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The molecular, electronic, bonding, and photophysical features of the $[(c\text{-}Pt_3)Tl(c\text{-}Pt_3)]^+$ inorganic metallocenes

Athanassios C. Tsipis and George N. Gkekas*

Laboratory of Inorganic and General Chemistry, Department of Chemistry, University of Ioannina, 451 10 Ioannina, Greece, E-mail: attsipis@uoi.gr

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List of authors in Ref. 14

Gaussian 09, Revision A.02, Frisch, M. J.; Schlegel, H. B.; Scusseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millan, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda. R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2009

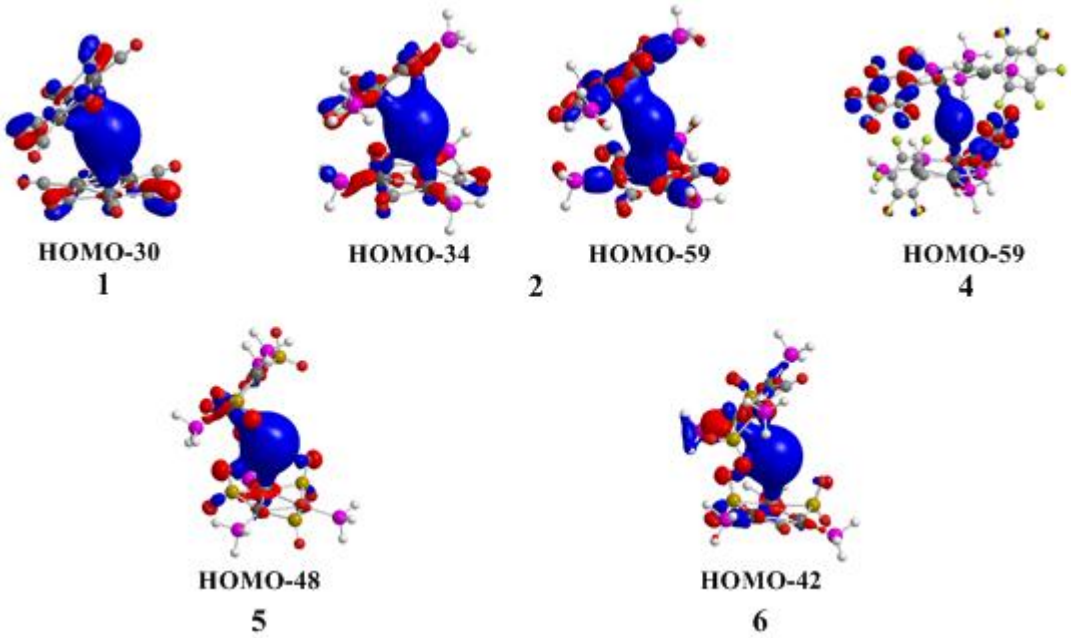

Fig. S1 3D contour plots of the bonding MOs related with $Pt_3\cdots Tl^+\cdots Pt_3$ covalent interactions.

