_3\text{-}Tl)]^+$ clusters at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p)(E) level.

1

Pt	0.000000	1.585028	0.000000
Pt	-1.372674	-0.792514	0.000000
Pt	1.372674	-0.792514	0.000000
O	-3.077988	1.770250	0.000000
O	0.005913	-3.550740	0.000000
O	3.072075	1.780491	0.000000
O	-4.007946	-2.331200	0.000000
O	4.022851	-2.305384	0.000000
O	-0.014905	4.636583	-0.000000
C	-2.068565	1.186742	0.000000
C	3.026541	-1.736978	0.000000
C	2.062031	1.198059	0.000000
C	0.006534	-2.384801	0.000000
C	-3.017538	-1.752573	-0.000000
C	-0.009004	3.489551	-0.000000

Sum of electronic and zero-point Energies= -1037.678664
Sum of electronic and thermal Energies= -1037.659486
Sum of electronic and thermal Enthalpies= -1037.658542
Sum of electronic and thermal Free Energies= -1037.730863

1_Tl

Pt	0.00000000	1.58409437	-0.55903142
Pt	-1.37186597	-0.79204719	-0.55903142
Pt	1.37186597	-0.79204719	-0.55903142
O	-3.07536311	1.77556172	-0.83779507
O	0.00000000	-3.55112344	-0.83779507
O	3.07536311	1.77556172	-0.83779507
O	-4.02810313	-2.32562643	-0.45961067
O	4.02810313	-2.32562643	-0.45961067
O	-0.00000000	4.65125286	-0.45961067
C	-2.07899718	1.20030958	-0.68675414
C	3.04124984	-1.75586641	-0.50183355
C	2.07899718	1.20030958	-0.68675414
C	0.00000000	-2.40061916	-0.68675414
C	-3.04124984	-1.75586641	-0.50183355
C	0.00000000	3.51173283	-0.50183355
Tl	0.00000000	0.00000000	2.26352669

Sum of electronic and zero-point Energies= -1039.471365
Sum of electronic and thermal Energies= -1039.449411
Sum of electronic and thermal Enthalpies= -1039.448467
Sum of electronic and thermal Free Energies= -1039.530009

2

Pt	0.44145736	1.49901133	0.00000000
Pt	1.07678599	-1.13494961	0.00000000
P	1.09935923	3.67742677	0.00000000
P	2.65138745	-2.77791207	0.00000000
O	-2.44678999	2.57948575	0.00000000
O	3.45641594	0.83154226	0.00000000
C	-1.63927184	1.72578946	0.00000000
C	2.31392486	0.55500503	0.00000000
Pt	-1.52205597	-0.36746772	0.00000000
C	-0.67718458	-2.28093185	0.00000000
P	-3.73689855	-0.88964723	0.00000000
O	-1.01063142	-3.40747885	0.00000000
H	0.13227476	4.70909899	0.00000000
H	1.90787359	4.14649137	-1.06158981
H	1.90787359	4.14649137	1.06158981
H	2.25786266	-4.13626896	0.00000000
H	3.58326410	-2.83051065	1.06381009
H	3.58326410	-2.83051065	-1.06381009
H	-4.14359142	-2.24386285	0.00000000
H	-4.55333162	-0.41265271	-1.05109738
H	-4.55333162	-0.41265271	1.05109738

Sum of electronic and zero-point Energies=	-1727.087993
Sum of electronic and thermal Energies=	-1727.066195
Sum of electronic and thermal Enthalpies=	-1727.065251
Sum of electronic and thermal Free Energies=	-1727.148013

