A Zwitterionic Gold(I) Complex from an Ambiphilic Diphosphino–Alane Ligand

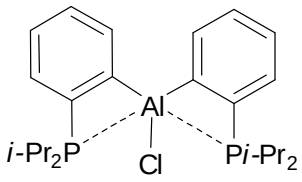
Marie Sircoglou, Ghenwa Bouhadir, Nathalie Saffon, Karinne Miqueu, and Didier Bourissou**

SUPPLEMENTARY INFORMATION

Contents

Experimental details and spectroscopic data

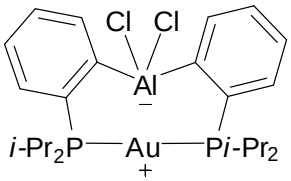
All reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques. Dry, oxygen–free solvents were employed. Diethyl ether was dried over sodium/benzophenone, CH_2Cl_2 was dried over CaH_2 and distilled prior to use. ^{1}H, ^{13}C, ^{27}Al and ^{31}P NMR spectra were recorded on Bruker Avance 300, 400WB or AMX 500 spectrometers. Chemical shifts are expressed with a positive sign, in parts per million, relative to residual ^{1}H and ^{13}C solvent signals, and external $Al(acac)_3$ and 85% H_3PO_4 respectively. Unless otherwise stated, NMR was recorded at −30°C. Mass spectra were recorded on Hewlett Packard 5989A. $AlCl_3$ (anhydrous powder, 99.999%) was purchased from Aldrich and used as received. 1−bromo−2−diisopropylphosphinobenzene was prepared as previously described.[1] The *N* values corresponding to ½ [*J*(AX)+*J*(BX)] are provided for the second–order AXX' systems observed in ^{13}C NMR.[2]



1

DPA ligand **1**: *n*-BuLi (1.6 M in hexanes, 0.289 mL, 0.46 mmol) was added at −40°C to a solution of 1−bromo−2−diisopropylphosphinobenzene (114 mg, 0.42 mmol) in diethyl ether (1 mL). A white precipitate appears after 5 min. After 30 min, the supernatant was removed by filtration. The residue was dissolved in 20 mL of toluene and was added slowly at room temperature to dry aluminium chloride (27 mg, 0.20 mmol). After removal of the solvent, the diphosphanyl–alane **1** was obtained as a white solid (63 mg, 70% crude yield). Compound **1** proved to be extremely sensitive, and was thus characterized without further purification. ^{31}P NMR (202.5 MHz, [D_8]Toluene): δ=24.4; ^{13}C NMR (125.8 MHz, [D_8]Toluene): *δ*=167.7 (AXX', *N*=60.7 Hz; C_{arom}), 140.9 (AXX', *N*=13.5 Hz; C_{arom}), 136.1 (AXX', *N*=17.4 Hz; CH_{arom}), 129.8 (s; CH_{arom}), 129.5 (s; CH_{arom}), 128.5 (s; CH_{arom}), 23.5 (s; *C*HCH_3), 19.2 (AXX', *N*=4.9 Hz; CH*C*H_3); ^{1}H NMR (500.3 MHz, [D_8]Toluene): *δ*=8.02 (d, 2H, ^{3}J(H,H)=7.2 Hz; H_{arom}), 7.44 (pseudo−t, 2H, ^{3}J(H,H)=6.4 Hz; H_{arom}), 7.27 (m, 2H; H_{arom}), 7.24 (m, 2H; H_{arom}), 2.02 (m, 4H; C*H*CH_3), 1.08 (m, 24H; CHC*H*$_3$); ^{27}Al RMN (104.13 MHz, Toluene, 293 K): δ=102.5 ($W_{½}$ ~ 1100 Hz).

[1] Tamm, M.; Dreβel, B.; Baum, K.; Lügger, T.; Pape, T. *J. Organomet. Chem.* **2003**, *677*, 1.
[2] (a) Nuclear Magnetic Resonance Spectroscopy, Ed. Bovey, F. A.; Academic Press, New–York **1969**; (b) Abraham, R. J.; Bernstein, H. J. *Can. J. Chem.* **1961**, *39*, 216.



2

Zwitterionic complex **2**: A solution of **1** (63 mg, 0.14 mmol) in toluene (2 mL) was added to a suspension of $AuCl(SMe_2)$ (41 mg, 0.14 mmol) in dichloromethane (300 μL) at −78°C. The solution became limpid, and after warming to room temperature, a white precipitate appeared. The supernatant was filtrated out and the volatile components were removed under vacuum to afford **2** (67 mg, 70% yield) as a white solid. Colorless crystals of **2** suitable for X−ray crystallography were obtained from a saturated dichloromethane solution at −4°C; mp: 196°C; ^{31}P NMR (202.5 MHz, $CDCl_3$): δ=70.4; ^{13}C NMR (125.8 MHz, $CDCl_3$): δ=160.7 (AXX', *N*=18.9 Hz; C_{arom}), 141.2 (AXX', *N*=10.5 Hz; CH_{arom}), 135.6 (AXX', *N*=27.7 Hz; C_{arom}), 130.2 (AXX', *N*=4.1 Hz; CH_{arom}), 129.5 (s; CH_{arom}), 127.3 (AXX', *N*=4.0 Hz; CH_{arom}), 29.1 (AXX', *N*=14.0 Hz; *C*HCH_3), 22.7 (AXX', *N*=15.0 Hz; *C*HCH_3), 21.4 (s; CH*C*H_3), 20.8 (s; CH*C*H_3), 20.5 (s; CH*C*H_3), 16.6 (s; CH*C*H_3); ^{1}H NMR (500.3 MHz, $CDCl_3$): δ=8.60 (d, 2H, ^3J(H,H)=7.5 Hz; H_{arom}), 7.42 (m, 2H; H_{arom}), 7.30 (m, 4H; H_{arom}), 3.11 (m broad, 2H; C*H*CH_3), 2.80 (m broad, 2H; C*H*CH_3), 1.52 (dd, 6H, ^3J(H,H)=9.1 Hz, ^3J(H,P)=25.5 Hz; CHC*H*$_3$), 1.42 (dd, 6H, ^3J(H,H)=8.2 Hz, ^3J(H,P)=23.4 Hz; CHC*H*$_3$), 1.30 (dd, 6H, ^3J(H,H)=7.3 Hz, ^3J(H,P)=21.3 Hz; CHC*H*$_3$), 1.08 (dd, 6H, ^3J(H,H)=8.5 Hz, ^3J(H,P)=24.2 Hz; CHC*H*$_3$); ^{27}Al RMN (104.13 MHz, DCM, 293 K): δ=111.7 ($W_{½}$ ~ 3800 Hz); Anal. Calcd. for $C_{24}H_{36}AlAuCl_2P_2$: C 42.31, H 5.33; found: C 42.34, H 5.30.