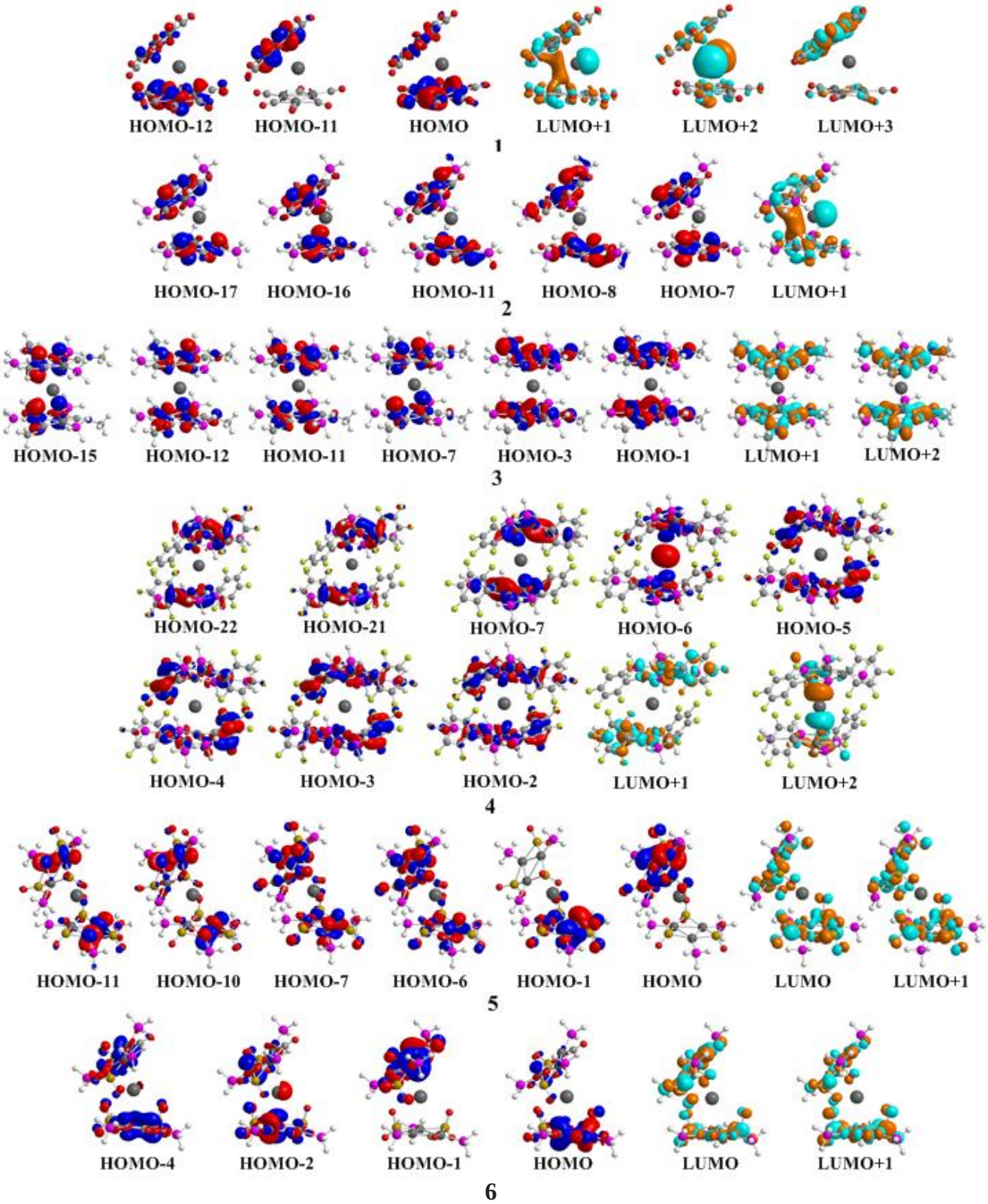

Fig. S2 3D contour plots of the MOs involved in the electronic transitions of the absorption spectra of the $\{[Pt_3(\mu_2\text{-}L)_3(L')_3]_2(\mu_6\text{-}Tl)]\}^+$ clusters at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p)(E) level.

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Table S1. Structural changes of selected structural parameters of the $\{[Pt_3(\mu_2\text{-}L)_3(L')_3]_2(\mu_6\text{-}Tl)\}^+$ sandwiches, upon $S_0 \rightarrow T_1$ excitation, calculated at the B3LYP/LANL2TZ(f)(Pt) $\cup$ 6-31G(d,p)(E) level.[a]