2_Tl

Tl	-0.01976700	-0.00443100	2.18046800
Pt	1.16262600	-1.06215800	-0.49579800
Pt	-1.49514500	-0.47275400	-0.50645900
P	2.86935100	-2.61338100	-0.52645300
P	-3.69811700	-1.15356700	-0.55691700
O	3.39102100	1.06715200	-0.77701300
O	-0.76510200	-3.46465100	-0.79973400
C	2.28702200	0.71818900	-0.61827400
C	-0.51373100	-2.33571800	-0.63489300
Pt	0.34357100	1.53450600	-0.49613800
C	-1.75785800	1.61938800	-0.63767500
P	0.85532500	3.78346800	-0.52793400
O	-2.61014400	2.40047600	-0.80751700
H	4.01803700	-2.37140700	0.25386200
H	3.47437300	-2.83190900	-1.78135800
H	2.58971800	-3.94377500	-0.15464300
H	-4.61662500	-0.53658400	0.31666700
H	-3.99766000	-2.50971700	-0.31726600

H	-4.37104900	-0.96511000	-1.78167300
H	-0.13126200	4.71397700	-0.14437500
H	1.21200300	4.31053800	-1.78636000
H	1.94439400	4.24177400	0.24077700

Sum of electronic and zero-point Energies= -1728.918979
Sum of electronic and thermal Energies= -1728.894616
Sum of electronic and thermal Enthalpies= -1728.893671
Sum of electronic and thermal Free Energies= -1728.982480

3

Pt	-0.0405529854	1.6293280975	-0.2913669301
Pt	1.4313160162	-0.7795441332	-0.2913669301
Pt	-1.3907630308	-0.8497839643	-0.2913669301
Sn	2.5634557605	1.5821926633	-0.2913669301
P	-3.3079151304	-2.0574637841	-0.2913669301
Sn	-2.6519469204	1.4289214785	-0.2913669301
Sn	0.0884911598	-3.0111141417	-0.2913669301
P	3.4357734696	-1.8360066444	-0.2913669301
P	-0.1278583393	3.8934704286	-0.2913669301
H	3.4834948636	2.1796751653	1.0472004023
H	3.4834948636	2.1796751653	-1.6299342624
H	-3.5485989815	-2.9553027557	-1.359609659
H	-4.5935739671	-1.4596934688	-0.2913669301
H	-3.5485989815	-2.9553027557	0.7768757989
H	-3.6294014969	1.9269574633	-1.6299342624
H	-3.6294014969	1.9269574633	1.0472004023
H	0.1459066332	-4.1066326285	1.0472004023
H	0.1459066332	-4.1066326285	-1.6299342624
H	3.5609186092	-3.2483050153	-0.2913669301
H	4.333666753	-1.5955254879	0.7768757989
H	4.333666753	-1.5955254879	-1.359609659
H	1.0326553578	4.7079984841	-0.2913669301
H	-0.7850677716	4.5508282437	0.7768757989
H	-0.7850677716	4.5508282437	-1.359609659

Sum of electronic and zero-point Energies= -1400.806158
Sum of electronic and thermal Energies= -1400.782561
Sum of electronic and thermal Enthalpies= -1400.781617
Sum of electronic and thermal Free Energies= -1400.868803

3_Tl

Pt	-0.060463013	1.6307891386	-0.2642664205
Pt	1.4425363287	-0.7630320641	-0.2642664205
Pt	-1.3820733158	-0.8677570745	-0.2642664205
Sn	2.5574712331	1.6054257974	-0.5746575684
P	-3.3208570322	-2.0781414158	-0.1033747125
Sn	-2.669075141	1.4121221586	-0.5746575684
Sn	0.1116039079	-3.017547956	-0.5746575684