Crystal data

X-Ray data collection, solution, and refinement for **2**: Data were collected at 173(2) K using an oil-coated shock-cooled crystal on a Bruker-AXS CCD 1000 diffractometer (λ = 0.71073 Å). Multiscan absorption corrections were employed.[3] The structures was solved by direct methods (SHELXS–97),[4] and refined using the least-squares method on F^2.[5] Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-671794. These data can be obtained free of charge via www.ccdc.cam.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Crystal data for **2**: $C_{24}H_{36}AlAuCl_2P_2$, M = 681.31, monoclinic, space group P2(1)/c, a = 13.1769(6), b = 11.8237(5), c = 18.8682(9) Å, α = 90°, β = 108.7250(10)°, γ = 90°, V =2784.1(2) Å^3, Z = 4, crystal size 0.05 x 0.05 x 0.02 mm^3, 21620 reflections collected (4093 independent, R_{int} = 0.0757), 279 parameters, $R1$ [I>2σ(I)] = 0.0300, $wR2$ [all data] = 0.0630, largest diff. peak and hole: 1.059 and –0.695 eÅ^{-3}.

[3] SADABS, Program for data correction, Bruker-AXS, 2003, version 2.10.
[4] Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467.
[5] SHELXL–97, Program for Crystal Structure Refinement, Sheldrick, G. M., University of Göttingen, **1997**.

Computational details

Calculations were performed with the Gaussian 03 program,[6] using the density functional method. The non local B3PW91[7] functional was used. B3PW91 is Becke's 3 parameter functional, with the non-local correlation provided by the Perdew 91 expression. All Gaussian calculations were done in combination with the 6-31G** basis set for C, P, B, Al, Cl, and H (all atoms were augmented with a single set of polarization functions) and the set-RECP (relativistic effective core potential) SDD[8] for Au, SDD being the combination of the Huzinaga-Dunning double ζ basis set on lighter elements with the Stuttgart/Dresden basis set-RECP on transition metals. Geometry optimizations were carried out without symmetry restrictions. The optimized structures were confirmed as true minima on the potential energy through vibrational analysis. The frequencies were calculated with analytical second derivatives. All total energies have been zero-point energy (ZPE) and temperature corrected using unscaled density functional frequencies. The free Gibbs energies, G, were calculated for T = 298.15 K. The electronic structure of the complexes was studied using Natural Bond Orbital (NBO) analysis.[9] The NBO-3.1 program was used to gain insight into the nature of the interaction between gold and aluminum or boron and to evaluate the energy of donor/acceptor interaction (interaction between filled and empty orbitals). The donor and acceptor NBO orbitals obtained from the second-order NBO analysis were plotted by using the molecular graphic package Molekel.[10] The ^{27}Al NMR chemical shifts were evaluated by employing the direct implementation of the Gauge Including Atomic Orbitals (GIAO) method[11] at the B3PW91 density functional level of theory, using as references the corresponding $Al(acac)_3$ ($\delta^{27}Al$ = 0 ppm) shielding constant calculated at the same level of theory.

---

[6] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, 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. X.; 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 03*, *Revision D-02*, Gaussian, Inc., Pittsburgh PA, **2003**.

[7] (a) Becke, A. D. *Phys. Rev*. **1988**, *A38*, 3098; (b) Perdew, J. P. *Phys. Rev.* **1986**, *B33*, 8822; (c) Perdew, J. P. *Phys. Rev.* **1986**, *B34*, 7406 (erratum); (d) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648; (e) Burke, K.; Perdew, J. P.; Wang, Y. *Electronic Density Functional Theory: Recent Progress and New Directions*, Ed. Dobson, J. F.; Vignale, G.; Das, M. P. (Plenum), **1998**.

[8] (a) Dolg, M. *Modern Methods and Algorithm of Quantum Chemistry*; Ed. Grotendorst, J.; John von Neuman Institute for Computing: Jülich, **2000**, *1*, 479; (b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866; (c) Andrae, D.; Häussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta.* **1990**, *77*, 123.

[9] (a) Reed, A. E.; Curtiss, L. A.; Weinhold, F. *Chem. Rev.* **1988**, *88*, 899; (b) Foster, J. P.; Weinhold, F. *J. Am. Chem. Soc.* **1980**, *102*, 7211.