Parameter	**1**	**2**	**3**	**4**	**5**	**6**
Pt_1-Pt_2	0.005	-0.009	-0.012	-0.009	-0.028	-0.108
Pt_2-Pt_3	0.016	-0.02	-0.012	-0.428	-0.03	-0.136
Pt_3-Pt_1	-0.018	-0.016	-0.012	0.184	-0.017	-0.074
Pt-L_1	-0.01	-0.002	0.004	-0.024	-0.004	0.009
Pt-L_2	0.004	0.003	0.003	0.009	-0.014	-0.004
Pt-L_3	0.002	-0.023	0.002	-0.04	-0.015	0.028
Pt_1-X_1	0.074	-0.083	-0.02	-0.121	-0.048	-0.046
Pt_2-X_1	-0.117	0.06	0.009	0.009	-0.038	-0.011
Pt_2-X_2	-0.097	0.017	-0.018	-0.036	-0.022	-0.036
Pt_3-X_2	0.051	-0.009	0.009	-0.028	-0.041	-0.129
Pt_3-X_3	-0.013	0.042	-0.018	0.134	-0.026	0.002
Pt_1-X_3	0.027	-0.099	0.008	-0.015	-0.017	0.054
Cd-Tl	0.078	-0.223	0.3	0.5	1.167	0.703
$<Pt_1$-Pt_2-Pt_3	-0.7	0	0	7	0.3	1
$<Pt_2$-Pt_3-Pt_1	0.2	0.2	0	-7.3	-0.1	0
$<Pt_2$-Pt_1-Pt_3	0.5	-0.1	0	0.3	-0.2	-1
<Pt-X_1-Pt	1.3	0.2	-0.2	-5.2	0.7	-2.3
$<X_1$-Pt-X_2	6.1	-3.6	1.4	8.7	-5.9	-2.1
$<X_1$-Pt-L_1	-0.7	-0.7	9.1	4.1	2.5	1.8
<Tl-Cd-Pt_1	-17.3	3.2	0.2	-2.6	9.7	-20.8

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

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Table S2. Absolute difference between the structural changes of selected structural parameters of the $\{[Pt_3(\mu_2\text{-}L)_3(L')_3]_2(\mu_6\text{-}Tl)\}^+$ sandwiches and $\{[Pt_3(\mu_2\text{-}L)_3(L')_3](\mu_3\text{-}Tl)\}^+$ half-sandwiches, upon $S_0 \rightarrow T_1$ excitation, calculated at the B3LYP/LANL2TZ(f)(Pt) $\cup$ 6-31G(d,p)(E) level.[a]

Parameter	**1**	**2**	**3**	**4**	**5**	**6**
Pt_1-Pt_2	0.004	0.003	0.063	0.009	0.049	0.101
Pt_2-Pt_3	0.007	0.018	0.035	0.419	0.014	0.028
Pt_3-Pt_1	0.009	0.076	0.088	0.135	0.024	0.036
Pt-L_1	0.008	0.008	0.004	0.005	0.012	0.004
Pt-L_2	0.002	0.008	0.007	0.011	0.011	0.011
Pt-L_3	0.000	0.008	0.015	0.002	0.002	0.027
Pt_1-X_1	0.062	0.001	0.107	0.060	0.022	0.035
Pt_2-X_1	0.105	0.015	0.075	0.047	0.012	0.040
Pt_2-X_2	0.085	0.058	0.084	0.017	0.034	0.007
Pt_3-X_2	0.039	0.073	0.162	0.026	0.027	0.109
Pt_3-X_3	0.001	0.47	0.055	0.063	0.008	0.043
Pt_1-X_3	0.015	0.079	0.054	0.016	0.039	0.016
Cd-Tl	0.194	0.008	0.600	0.39	0.104	0.499
<Pt_1-Pt_2-Pt_3	0.7	2.1	0.0	5.5	0.1	0.6
<Pt_2-Pt_3-Pt_1	0.2	0.8	1.0	1.4	0.7	1.7
<Pt_2-Pt_1-Pt_3	0.5	1.0	1.5	7.1	0.2	1.1
<Pt-X_1-Pt	1.1	0.8	3.3	4.9	13	1.4
<X_1-Pt-X_2	5.2	7.7	3.8	5.0	5.3	22.9
<X_1-Pt-L_1	0.6	2.3	9.025	2.0s	1.5	6.6
<Tl-Cd-Pt_1	17.3	12.3	0.153	9.5	2.9	10.3

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Table S3. Cartesian coordinates and energetic results of the $\{[Pt_3(\mu_2\text{-}L)_3(L')_3]_2(\mu_6\text{-}Tl)]\}^+$ sandwich-type clusters at the B3LYP/LANL2TZ(f)(Pt)∪6-31G(d,p)(E) level.