P	3.4601517748	-1.8368758443	-0.1033747125
P	-0.1392947427	3.9150172601	-0.1033747125
H	3.6439153747	2.2968096611	0.5653959471
H	3.2040677684	2.013633136	-2.1091795019
H	-3.934810826	-2.4783706295	-1.3095848295
H	-4.4455192962	-1.5169559853	0.5404760073
H	-3.3155738889	-3.3217241621	0.5654808149
H	-3.3458913339	1.7679875149	-2.1091795019
H	-3.8110532015	2.0073184532	0.5653959471
H	0.1671378268	-4.3041281143	0.5653959471
H	0.1418235654	-3.7816206509	-2.1091795019
H	3.5364820678	-3.0914546508	0.5404760073
H	4.5344844531	-1.2105091348	0.5654808149
H	4.1137373381	-2.1684608196	-1.3095848295
H	0.9090372283	4.6084106362	0.5404760073
H	-1.2189105643	4.5322332969	0.5654808149
H	-0.1789265122	4.6468314492	-1.3095848295
Tl	0.	0.	2.2849601022

Sum of electronic and zero-point Energies= -1402.656325
Sum of electronic and thermal Energies= -1402.629690
Sum of electronic and thermal Enthalpies= -1402.628745
Sum of electronic and thermal Free Energies= -1402.720521

4

Pt	0.000000	1.581235	0.000000
Pt	1.369390	-0.790617	0.000000
Pt	-1.369390	-0.790617	0.000000
Si	2.372115	1.385478	0.000000
P	-3.313290	-1.953014	0.000000
Si	-2.385916	1.361573	0.000000
Si	0.013801	-2.747051	0.000000
P	3.348004	-1.892886	0.000000
P	-0.034715	3.845900	0.000000
H	3.179079	1.869790	1.171201
H	3.179079	1.869790	-1.171201
H	-3.568252	-2.843492	-1.069463
H	-4.572624	-1.305823	0.000000
H	-3.568252	-2.843492	1.069463
H	-3.208826	1.818268	-1.171201
H	-3.208826	1.818268	1.171201
H	0.029746	-3.688059	1.171201
H	0.029746	-3.688059	-1.171201
H	3.417188	-3.307097	0.000000
H	4.246663	-1.668451	1.069463
H	4.246663	-1.668451	-1.069463
H	1.155436	4.612920	0.000000
H	-0.678410	4.511943	1.069463

H -0.678410 4.511943 -1.069463

Sum of electronic and zero-point Energies= -2259.170841
Sum of electronic and thermal Energies= -2259.149177
Sum of electronic and thermal Enthalpies= -2259.148233
Sum of electronic and thermal Free Energies= -2259.228650

4_Tl

Pt	0.3753677417	1.5417901296	-0.29531027
Pt	1.1475455487	-1.0959730648	-0.29531027
Pt	-1.5229132903	-0.4458170647	-0.29531027
Si	2.63941302	0.7749327583	-0.5620962852
P	-3.7199477256	-1.0959174385	-0.2426048326
Si	-1.9908179649	1.8983323473	-0.5620962852
Si	-0.6485950551	-2.6732651055	-0.5620962852
P	2.8090662051	-2.6736105118	-0.2426048326
P	0.9108815206	3.7695279505	-0.2426048326
H	3.7386276607	1.0963534121	0.4005025035
H	3.2501797744	0.9542100862	-1.9124609335
H	-4.3289218401	-1.3239473839	-1.4938734511
H	-4.6842369822	-0.2439500275	0.3353735171
H	-4.068252659	-2.2961289444	0.4113614277
H	-2.4514600624	2.3376332084	-1.9124609335
H	-2.8187837368	2.6895698234	0.4005025035
H	-0.919843924	-3.7859232355	0.4005025035
H	-0.798719712	-3.2918432946	-1.9124609335
H	2.5533854122	-3.9346932101	0.3353735171
H	4.0226323257	-2.3751456794	0.4113614277
H	3.3110329878	-3.0869825925	-1.4938734511
H	2.13085157	4.1786432377	0.3353735171
H	0.0456203332	4.6712746239	0.4113614277
H	1.0178888523	4.4109299765	-1.4938734511
Tl	0.	0.	2.3284460382

Sum of electronic and zero-point Energies= -2261.015917
Sum of electronic and thermal Energies= -2260.991978
Sum of electronic and thermal Enthalpies= -2260.991034
Sum of electronic and thermal Free Energies= -2261.074684