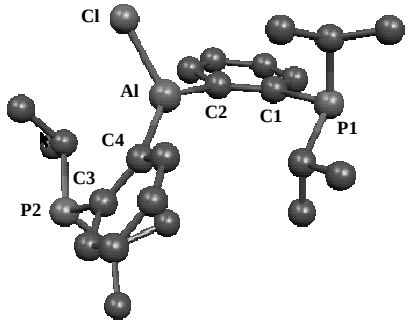
[10] (a) Flükiger, P.; Lüthi, H. P.; Portmann, S.; Weber, J. Swiss Molekel 4.3, Center for Scientific Computing, Manno, Switzerland, **2000–2002**; (b) Portmann, S.; Lüthi, H. P. *Chimica* **2000**, *54*, 766.

[11] (a) London, F. *J. Phys. Radium* **1937**, *8*, 3974; (b) Ditchfield, R. *Mol. Phys.* **1974**, *27*, 789; (c) Wolinski, K.; Hilton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.

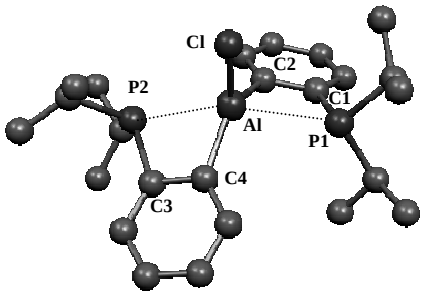
Theoretical results

I- Diphosphanyl-alane:

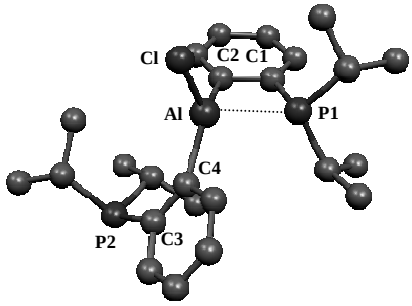
Table S1. Selected bond lengths and bond angles (in Å and °, respectively) for the different forms (**a**: without P→Al interaction; **b**: with two P→Al interactions; **c**: with one P→Al interaction) of the diphosphanyl-alane **I** at the B3PW91/ 6-31G** level of theory. Energetic difference (ΔE) and Gibbs energetic difference (ΔG) between the different forms in kcal/mol.



form a (without P→Al)



form b (with 2 P→Al)



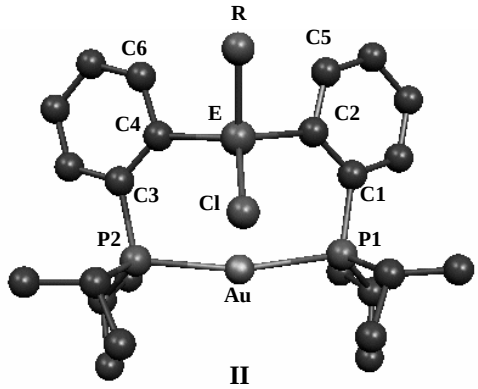
form c (with 1 P→Al)

complex	AlP1	AlP2	P1C1	P2C3	C1C2	C3C4	AlR	ΣP1	ΣP2	ΣAl	ΔE	ΔG
a-I	4.026	3.855	1.865	1.857	1.422	1.419	2.145	313.4	311.4	359.9	28.7	28.3
b-I	2.782	2.664	1.831	1.829	1.412	1.414	2.179	314.7	326.4	359.8	0	0
c-I	2.518	4.063	1.825	1.861	1.417	1.420	2.169	330.9	311.7	357.3	11.4	10.2

II- Gold complexes of diphosphanyl-alanes and -boranes

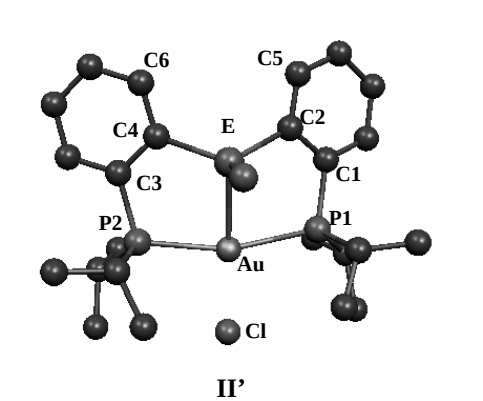
Geometrical parameters of the neutral and zwitterionic forms :

Table S2. Selected bond lengths and bond angles (in Å and °, respectively) for the actual complexes at the B3PW91/SDD(Au)-6-31G**(other atoms) level of theory. Energetic difference (ΔE) between the different forms in kcal/mol.