1

Pt	-1.4309523655	0.9508380498	-2.2778883604
Pt	-0.1319075362	-1.1690464981	-3.4347748765
Pt	1.3029807354	0.9419837613	-2.4212572759
O	-3.2128072739	-1.1845526415	-3.6443278952
O	2.9270589803	-1.2699431576	-3.8502703396
O	0.0048344384	3.5144097278	-1.3166250206
O	-0.1894873409	-3.916950797	-4.7890211964
O	4.0184293399	2.2303290602	-1.8253166783
O	-4.0369208145	2.2922339021	-1.3871751369
C	-2.188852744	-0.7623407951	-3.295061768
C	3.0062830586	1.7516519313	-2.0498598432
C	-0.0093091525	2.4275414988	-1.7314349687
C	1.9457704703	-0.7998892437	-3.443215395
C	-0.1672037412	-2.8922517236	-4.286177153
C	-3.0671802986	1.7912052878	-1.7245122378
Tl	-0.172327554	-0.9834369318	-0.048568264
Pt	-0.3448901346	1.5025053966	2.4837736913
Pt	-0.934099773	-1.0931582954	3.1594256763
Pt	1.6358911294	-0.393798075	2.5243675588
O	-3.2696225928	0.9284650194	3.2931012292
O	1.2275866978	-3.2435902533	3.6681912604
O	2.5108487427	2.5026757895	1.8816248269
O	-3.0147468297	-3.1928303087	3.9666813719
O	4.5755196408	-1.1456744416	2.1005945593
O	-1.2694834907	4.3875873464	2.0248194186
C	-2.1674226505	0.6328125241	3.0734920898
C	3.4798759842	-0.8655834411	2.2617229465
C	1.7091167374	1.6970081931	2.1276074503
C	0.8477060739	-2.2123737448	3.2928749257
C	-2.2400783199	-2.4089690659	3.6679256445
C	-0.9231114164	3.312948926	2.1939377601

Zero-point correction= 0.098913 (Hartree/Particle)
Thermal correction to Energy= 0.142719
Thermal correction to Enthalpy= 0.143664
Thermal correction to Gibbs Free Energy= 0.000322
Sum of electronic and zero-point Energies= -2077.167235
Sum of electronic and thermal Energies= -2077.123429
Sum of electronic and thermal Enthalpies= -2077.122484
Sum of electronic and thermal Free Energies= -2077.265826

2

Tl	0.008646448	0.9891912478	-0.052472736
Pt	2.6024054329	-0.1036429568	-1.4123632688
Pt	2.1972579747	-1.3245848997	0.9728514255
Pt	3.0682009181	1.2465754847	0.8969864856
P	2.6604962762	-0.1676548717	-3.7068138791
P	1.6550897397	-3.1863297906	2.2078341837
P	3.7858480842	3.1148378578	2.0215762969
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O	2.8236478505	-0.0232129799	3.7075462374
O	3.9542373318	2.6756526908	-1.6961910537
C	2.0074297979	-2.0762283533	-0.9653081785
C	2.7223668887	-0.0316018291	2.5401330241
C	3.455720157	1.8107568912	-1.0860685141
Pt	-2.5950664431	0.0967877143	1.4300010739
Pt	-3.0629170202	1.2791431301	-0.9695745268
Pt	-2.2571066818	-1.3123416402	-0.8598865462
P	-2.6146490743	0.2141129608	3.7230170553
P	-3.7486645472	3.0759565337	-2.2230795288
P	-1.7734186117	-3.2726562525	-1.9590412955
O	-3.8690462874	2.9252215954	1.5183035155
O	-2.9121471635	-0.2121099631	-3.6755494076
O	-1.8323002273	-2.8788786017	1.7661166901
C	-3.4025620069	2.0035866649	0.9688585554
C	-2.7829907056	-0.1297314656	-2.5138542787
C	-2.06753176	-1.9213714628	1.128294467
H	3.9305608857	-0.0519302232	-4.3106606104
H	1.9756568947	0.8252299357	-4.4402422991
H	2.1888178177	-1.3155627522	-4.3783468342
H	2.7419190346	-3.8672285986	2.7968288442
H	1.0086905618	-4.2708622919	1.581297967
H	0.8319252001	-3.04227514	3.3431005826
H	4.1681223822	4.2558060183	1.2854511927
H	4.9290099715	2.965854874	2.834990721
H	2.9225732744	3.7204103337	2.9600087113
H	-2.1542132073	-0.8868842668	4.4759803281
H	-3.8717287579	0.4034761181	4.3353563408
H	-1.89805922	1.2471736342	4.3648555058
H	-4.1004212787	4.2753671756	-1.5692858217
H	-4.9006718295	2.8938016802	-3.0170011202
H	-2.8792066341	3.5926054495	-3.2078073567
H	-1.1616422104	-4.3302134428	-1.2562260451
H	-0.9449325319	-3.2342920823	-3.0989970839
H	-2.8801966211	-3.9590967342	-2.5026370649