5

Pt	2.077974977	5.3744349311	2.767827743
Pt	0.0737872679	5.6105692262	1.0027133677
Pt	2.6155631761	5.8683699721	0.1895757316
P	2.5869256955	5.017480207	4.9494130929
P	-2.0940417104	5.6455179266	0.3378684299
P	4.2741938561	6.2226201244	-1.3161566998
N	-0.7225892249	5.0033873514	4.0229659286
C	0.0094473084	5.2233295603	3.0628113066
C	-2.1604149217	4.9088591635	4.1089187254

N	0.3527807922	6.1618334041	-2.0262333205
C	0.8356991695	5.9866057958	-0.9114191076
C	0.9879582488	6.4167500742	-3.2977253562
N	5.1427482214	5.6312968122	1.9559143976
C	3.9241740308	5.6200836675	1.8082882138
C	5.9513943264	5.4421063291	3.136912818
H	3.3417856381	3.8902354296	5.3611869645
H	1.4789939752	4.8409569089	5.8097815668
H	3.2869505299	5.9826740709	5.7167457346
H	-2.307455982	5.9199000922	-1.0331523258
H	-3.0255674867	6.5703085378	0.8735642989
H	-2.9156906386	4.4947216727	0.4402643044
H	4.3763397718	7.4404087813	-2.0349762096
H	4.4746894681	5.3541797866	-2.4188291911
H	5.588195778	6.1876393042	-0.7941298385
H	-2.5352907492	5.6510915523	4.8210629404
H	-2.441125126	3.9193858114	4.4842000912
H	-2.6469556451	5.070892842	3.1381192404
H	0.6327165237	7.3707017304	-3.7008047647
H	0.7110948737	5.6331562661	-4.0103456188
H	2.0824226645	6.4515409767	-3.2171968103
H	6.5519977054	6.33955541	3.3176504823
H	6.6431743561	4.6085432119	2.9783017978
H	5.3463261301	5.2348540694	4.0292820665

Sum of electronic and zero-point Energies=	-1785.198876
Sum of electronic and thermal Energies=	-1785.171680
Sum of electronic and thermal Enthalpies=	-1785.170736
Sum of electronic and thermal Free Energies=	-1785.261276

5_Tl

Pt	-0.2433090749	-1.544362343	-0.1640034986
Pt	1.4591115566	0.5614693331	-0.1640034986
Pt	-1.2158024867	0.9828930099	-0.1640034986
P	-0.4340656532	-3.8277346935	-0.1148683173
P	3.5319483076	1.5379554656	-0.1148683173
P	-3.0978826594	2.2897792279	-0.1148683173
N	2.7308608665	-2.3476437783	-0.4793417802
C	1.862018206	-1.5169683112	-0.2980253349
C	4.1598558168	-2.331353652	-0.6763084927
N	0.6676887153	3.5388167752	-0.4793417802
C	0.3827239888	2.3710392259	-0.2980253349
C	-0.060916423	4.7682176409	-0.6763084927
N	-3.3985495869	-1.1911729968	-0.4793417802
C	-2.2447421998	-0.8540709145	-0.2980253349
C	-4.0989393988	-2.4368639888	-0.6763084927
H	-1.2651680355	-4.4775947002	0.8241985994
H	0.7654825654	-4.5351822356	0.1084853368
H	-0.8726563235	-4.4914989796	-1.2822465543

H	3.5448417417	2.9305184671	0.1084853368
H	4.3260803767	1.4900069464	-1.2822465543
H	4.5102947734	1.1431296928	0.8241985994
H	-3.4534240582	3.0014920333	-1.2822465543
H	-3.245126743	3.3344650074	0.8241985994
H	-4.3103243121	1.6046637686	0.1084853368
H	4.3947277119	-2.7745331893	-1.6477739409
H	4.6397371815	-2.9410492985	0.0939778396
H	4.5670467181	-1.3134348371	-0.6388003278
H	0.2054523671	5.1932124374	-1.6477739409
H	0.227154813	5.4886549168	0.0939778396
H	-1.1460554264	4.6118958981	-0.6388003278
H	-4.6001800841	-2.418679248	-1.6477739409
H	-4.8668919996	-2.5476056183	0.0939778396
H	-3.4209912967	-3.298461061	-0.6388003278
Tl	-0.0000000017	0.	2.4776874484