II

ER
a: AlCl
b: BPh
c: BCl
d: AlPh



II'

	P-Au	Au…E	Au…Cl	E...Cl	E…R	Au…R	PAuP	ΣAu_α	ΣE_α	C4EC2	ClAuER	$C_5C_2C_4C_6$	ΔE
IIa	2.374 2.374	3.178	3.101	2.225	2.196	5.348	166.7	/	/	115.9	-0.04	0	0
II'a	2.391 2.393	2.539	2.535	6.067	2.184	3.804	161.7	359.8	344.1	121.0	14.7	-1.7	+7.8
IIb	2.328 2.322	3.339	2.884	1.996	1.641	4.868	155.3	/	/	111.4	31.4	-20.5	0
II'b	2.352 2.367	2.323	2.564	4.884	1.617	3.160	161.9	357.2	339.8	116.1	1.2	32.6	–14.3
IIc	2.330 2.323	3.288	2.916	1.934	1.921	5.105	155.2	/	/	113.6	44.1	-24.6	0
II'c	2.354 2.376	2.256	2.537	4.737	1.902	3.080	154.9	353.4	337.0	122.0	-10.8	26.1	–9.1
IId	2.369 2.369	3.300	3.057	2.256	2.032	5.291	166.7	/	/	115.4	1.5	-0.5	0
II'd	2.385 2.385	2.581	2.563	5.137	1.996	3.835	163.1	358.7	343.2	120.3	0.2	0.2	+4.8

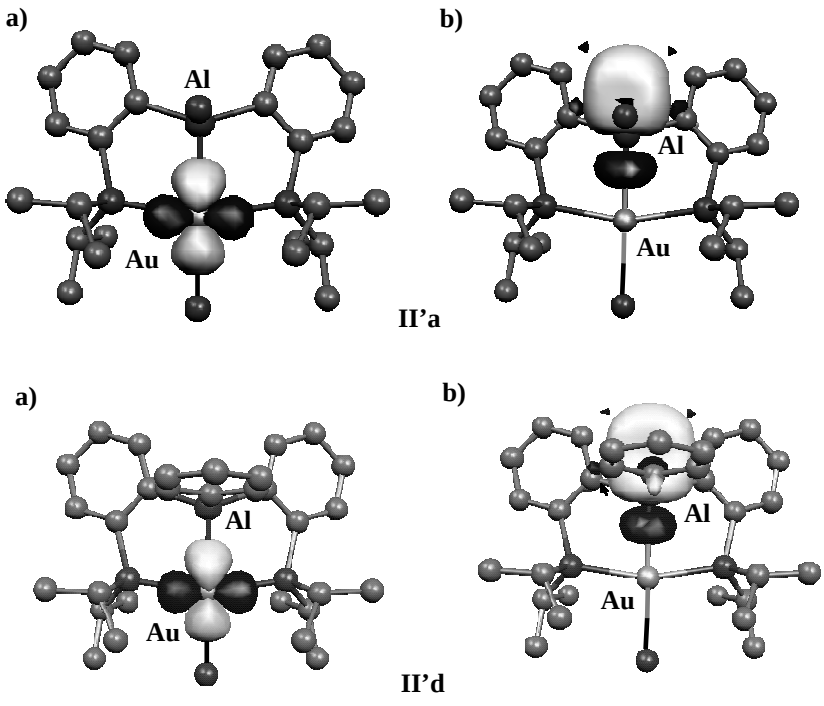
NBO analyses for the neutral forms :

In order to have further insights into the nature of the Au→E interactions in the neutral forms **II'a-d**, NBO calculations were carried out, second−order perturbation theory being particularly adapted to the description of donor/acceptor interactions. The stabilizing interactions 5d(Au) → p^{π} (E) are presented in Table S3.

Table S3. Stabilizing interaction 5d(Au) → p^{π} (E) in kcal/mol for complexes **II'a-d** (E : Al, B).

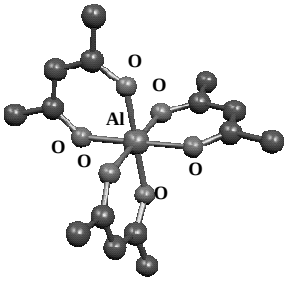
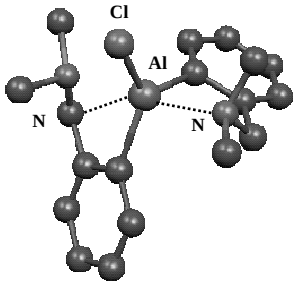
	5d (Au) → p^{π}(E)
	stabilizing interaction (kcal/mol)
II'a	19.0
II'b	32.8
II'c	75.2
II'd	9.8

Figure S1. Molekel plots (cutoff : 0.05) for the a) donor NBO and b) acceptor NBO associated with the Au→Al interaction for **II'a** and **II'd**.



III- ^{27}Al NMR:

Reference compounds:

	
$Al(acac)_3$	**$Al(C_6H_4$-*o*-$CH_2NMe_2)_2Cl$**
σ(B) = 597.0704 ppm	σ(Al) = 506.29 ppm
	δ(Al) = 90.8 ppm (exp.[12]: 96 ppm)

Ligand: exp. δ=102.5 ($W_{½}$ ~ 1100 Hz)

a-I	b-I	c-I
σ(Al) = 425.8144 ppm	σ(Al) = 490.42 ppm	σ(Al) = 468.65 ppm
δ (Al) = 171.3 ppm	δ(Al) = 106.6 ppm	δ(Al) = 128.4 ppm

Complex: δ=111.7 ($W_{½}$ ~ 3800 Hz)

IIa	II'a
σ(Al) = 485.40 ppm	σ(Al) = 438.30 ppm
δ (Al) = 111.7 ppm	δ (Al) = 151.8 ppm

[12] Müller, J.; Englert, U. *Chem. Ber.* **1995**, *128*, 493.