Zero-point correction= 0.217979 (Hartree/Particle)
Thermal correction to Energy= 0.265417
Thermal correction to Enthalpy= 0.266361
Thermal correction to Gibbs Free Energy= 0.119008

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Sum of electronic and zero-point Energies= -3456.039592
Sum of electronic and thermal Energies= -3455.992155
Sum of electronic and thermal Enthalpies= -3455.991211
Sum of electronic and thermal Free Energies= -3456.138563

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3

Pt	1.4493314742	-0.5658295342	-2.829271848
Pt	-0.2338715088	1.5381202252	-2.830771315
Pt	-1.2148393295	-0.971490498	-2.8276477736
P	3.6339846758	-1.2199147806	-2.8203030457
P	-0.7604544828	3.7570252408	-2.8219351834
P	-2.8740933184	-2.5358525901	-2.8126493172
N	2.8742584578	2.1577579825	-3.1704192266
C	1.8722842044	1.4872090222	-2.9789482368
C	3.1036413562	3.5683042409	-3.372870795
N	-3.3057828249	1.4097461986	-3.1696827062
C	-2.223863263	0.8777290197	-2.9784031342
C	-4.6418692914	0.9018663551	-3.3715690749
N	0.431084542	-3.5698084194	-3.1510102615
C	0.3517968679	-2.3653099821	-2.9694513958
C	1.5363583327	-4.4776360539	-3.3455024945
H	4.1446743734	-2.1327910637	-1.8673656675
H	4.5816994635	-0.1854877871	-2.6598506782
H	4.1761399057	-1.8253371859	-3.9775376044
H	-2.1271789632	4.062117756	-2.6409735674
H	-0.5247398035	4.5225691039	-3.9872711653
H	-0.2097858473	4.6605399039	-1.8819866704
H	-3.6631969616	-2.7135623564	-3.9725515123
H	-3.9251594519	-2.5131154601	-1.8654974882
H	-2.4514073958	-3.8713960437	-2.6366765079
H	3.5496100898	3.7252017761	-4.3592545246
H	3.8134781942	3.9346045683	-2.6255864094
H	2.1760872976	4.1508393221	-3.3051627668
H	-4.999070338	1.2045682473	-4.3600457702
H	-5.3152609189	1.3366088767	-2.627341289
H	-4.6818866406	-0.1923592483	-3.2984112295
H	1.4497543549	-4.9483402077	-4.3289951407
H	1.4954207365	-5.2703249261	-2.5930317053
H	2.5059469151	-3.9678901595	-3.2793664356
Pt	1.4553994406	-0.550315124	2.8266858965
Pt	-0.2480917002	1.5374996985	2.8294678038
Pt	-1.2047556688	-0.9819011472	2.8260118996
P	3.6457141123	-1.1838654434	2.8129369481
P	-0.7961569362	3.7511692922	2.8119814435
P	-2.8485409873	-2.5625207002	2.809805171
N	2.8523673446	2.1868255544	3.1768016577
C	1.8582848458	1.506190989	2.9803235344
C	3.0664353433	3.5988408746	3.3873991313
N	-3.3165521641	1.3796600321	3.1783581075
C	-2.2308043201	0.8574733971	2.9817321041
C	-4.6471785895	0.859288317	3.3840590628
N	0.4660789275	-3.5635892608	3.1540394751
C	0.3754301946	-2.3602890445	2.9690174804
C	1.5797949939	-4.4595989581	3.3536791694