Sum of electronic and zero-point Energies=	-1787.052841
Sum of electronic and thermal Energies=	-1787.022611
Sum of electronic and thermal Enthalpies=	-1787.021667
Sum of electronic and thermal Free Energies=	-1787.120313

6

Pt	7.1121306751	10.6497114969	1.9371891256
Pt	5.1386575453	11.5743015964	3.9727112136
Pt	6.2032108355	9.1025840611	4.3201004771
P	5.9532826577	12.5889190608	2.0987694484
P	7.687447488	8.582148921	2.6639368907
P	3.758968857	13.2397183565	4.6506251508
P	6.3772099644	7.1759350391	5.499741615
F	10.2585269663	10.3521996256	1.3600046043
F	11.7092482751	10.6758812664	-0.8801883677
F	10.4952879196	11.3743105073	-3.2295965403
F	7.7872602356	11.7529185815	-3.296607749
F	6.3131923274	11.4505233697	-1.0685946581
F	6.4157634323	11.0406053894	7.0233569672
F	4.9224960826	10.7941076871	9.2503378045
F	2.4169161163	9.7414993057	9.1004722664
F	1.3964849932	8.9320945952	6.7100443362
F	2.8674051711	9.17058303	4.4674366872
C	8.2205742386	10.8870260614	0.2452448979
C	9.6040656899	10.7055367844	0.2290447387
C	10.3799570733	10.8634604734	-0.917558548
C	9.7660262588	11.2181440285	-2.1155659379
C	8.3874082572	11.4091048029	-2.1454252672
C	7.6475545804	11.242341603	-0.976481051
C	4.7152135051	10.1208835552	5.6321532108
C	5.1835204079	10.5174651079	6.8989861692
C	4.4361249382	10.4012951343	8.0651473063

C	3.150472217	9.86197527	7.9936621649
C	2.6318470862	9.4482333551	6.7654613003
C	3.4141826812	9.5831616026	5.6243895863
H	4.970202404	12.9905615551	1.1646994812
H	6.5734881921	13.8404184364	2.330474234
H	8.9877137041	8.247813981	3.1082579975
H	7.3827677848	7.4051010915	1.9386970741
H	3.0793206071	13.1039939157	5.8834521302
H	2.6505215098	13.5850649828	3.843033638
H	4.2811912214	14.5388307055	4.8485557905
H	5.7095209131	7.0715252707	6.7418975901
H	7.6516596672	6.7255930093	5.9152777507
H	5.91417752	5.9734273835	4.9168564716

Sum of electronic and zero-point Energies=	-3184.500345
Sum of electronic and thermal Energies=	-3184.464151
Sum of electronic and thermal Enthalpies=	-3184.463207
Sum of electronic and thermal Free Energies=	-3184.577910