Z-matrix:

• **a-I**

C	0.1694	-0.00408	-0.08382
C	0.10558	0.0097	1.33701
C	1.33223	-0.03108	2.03535
C	2.57311	-0.04675	1.39975
C	2.62105	-0.02913	0.01294
C	1.42923	-0.01265	-0.70782
Al	-1.3561	0.02614	2.66833
C	-2.85333	1.22787	3.12979
C	-2.88577	2.39803	3.93135
C	-4.11108	3.05262	4.1434
C	-5.29816	2.59889	3.57523
C	-5.28642	1.4385	2.81047
C	-4.08083	0.76945	2.60761
P	-1.48979	3.19075	4.86521
C	-0.6778	4.32228	3.59479
C	-0.23962	3.67475	2.28677
P	-1.19299	-0.11436	-1.35228
C	-1.83583	-1.87156	-1.07786
C	-2.56248	-2.36455	-2.33606
Cl	-1.34972	-1.77118	3.83948
C	-0.26964	1.78998	5.08047
C	1.1309	2.30794	5.4171
C	-0.7855	0.85848	6.1806
C	-2.50427	1.06493	-0.7221
C	-3.83172	0.8883	-1.46428
C	-1.97397	2.48775	-0.93139
C	-2.64856	-2.14617	0.1836
C	-1.59675	5.52168	3.34059
H	-6.20599	1.04609	2.38493
H	-4.11129	-0.14932	2.0221
H	1.4667	-0.00796	-1.79457
H	-6.2268	3.13352	3.75538
H	3.57357	-0.03449	-0.50998
H	-4.13142	3.92737	4.78973
H	1.33497	-0.07223	3.12507
H	3.48616	-0.0759	1.98822
H	-2.68439	0.9151	0.35018
H	-0.89747	-2.43836	-1.00144
H	-2.67263	3.22258	-0.5149
H	-1.00078	2.63868	-0.45641
H	-1.85737	2.70065	-1.99975
H	-4.54003	1.66539	-1.15453
H	-3.69118	0.98093	-2.54741
H	-4.30096	-0.07976	-1.26971
H	-2.93314	-3.20397	0.24043
H	-2.06959	-1.94417	1.09078
H	-3.5748	-1.56264	0.21199
H	-2.78453	-3.43501	-2.25153
H	-3.51386	-1.84579	-2.49122
H	-1.95389	-2.21307	-3.23224
H	-0.16946	1.21853	4.13042
H	0.20839	4.69286	4.12906
H	1.79763	1.47208	5.6567
H	1.58151	2.87047	4.59517
H	1.09471	2.96153	6.29614
H	-0.1279	-0.00917	6.29663
H	-0.81615	1.39639	7.13385
H	-1.79187	0.48621	5.97207
H	-1.09516	6.25568	2.6995
H	-2.51629	5.21388	2.83098
H	-1.87821	6.0225	4.27229
H	0.23809	4.41368	1.63137
H	0.47741	2.86178	2.43385
H	-1.10245	3.27069	1.74933

Etot : -2321.15375124 ua Erep : 3553.8412073781 Hartrees
Etot (ZPE) : -2320.610948 ua G (ZPE) : -2320.678028 ua

• **b-I**

Cl	0.08277	0.04653	1.79081
Al	-1.78638	0.04207	2.91086
C	-1.61927	0.6644	4.80135
C	-1.82577	2.0579	4.90295
C	-1.77095	2.72205	6.13515
C	-1.49471	1.99681	7.29108
C	-1.26664	0.62037	7.21285
C	-1.32829	-0.03366	5.98363
P	-2.14477	2.77996	3.25113
C	-0.79447	4.04968	2.91677
C	0.53208	3.66452	3.57623
C	-3.43219	-0.43835	1.88904
C	-4.26234	0.30242	1.03554
C	-5.35945	-0.28633	0.40981
C	-5.65833	-1.63309	0.63219
C	-4.8556	-2.39791	1.4743
C	-3.74569	-1.80248	2.09245
P	-2.47704	-2.537	3.18602
C	-1.71997	-4.02674	2.33758
C	-2.63384	-5.22746	2.08398
C	-3.30799	-3.11342	4.77152
C	-2.3551	-3.99886	5.58243
C	-4.70142	-3.73157	4.64879
C	-3.68328	3.82526	3.51819
C	-4.84336	2.93846	3.97778
C	-4.06353	4.63355	2.2758
C	-0.60999	4.19984	1.40107
C	-1.04906	-3.56521	1.03873
H	-2.75322	-4.15274	6.59146
H	-2.23373	-4.98642	5.12552
H	-1.35973	-3.55322	5.68353
H	-5.11839	-3.89768	5.6495
H	-3.07876	-5.62389	2.99992
H	-4.68475	-4.69945	4.13913
H	-2.05513	-6.03721	1.62319
H	-0.92945	-4.33194	3.03747
H	-3.44105	-4.97358	1.3903
H	-3.41844	-2.16421	5.31347
H	-5.38733	-3.07376	4.10933
H	-1.04039	0.06097	8.11757
H	-1.13943	-1.10463	5.9453
H	-0.49295	-4.39781	0.5932
H	-0.35488	-2.73757	1.20458
H	-5.0996	-3.4427	1.6421
H	-1.79532	-3.23406	0.30918
H	-1.44949	2.50166	8.25268
H	0.45873	3.62843	4.66565
H	-6.51728	-2.08656	0.1443
H	-1.93603	3.79579	6.19824
H	0.8749	2.68432	3.22944
H	1.30067	4.39994	3.31069
H	-4.60408	2.40402	4.90105
H	-4.03985	1.3511	0.84853
H	-5.98745	0.30009	-0.2568
H	-1.13749	5.00562	3.33826
H	-5.09936	2.19493	3.21583
H	-3.43766	4.52966	4.32618
H	-5.73389	3.55054	4.16265
H	-0.24283	3.26403	0.96806
H	0.12567	4.98393	1.18685
H	-1.53688	4.46414	0.88403
H	-4.24796	3.98143	1.41482
H	-3.29189	5.35575	1.995
H	-4.98498	5.19647	2.46461