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H	4.1578117987	-2.1171454768	1.8806055396
H	4.5820012248	-0.1453220875	2.6173804851
H	4.201738649	-1.7523782554	3.9821580037
H	-2.1569427338	4.0453368549	2.5778281625
H	-0.6170111535	4.5085813189	3.9926419823
H	-0.2173733854	4.669064053	1.9035908073
H	-3.6382223662	-2.7458002924	3.9683811789
H	-3.8975652335	-2.5501158731	1.8602748288
H	-2.4139090113	-3.8947086485	2.6365722492
H	3.5156724611	3.7541748963	4.3724596168
H	3.7679459106	3.9781345794	2.6388463912
H	2.1321127291	4.1713740747	3.3287030819
H	-5.0046572132	1.1589281911	4.3733775128
H	-5.326635606	1.2875186155	2.6415213577
H	-4.6771174332	-0.2353841655	3.3114595177
H	1.4910599959	-4.9351728054	4.3346825057
H	1.5536153165	-5.250010279	2.5979930097
H	2.5438931894	-3.9385479284	3.2969861204
Tl	0.0030674999	0.0082430729	-0.0004192946

Zero-point correction=	0.455852 (Hartree/Particle)
Thermal correction to Energy=	0.515971
Thermal correction to Enthalpy=	0.516915
Thermal correction to Gibbs Free Energy=	0.339946
Sum of electronic and zero-point Energies=	-3572.281699
Sum of electronic and thermal Energies=	-3572.221580
Sum of electronic and thermal Enthalpies=	-3572.220636
Sum of electronic and thermal Free Energies=	-3572.397605

4

Pt	-2.11021	1.11185	-1.65503
Pt	-3.82041	0.361	0.66736
Pt	-3.46333	-1.52304	-1.33098
P	-2.8634	2.33479	0.12103
P	-2.35155	-0.62809	-3.12986
P	-4.83995	0.99803	2.60113
P	-4.01568	-3.53052	-2.23676
F	0.98942	1.04197	-2.62904
F	2.44008	2.79751	-4.05652
F	1.32316	5.12934	-4.94538
F	-1.29529	5.68401	-4.37122
F	-2.76981	3.95149	-2.93217
F	-2.15128	-2.43981	1.53207
F	-3.22493	-3.74839	3.61694
F	-5.92665	-3.97117	3.84733
F	-7.57186	-2.86833	1.98149
F	-6.5246	-1.55607	-0.12724
C	-0.962	2.42513	-2.72279
C	0.37179	2.19034	-3.04307
C	1.14931	3.07781	-3.78058
C	0.58923	4.26711	-4.23762
C	-0.74442	4.54489	-3.9425
C	-1.48565	3.629	-3.19694
C	-4.29111	-1.89271	0.61787
C	-3.49927	-2.50747	1.60863
C	-4.02011	-3.19952	2.69307
C	-5.40738	-3.318	2.81479
C	-6.2481	-2.74946	1.85484
C	-5.68096	-2.06698	0.78396
H	-3.76196	3.39429	-0.13197
H	-2.087	2.91843	1.14952
H	-1.28071	-1.36825	-3.68291
H	-3.09151	-0.36703	-4.30405
H	-4.66444	0.17146	3.73129
H	-6.2495	1.06227	2.56487
H	-4.55432	2.24913	3.17885
H	-4.60497	-4.50695	-1.40521
H	-3.01283	-4.32255	-2.83731
H	-4.96028	-3.52127	-3.28518
Tl	-0.0052	-0.41749	-0.04293
Pt	2.14828	0.78234	1.7711
Pt	3.40886	-1.82198	1.05947
Pt	3.83671	0.32134	-0.64091
P	2.32452	-1.16302	2.97324
P	2.9486	2.22592	0.19217
P	3.88824	-3.95895	1.65884
P	4.88297	1.19894	-2.46297
F	2.90488	3.37789	3.45047