6_Tl

Pt	-1.720499369	-0.0530196898	-0.1721946872
Pt	0.9466660919	-1.3392042051	0.0630846404
Pt	0.8656787905	1.3730509575	-0.4804227922
P	-1.1422466799	-2.2559770347	0.0504063701
P	-1.2870389324	2.0848811618	-0.8789847967
P	2.1519741583	-3.2485188112	0.4063121699
P	1.9563472477	3.3319017602	-0.9126936331
F	-3.5984651776	1.5086956828	1.8678974679
F	-6.2791993835	1.5402269418	2.1759458148
F	-7.8794517243	0.0362938308	0.5466356326
F	-6.759388254	-1.5177383225	-1.3998471143
F	-4.0750998367	-1.5775074664	-1.7211189435
F	2.4950826246	0.6430341673	2.3222739322
F	5.125701718	0.2329367257	2.6875210633
F	6.7137296196	-0.4061844324	0.5749526263
F	5.67012915	-0.6450688781	-1.9234772108
F	3.0344874002	-0.2341882819	-2.3236682801
C	-3.7476091713	-0.0313335129	0.048253762
C	-4.3608909912	0.7419054002	1.0292647487
C	-5.7392181289	0.7812266209	1.217558963
C	-6.5563354267	0.0143833003	0.3876491808
C	-5.981743183	-0.7775768401	-0.6061787788
C	-4.5961279214	-0.7892412746	-0.7556034422
C	2.6304359519	0.1955731579	-0.0207690492
C	3.2435394368	0.3182885085	1.2423537625
C	4.5979303128	0.1199253662	1.4683781663
C	5.418421014	-0.2087460011	0.3837617847
C	4.8767606634	-0.3312988234	-0.8999013805
C	3.5144897768	-0.1216363873	-1.0762821269

H	-1.395933228	-3.1246837074	-1.0322738715
H	-1.4429553812	-3.1120155927	1.1352833092
H	-1.7394544323	3.2656109032	-0.248540841
H	-1.611390591	2.3721732238	-2.2214400008
H	3.4874428044	-3.1131992192	0.8423133263
H	2.3452704405	-4.091535139	-0.707973079
H	1.692380846	-4.1940847451	1.3462475695
H	3.2805098335	3.4715206114	-0.4482873414
H	1.4105655629	4.5436950554	-0.4416721115
H	2.1395131181	3.6603785874	-2.2721444222
Tl	-0.6713777495	0.670821402	2.4943946122

Sum of electronic and zero-point Energies= -3184.500345
Sum of electronic and thermal Energies= -3184.464151
Sum of electronic and thermal Enthalpies= -3184.463207
Sum of electronic and thermal Free Energies= -3184.577910

7

Pt	-1.3633655068	-0.8501930257	-0.0233136087
Pt	-0.0529383212	1.6055486868	0.0043972797
Pt	1.4189749267	-0.7568546844	-0.0349291696
S	-2.3731598612	1.2656940503	-0.0532999338
P	3.4514742702	-1.8382286369	-0.0172610323
S	0.0916787693	-2.688670343	-0.0755308536
S	2.2848632622	1.4229349058	-0.017554837
P	-0.1333283575	3.904129927	0.0959225257
P	-3.3166856053	-2.0676777517	0.040166305
O	-3.0859150115	1.6293865489	1.1873862177
O	-3.0080254262	1.6200622741	-1.3372255174
O	0.1115695651	-3.4157021095	-1.3595728624
O	0.1202429812	-3.4876680457	1.1653996505
O	2.9427841881	1.8179645484	1.2433807698
O	2.9220049577	1.8373767913	-1.2823997497
H	4.067994537	-2.0976890677	-1.259034078
H	3.5076097641	-3.1234572337	0.559365856
H	4.517321647	-1.2131706084	0.6616212204
H	0.9355883982	4.628621917	-0.4703911183
H	-0.1850283283	4.5000550513	1.3730676123
H	-1.223890965	4.5512047016	-0.519957549
H	-4.4640575116	-1.5071275358	-0.5573352297
H	-3.8339473904	-2.3914023933	1.3115763825
H	-3.3225099818	-3.3432119667	-0.5608402801

Sum of electronic and zero-point Energies= -3032.853114
Sum of electronic and thermal Energies= -3032.826932
Sum of electronic and thermal Enthalpies= -3032.825987
Sum of electronic and thermal Free Energies= -3032.916239