Etot : -2321.20100408 ua Erep : 3539.3569358139 Hartrees
Etot (ZPE) : -2320.656655 ua G (ZPE) : -2320.723097 ua

• **c-I**

Cl	0	0.40614	-1.03496	1.55787
Al	0	-1.48146	-0.46772	2.46118
C	0	-1.17332	0.66895	4.07131
C	0	-1.41732	2.0147	4.45228
C	0	-1.02981	2.45193	5.73259
C	0	-0.37163	1.62243	6.63505
C	0	-0.09932	0.30955	6.27018
C	0	-0.50669	-0.14244	5.01664
P	0	-2.14403	3.42005	3.47376
C	0	-0.61572	3.95982	2.49339
C	0	-0.13071	3.0183	1.39358
C	0	-3.03984	-0.77146	1.2321
C	0	-3.54788	-0.21605	0.04786
C	0	-4.67246	-0.75504	-0.57338
C	0	-5.32962	-1.85923	-0.02214
C	0	-4.8533	-2.44115	1.14804
C	0	-3.71163	-1.90235	1.75927
P	0	-2.79659	-2.47191	3.23092
C	0	-2.30008	-4.26399	3.04574
C	0	-3.43536	-5.28876	3.0956
C	0	-3.84383	-2.25488	4.76768
C	0	-3.16703	-2.91083	5.97587
C	0	-5.31951	-2.63621	4.63972
C	0	-3.28591	2.59396	2.24817
C	0	-3.79958	3.58789	1.20276
C	0	-4.45849	1.98311	3.02103
C	0	-0.77291	5.39969	1.99097
C	0	-1.46837	-4.422	1.7675
H	0	-3.70484	-2.64051	6.89083
H	0	-3.17179	-4.00328	5.90415
H	0	-2.13188	-2.57654	6.09405
H	0	-5.85103	-2.34767	5.55388
H	0	-3.99057	-5.26089	4.03611
H	0	-5.46143	-3.71225	4.50505
H	0	-3.01901	-6.29732	2.99028
H	0	-1.63947	-4.43065	3.90791
H	0	-4.14146	-5.14318	2.27268
H	0	-3.79056	-1.16765	4.91399
H	0	-5.79682	-2.12084	3.80249
H	0	0.42063	-0.35979	6.95095
H	0	-0.27224	-1.17694	4.75976
H	0	-1.07661	-5.4434	1.70979
H	0	-0.62337	-3.72968	1.73321
H	0	-5.36851	-3.29834	1.57199
H	0	-2.08038	-4.24756	0.87689
H	0	-0.08101	2.00007	7.61188
H	0	0.07268	2.01365	1.77548
H	0	-6.21038	-2.26657	-0.51122
H	0	-1.25577	3.47637	6.02188
H	0	-0.85327	2.93687	0.57383
H	0	0.80541	3.38921	0.95823
H	0	-3.00408	3.95389	0.54796
H	0	-3.05909	0.64385	-0.40471
H	0	-5.04496	-0.31573	-1.49553
H	0	0.14889	3.97362	3.28283
H	0	-4.26842	4.45656	1.67921
H	0	-2.75345	1.78999	1.72566
H	0	-4.55498	3.10887	0.56864
H	0	-1.5231	5.4788	1.19796
H	0	0.17574	5.76339	1.578
H	0	-1.0735	6.07451	2.79809
H	0	-5.03274	2.76376	3.5325
H	0	-4.11997	1.27169	3.78039
H	0	-5.13285	1.4539	2.33862

Etot : -2321.18244283 ua Erep : 3562.1679147505 Hartrees
Etot (ZPE) : -2320.638455 ua G (ZPE) : -2320.706854 ua