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F	1.48899	4.93104	5.13264
F	-1.149	4.39125	5.62576
F	-2.34566	2.25674	4.40634
F	-0.95448	0.68003	2.73223
F	6.47015	-1.78524	-0.14493
F	7.47535	-2.81324	-2.42493
F	5.79666	-3.57318	-4.42712
F	3.10405	-3.28984	-4.15971
F	2.0724	-2.26107	-1.90381
C	1.04456	1.96417	3.02342
C	1.60937	3.06578	3.66822
C	0.89916	3.88771	4.54238
C	-0.44429	3.61706	4.79689
C	-1.04504	2.52862	4.17126
C	-0.29757	1.73232	3.30913
C	4.22802	-1.92994	-0.92522
C	5.61117	-2.12766	-1.11857
C	6.15636	-2.6668	-2.27886
C	5.29837	-3.05911	-3.30915
C	3.9159	-2.91009	-3.16786
C	3.4173	-2.36512	-1.99287
H	1.22708	-1.93877	3.414
H	3.0702	-1.10396	4.17112
H	3.88319	3.20441	0.59596
H	2.19567	2.98152	-0.73701
H	4.44341	-4.82308	0.69074
H	2.85718	-4.79457	2.14085
H	4.83135	-4.13697	2.69345
H	4.67971	0.55508	-3.70208
H	6.29385	1.20549	-2.42224
H	4.64471	2.53117	-2.84897

Zero-point correction= 0.390117 (Hartree/Particle)
Thermal correction to Energy= 0.466661
Thermal correction to Enthalpy= 0.467605
Thermal correction to Gibbs Free Energy= 0.255986
Sum of electronic and zero-point Energies= -6370.875892
Sum of electronic and thermal Energies= -6370.799348
Sum of electronic and thermal Enthalpies= -6370.798404
Sum of electronic and thermal Free Energies= -6371.010023

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Pt	1.2097684799	1.2895032055	3.6921577126
Pt	-1.2079154682	0.2218309217	2.8306102882
Pt	0.6163041669	-1.3982739401	4.1621475595
S	-0.3473342036	2.3318200935	2.3153540575
P	1.0473296755	-3.3171363657	5.3826640148
S	2.6600510033	-0.3300451181	4.6004471585
S	-1.319679685	-2.1161630947	3.0756380824
P	-3.421815978	0.5550960724	2.2017467162
P	2.4946294312	3.1235313818	4.2763178852
O	0.1120372846	2.3523005943	0.8927762811
O	-1.0416275104	3.5406445463	2.7930401494
O	3.0074891932	-0.1581919575	6.0216977752
O	3.7160721457	-0.7291548615	3.6556209464
O	-1.0135370912	-2.7704670345	1.7803304229
O	-2.4027280533	-2.6870113348	3.8934294452
H	0.6297230728	-3.2611060055	6.726154639
H	2.3867105678	-3.724265767	5.5358697945
H	0.4490304599	-4.5220795668	4.9669730879
H	-4.0870753378	-0.4734410405	1.5136223468
H	-3.7422151348	1.6724360971	1.4128428689
H	-4.2748236928	0.7440861962	3.3069388013
H	2.3707213766	4.3014546694	3.5144995993
H	3.894980487	2.9760510844	4.3071279036
H	2.2511818642	3.6199797263	5.5713015389
Tl	0.405341041	-0.5602122863	-0.02484714
Pt	-0.2832436252	1.2965682332	-2.7540945919
Pt	-1.7093803008	-0.9065932097	-3.6705203494
Pt	1.008778913	-0.652145039	-4.2570493236
S	-2.4638932384	0.6983755507	-2.1667364024
P	2.7912827843	-1.2677050294	-5.599179395
S	2.033995719	1.1084267	-3.1197773739
S	-0.3469472238	-2.5082426524	-4.733471447
P	-3.7267366644	-1.9014623392	-4.214896264
P	-0.2820737447	3.4976961502	-2.0038463739
O	-2.4793542452	0.1690775133	-0.7685858683
O	-3.5883103124	1.5726724117	-2.5446030062
O	2.7076750554	2.148581171	-3.9146917595
O	2.7009963858	0.6473255005	-1.8779516377
O	-0.0505821383	-3.6579061184	-3.8630563705
O	-0.6317895299	-2.7517394541	-6.1581715404
H	2.72972854	-0.7723517567	-6.915741882
H	4.0848230004	-0.8601424099	-5.2206311916
H	3.0040780431	-2.6389324466	-5.8392163645
H	-3.7732493726	-3.3053140043	-4.3184674766
H	-4.8399205215	-1.6616100036	-3.386336518
H	-4.2451499707	-1.5252019613	-5.4688428575
H	-1.3068987469	3.9211057246	-1.1413359745
H	0.8587911673	3.9813778418	-1.3416972696