7_Tl

Pt	1.6131926238	-0.0053370532	-0.0170670209
Pt	-0.811218284	-1.3943972369	-0.0170670209
Pt	-0.8019742366	1.3997342902	-0.0170670209
S	1.3112672414	-2.2855519642	0.4119225577
P	-1.9444860731	3.3679029246	-0.4728047728
S	1.3237124936	2.2783666945	0.4119225577
S	-2.6349796317	0.0071852697	0.4119225577
P	-1.944446402	-3.3679258287	-0.4728047728
P	3.8889325783	0.0000229041	-0.4728047728
O	1.4255040311	-2.4874497126	1.8808834496
O	1.8916457121	-3.3023152599	-0.475800732
O	1.9140661019	3.2893708418	-0.475800732
O	1.4414426778	2.4782475306	1.8808834496
O	-2.8669466057	0.009202182	1.8808834496
O	-3.8057117108	0.0129444181	-0.475800732
H	-2.4047515033	3.4692960933	-1.7991761318
H	-1.2489225301	4.582455071	-0.3266297267
H	-3.1250920013	3.6358104415	0.245802071
H	-3.3440611865	-3.3728262037	-0.3266297267
H	-1.5861581535	-4.5243143129	0.245802071
H	-1.8021227468	-3.8172239681	-1.7991761318
H	4.5929838198	-1.2096288673	-0.3266297267
H	4.711250258	0.8885038713	0.245802071
H	4.2068743533	0.3479278748	-1.7991761318
Tl	0.0000000344	0.	3.1586108938

Sum of electronic and zero-point Energies= -3034.678244
Sum of electronic and thermal Energies= -3034.649290
Sum of electronic and thermal Enthalpies= -3034.648346
Sum of electronic and thermal Free Energies= -3034.749627

8

Pt	1.347020	-0.952410	-0.007604
Pt	-1.346952	-0.952478	-0.007641
Pt	-0.000042	1.483666	-0.004126
P	3.269097	-2.202824	-0.064330
P	-3.268996	-2.202943	-0.064527
P	-0.000125	3.776374	-0.090495
C	0.000068	-2.497397	0.054525
S	-2.344057	1.193117	0.052900
S	2.343987	1.193272	0.052724
O	0.000101	-3.669226	0.129741
O	-2.964504	1.553156	1.344453
O	-3.048814	1.606674	-1.179021
O	3.048581	1.606807	-1.179304
O	2.964530	1.553462	1.344191
H	4.305526	-1.900348	0.844940
H	4.017057	-2.215851	-1.261794
H	3.159338	-3.592372	0.155786
H	-4.307163	-1.898009	0.841925

H	-3.159770	-3.591921	0.159419
H	-4.014623	-2.219098	-1.263407
H	-1.079560	4.467763	0.497855
H	-0.000344	4.373349	-1.368575
H	1.079443	4.467837	0.497523

Sum of electronic and zero-point Energies= -2597.604853
Sum of electronic and thermal Energies= -2597.580179
Sum of electronic and thermal Enthalpies= -2597.579235
Sum of electronic and thermal Free Energies= -2597.666348

8_Tl

Pt	1.3537817281	-0.8361119235	-0.0216234686
Pt	-1.353760561	-0.8361728831	-0.0217737079
Pt	-0.0000471071	1.5954908669	0.0326051746
P	3.2594048128	-2.1116361728	-0.329597629
P	-3.2592932553	-2.1117791896	-0.3299677878
P	-0.0000765649	3.8735939103	-0.4214064891
C	0.0000423565	-2.3876366357	0.0346704796
S	-2.3295634792	1.2588570933	0.367905053
S	2.3294452874	1.2589618605	0.368167946
O	0.0000610904	-3.5492580732	0.1648667559
O	-2.5843981517	1.4665796127	1.8250547259
O	-3.305785218	1.8233974815	-0.5752654243
O	3.3057470355	1.823546536	-0.5748932201
O	2.5841069925	1.4666936846	1.8253460266
H	4.3726941577	-1.8662429069	0.4976837496
H	3.858150812	-2.0213076864	-1.6014062965
H	3.1265298803	-3.5066602465	-0.192406465
H	-4.3726138948	-1.8665667745	0.4973257561
H	-3.126330766	-3.5068124821	-0.1929569617
H	-3.8580215436	-2.0213198194	-1.6017751989
H	-1.086607644	4.6557965078	0.0151980968
H	-0.0000556631	4.1628560334	-1.7995043258
H	1.0864122964	4.6558319073	0.0152395579
Tl	-0.0002206011	1.1898622992	3.1521846527