• **IIa**

Cl	0	-3.05802	-1.27982	0.69041
Cl	0	-2.23185	-1.00425	3.99352
Au	0	-0.4614	1.51736	4.41105
C	0	-2.84033	1.83943	1.88596
C	0	-0.00095	-0.07182	1.34141
P	0	1.38598	0.22949	3.78576
P	0	-2.42394	2.78233	4.51765
Al	0	-1.91955	0.02149	2.04475
C	0	0.03297	-0.26102	-0.05665
C	0	1.26913	-0.00121	1.97097
C	0	2.46184	-0.13345	1.2406
C	0	2.43993	-0.30874	-0.13874
C	0	1.21326	-0.36429	-0.79011
C	0	3.02023	1.05137	4.14415
C	0	3.08019	2.4143	3.44759
C	0	-3.0563	2.90191	2.80171
C	0	-3.77419	4.05323	2.43861
C	0	-4.27809	4.2054	1.15159
C	0	-4.0697	3.19152	0.22375
C	0	-3.37897	2.04036	0.59729
C	0	-3.81295	1.98894	5.48458
C	0	-5.02237	2.9096	5.65374
C	0	1.38487	-1.50364	4.48462
C	0	2.66696	-2.27608	4.16974
C	0	-2.14925	4.51963	5.13646
C	0	-1.11663	5.23213	4.25698
C	0	1.00282	-1.56953	5.96516
C	0	3.25108	1.19778	5.651
C	0	-1.70681	4.52473	6.60313
C	0	-3.35791	1.35907	6.80283
H	0	2.54436	-3.32404	4.46374
H	0	2.90205	-2.26	3.10158
H	0	3.52768	-1.88195	4.72138
H	0	0.84217	-2.61518	6.24929
H	0	1.78323	-1.16935	6.61891
H	0	0.07337	-1.02742	6.15946
H	0	4.1853	1.74243	5.82675
H	0	2.44101	1.76402	6.1238
H	0	3.33197	0.23273	6.1562
H	0	4.05105	2.88533	3.63758
H	0	2.94552	2.33411	2.3664
H	0	2.30071	3.07941	3.83502
H	0	-1.47106	5.54971	6.91015
H	0	-2.4814	4.15027	7.27622
H	0	-0.806	3.91794	6.74756
H	0	-0.98709	6.2639	4.60223
H	0	-0.14445	4.73131	4.32079
H	0	-1.41203	5.25885	3.20548
H	0	-4.18058	0.77184	7.22511
H	0	-2.51409	0.68201	6.64621
H	0	-3.07199	2.10617	7.54882
H	0	-5.85544	2.3441	6.08489
H	0	-4.80944	3.74361	6.33169
H	0	-5.36236	3.3175	4.6974
H	0	0.55735	-1.94664	3.91558
H	0	3.42474	-0.09396	1.74242
H	0	3.37101	-0.40098	-0.69119
H	0	1.1704	-0.49875	-1.86795
H	0	-0.90636	-0.34902	-0.59612
H	0	-3.26896	1.25371	-0.14451
H	0	-4.45204	3.28839	-0.7892
H	0	-4.8252	5.10502	0.88327
H	0	-3.94096	4.84953	3.15854
H	0	-4.08744	1.16779	4.80983
H	0	3.80734	0.4044	3.73756
H	0	-3.1083	5.04821	5.06458

Etot : = -2917.31334815 ua Erep : 4578.8248371974 Hartrees
Etot (ZPE) : -2916.764914 ua G (ZPE) : -2916.833944 ua

• **II'a**

P	0	0.78108	0.15765	3.91824
P	0	-3.29584	-2.09973	4.6896
C	0	-3.36404	-1.60638	1.95397
Cl	0	-0.29954	-1.83877	6.91293
Cl	0	-2.99572	1.71073	2.79674
Au	0	-1.14873	-1.04353	4.66101
C	0	-0.34591	-0.00749	1.3852
Al	0	-2.02857	-0.21214	2.42859
C	0	-0.28974	0.03144	-0.01749
C	0	0.87726	0.10178	2.08208
C	0	2.09336	0.22853	1.39621
C	0	2.11184	0.24299	0.0037
C	0	0.91699	0.14777	-0.70545
C	0	2.41547	-0.49774	4.52993
C	0	2.70349	-0.19075	6.00175
C	0	-3.85729	-1.8119	0.65507
C	0	-4.78429	-2.81181	0.36678
C	0	-5.25633	-3.63303	1.38796
C	0	-4.80463	-3.44544	2.6916
C	0	-3.86526	-2.44318	2.97428
C	0	-4.58521	-0.935	5.37788
C	0	-4.11434	-0.21944	6.64711
C	0	-3.36155	-3.7408	5.57208
C	0	-3.33238	-3.6433	7.09946
C	0	-2.2365	-4.63776	5.04311
C	0	0.62856	1.98008	4.30397
C	0	0.11666	2.24554	5.72219
C	0	1.89041	2.77597	3.96515
C	0	-5.96535	-1.57685	5.53396
C	0	2.49477	-2.00148	4.24311
H	0	-6.6935	-0.80622	5.80951
H	0	-6.31099	-2.03718	4.60402
H	0	-5.9786	-2.33516	6.32317
H	0	-4.84216	0.55441	6.91438
H	0	-4.01504	-0.89673	7.49855
H	0	-3.1461	0.26588	6.49749
H	0	-3.33803	-4.65794	7.51398
H	0	-2.4281	-3.13768	7.44748
H	0	-4.20768	-3.12493	7.4989
H	0	-2.34686	-5.64486	5.45985
H	0	-2.25193	-4.72268	3.95203
H	0	-1.2622	-4.24855	5.35397
H	0	3.66442	-0.6435	6.27148
H	0	2.78342	0.88196	6.19483
H	0	1.93293	-0.61447	6.6506
H	0	3.49867	-2.36576	4.48747
H	0	1.77767	-2.54589	4.86488
H	0	2.29967	-2.23371	3.19168
H	0	-0.0703	3.3183	5.84174
H	0	-0.82306	1.71961	5.91247
H	0	0.83047	1.94095	6.49114
H	0	1.68434	3.846	4.07644
H	0	2.72186	2.53239	4.63358
H	0	2.21422	2.60983	2.93366
H	0	-4.64277	-0.18485	4.57712
H	0	-5.19055	-4.09196	3.4742
H	0	-5.97631	-4.41797	1.17364
H	0	-5.13592	-2.95372	-0.65188
H	0	-3.50692	-1.18212	-0.16032
H	0	-1.20859	-0.04114	-0.59601
H	0	0.92709	0.15962	-1.79229
H	0	3.05817	0.32958	-0.52301
H	0	3.03472	0.31063	1.93178
H	0	-0.16511	2.27949	3.60595
H	0	-4.32655	-4.17316	5.27699
H	0	3.16746	0.01905	3.91889

Etot : = -2917.29967961 ua Erep : 4602.9060058925 Hartrees.
Etot (ZPE) : -2916.751682 ua G (ZPE) : -2916.822828 ua