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H -0.4052420678 4.4269514113 -3.0555606973

Zero-point correction= 0.227343 (Hartree/Particle)
Thermal correction to Energy= 0.284203
Thermal correction to Enthalpy= 0.285147
Thermal correction to Gibbs Free Energy= 0.115839
Sum of electronic and zero-point Energies= -6067.569000
Sum of electronic and thermal Energies= -6067.512140
Sum of electronic and thermal Enthalpies= -6067.511196
Sum of electronic and thermal Free Energies= -6067.680503

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Pt	3.8317051274	0.4944879711	-1.4868641212
Pt	2.9537407086	1.4040323904	0.8978642337
Pt	3.2100068179	-1.3384854195	0.5147746116
P	4.7773459028	1.0340631837	-3.5201791137
P	2.4220351354	3.2913367636	2.1221072236
P	3.3968516434	-3.4925376357	1.3420091176
C	3.4052366462	2.4014179613	-0.8472152377
S	2.3753342	-0.2575653592	2.4409920532
S	3.6472156794	-1.8348433747	-1.7718104315
O	3.3431923908	3.4815031823	-1.2935626196
O	0.8957705192	-0.4807266711	2.5141952996
O	3.1128134893	-0.368901047	3.7116961867
O	4.8561421161	-2.6145678547	-2.0885006153
O	2.3859227836	-2.1988327134	-2.4592074499
H	4.3127974308	0.3827206996	-4.6806274539
H	6.1618317872	0.8014334768	-3.6439018026
H	4.7035632409	2.3785143763	-3.935427589
H	1.4296713064	3.1889286495	3.1144765821
H	1.9480962961	4.394891878	1.3890119801
H	3.4606116374	3.8952329051	2.8601734401
H	2.6311161034	-3.8558155692	2.4673747043
H	4.689040693	-3.8333869589	1.787127459
H	3.1236320958	-4.576713609	0.4850702896
Pt	-4.056878761	-1.0312488341	-0.8355360079
Pt	-3.4670200632	1.6005665377	-0.6425870113
Pt	-2.6269640318	-0.1180284448	1.3655447099
P	-5.2902076451	-2.63680108	-1.9442768887
P	-3.8982072873	3.7078364938	-1.4743828669
P	-1.9892141253	-0.4516066483	3.5706656627
C	-4.3741455386	0.5193515346	-2.1428213655
S	-2.0058331436	2.1500981696	1.1213867545
S	-3.0545374571	-2.3788825457	0.8121025387
O	-4.7562722443	0.6894006645	-3.2360815082
O	-0.5884447338	2.2549945476	0.6690539021
O	-2.4403586149	3.1140709782	2.150581102
O	-3.90983831	-3.1836400079	1.7019548707
O	-1.7855914474	-3.0069804364	0.3445832078
H	-4.7101510505	-3.8997582404	-2.1784258551
H	-6.497080392	-3.0286839817	-1.331059481
H	-5.748393824	-2.3212275575	-3.2386674171
H	-2.8422977786	4.6372536672	-1.5701748342
H	-4.4301396815	3.7959581672	-2.7763472586
H	-4.8377247799	4.4797882824	-0.7614852007
H	-1.1938288043	0.5182335789	4.2025241295
H	-3.0913608546	-0.5136295254	4.4463921443
H	-1.3077986116	-1.6323968034	3.9112049241
Tl	0.084828429	-0.7544517414	-0.362729998

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Zero-point correction= 0.224543 (Hartree/Particle)
Thermal correction to Energy= 0.278342
Thermal correction to Enthalpy= 0.279286
Thermal correction to Gibbs Free Energy= 0.117029
Sum of electronic and zero-point Energies= -5197.077251
Sum of electronic and thermal Energies= -5197.023453
Sum of electronic and thermal Enthalpies= -5197.022509
Sum of electronic and thermal Free Energies= -5197.184766