Sum of electronic and zero-point Energies= -2599.433727
Sum of electronic and thermal Energies= -2599.406631
Sum of electronic and thermal Enthalpies= -2599.405686
Sum of electronic and thermal Free Energies= -2599.500300

9

Pt	1.063502318	-1.1867038816	0.0097850599
Pt	0.4792106115	1.473497219	0.0408307029
Pt	-1.5066677946	-0.3454255652	0.0215384384
N	3.494184012	0.846850737	0.0300848393
N	-2.5058796479	2.5823494109	0.0581182175
N	-1.2034946724	-3.4175063332	-0.0161031982

N	1.359213088	4.4372242318	0.075249547
N	-4.5438446606	-0.9857722645	0.0219350253
N	3.2661537414	-3.3457530527	-0.0137959533
C	2.3083452972	0.5251035825	0.027752944
C	-3.3953915396	-0.7430317055	0.0206184715
C	-0.772662044	-2.2661680662	-0.0023322883
C	-1.6345504825	1.7161015159	0.0465235043
C	1.0533176495	3.2912628821	0.0618141902
C	2.3674724195	-2.5665005632	-0.0052143956
H	4.2214943149	0.1348931947	0.0211088528
H	-2.2531216191	3.5684276304	0.0698906946
H	-0.5657349865	-4.2100468678	-0.0262696021
H	2.0653191972	5.1470658754	0.079092545
H	-5.5229108829	-1.1670685907	0.0186622046
H	3.598482681	-4.2898273892	-0.0180967999

Sum of electronic and zero-point Energies=	-918.203857
Sum of electronic and thermal Energies=	-918.181038
Sum of electronic and thermal Enthalpies=	-918.180094
Sum of electronic and thermal Free Energies=	-918.259532

9_Tl

Pt	0.0161418532	1.6017725357	0.0785274771
Pt	1.3781792295	-0.7439824813	0.1221007757
Pt	-1.341031645	-0.735076349	0.1274037546
N	3.0714921059	1.9388409053	-0.2502075788
N	-0.1081975081	-3.5489086744	-0.1686324303
N	-3.0419458508	1.9446232345	-0.2311497338
N	4.0755864068	-2.2749650379	0.2518635994
N	-4.0122490534	-2.3253631947	0.233445181
N	-0.0014622841	4.7183437965	0.0504757401
C	2.0675807666	1.2764647708	-0.0545358507
C	-3.0123712369	-1.718383605	0.196618233
C	-2.0433661915	1.269816548	-0.0429188633
C	-0.0169158713	-2.3461300133	0.0041019311
C	3.0562639229	-1.698139716	0.2016478633
C	0.0061135165	3.5508348575	0.0686372612
H	4.0130571713	1.5757190101	-0.3648245248
H	0.6674846478	-4.1940348483	-0.2856638781
H	-3.9840390875	1.5779839435	-0.3363032099
H	4.9427774997	-2.7710237126	0.2845839063
H	-4.8063995275	-2.9330372484	0.23660671
H	-0.0108768697	5.7167816041	-0.0005945592
Tl	-0.0058219938	0.1171349905	2.7979187585

Sum of electronic and zero-point Energies=	-920.047721
Sum of electronic and thermal Energies=	-920.022997
Sum of electronic and thermal Enthalpies=	-920.022053
Sum of electronic and thermal Free Energies=	-920.107294