• **IIb**

C	0.04316	-1.01744	0.24262
C	0.04654	-0.44097	1.53282
C	1.34916	-0.17418	2.05026
C	2.49647	-0.37136	1.25808
C	2.42712	-0.8994	-0.02321
C	1.17971	-1.25885	-0.51929
B	-1.51839	-0.0843	1.9966
Cl	-1.74326	0.96875	3.67734
P	1.65779	0.27207	3.81281
C	3.41005	-0.22363	4.2287
C	3.76495	0.2189	5.65283
C	-2.44808	-1.45788	2.10397
C	-3.12675	-1.7746	0.90583
C	-3.92135	-2.9002	0.71796
C	-4.10283	-3.79141	1.7659
C	-3.47182	-3.52354	2.97338
C	-2.65166	-2.39423	3.16266
P	-1.96622	-2.25082	4.87571
C	-3.32918	-1.40941	5.84927
C	-2.81491	-0.71719	7.1139
C	-1.73769	-3.98883	5.52151
C	-1.21989	-3.95934	6.96326
Au	0.00427	-1.02362	4.81527
C	-0.77098	-4.75916	4.6171
C	-2.1416	1.01481	0.94979
C	1.51102	2.13275	3.90561
C	1.19417	2.65287	5.30884
C	2.694	2.84792	3.25032
C	-4.53573	-2.30787	6.12432
C	3.57917	-1.73939	4.08668
H	-5.33743	-1.71431	6.57756
H	-4.9342	-2.75046	5.20723
H	-4.29499	-3.11578	6.82419
H	-3.61989	-0.11857	7.555
H	-2.48093	-1.42909	7.8745
H	-1.98252	-0.04566	6.88483
H	-1.01881	-4.98268	7.2997
H	-0.28518	-3.39215	7.03427
H	-1.93882	-3.52045	7.65961
H	-0.63101	-5.77427	5.0053
H	-1.13351	-4.83354	3.5891
H	0.20802	-4.26807	4.59487
H	4.75838	-0.16194	5.91452
H	3.79085	1.30562	5.76116
H	3.0521	-0.18144	6.38214
H	4.61202	-2.02015	4.32196
H	2.91709	-2.26294	4.78493
H	3.35054	-2.09401	3.0791
H	0.97501	3.72513	5.25755
H	0.31432	2.15196	5.7213
H	2.02631	2.52033	6.00598
H	2.4803	3.92011	3.18089
H	3.61697	2.73696	3.82938
H	2.87717	2.48377	2.23466
H	-3.62757	-0.6239	5.14441
H	-3.62254	-4.22421	3.78797
H	-4.72395	-4.67601	1.65685
H	-4.40244	-3.06739	-0.24236
H	-3.04088	-1.07935	0.07689
H	-0.91441	-1.26968	-0.20026
H	1.08361	-1.70573	-1.50544
H	3.33094	-1.0406	-0.60913
H	3.47487	-0.12275	1.65637
H	0.61924	2.29761	3.28994
H	-2.71235	-4.49152	5.52061
H	4.08865	0.28664	3.53387
C	-3.51693	1.32016	0.97639
C	-4.07645	2.30758	0.17159
C	-3.26952	3.04579	-0.69515
C	-1.90474	2.77985	-0.73553
C	-1.35787	1.78077	0.07307
H	-4.16577	0.76943	1.65382
H	-5.14475	2.50577	0.22243
H	-3.70094	3.81903	-1.32589
H	-1.25791	3.34947	-1.39918
H	-0.28811	1.59969	0.01477

Etot : -2471.05975690 ua Erep : 5062.3171078417 Hartrees
Etot (ZPE) : -2470.417861 ua G (ZPE) : -2470.489243 ua

• **II'b**

P	0	1.00918	-0.50636	2.04864
P	0	-1.70651	-0.41217	-1.73824
Cl	0	-0.82339	-3.2949	0.39087
B	0	0.39598	1.39047	-0.25577
Au	0	-0.26381	-0.8123	0.0761
C	0	2.32439	0.4366	-1.81417
C	0	1.92411	1.30141	-0.77793
C	0	2.91338	2.1648	-0.27033
C	0	4.21858	2.16753	-0.76541
C	0	4.58409	1.2886	-1.78208
C	0	3.62757	0.41784	-2.30455
C	0	-0.56614	2.04999	-1.37994
C	0	-1.62658	1.3846	-2.02102
C	0	-2.49098	2.05469	-2.90168
C	0	-2.28296	3.39486	-3.20279
C	0	-1.1849	4.05382	-2.64846
C	0	-0.34489	3.3886	-1.76167
C	0	-1.14572	-1.18343	-3.35118
C	0	-2.13558	-1.00781	-4.50584
C	0	0.33506	-1.37445	3.55741
C	0	-1.18441	-1.18422	3.61879
C	0	0.28235	2.01831	1.24185
C	0	-0.1108	3.3423	1.48988
C	0	-0.03707	3.9141	2.76106
C	0	0.44284	3.17395	3.83676
C	0	0.81403	1.84584	3.63488
C	0	0.71954	1.27301	2.3631
C	0	2.84965	-0.78204	1.93264
C	0	3.58104	-0.56697	3.25931
C	0	3.19905	-2.11591	1.26486
C	0	0.706	-2.85754	3.64059
C	0	-3.49977	-0.80798	-1.42803
C	0	-3.92646	-0.15678	-0.10794
C	0	-3.82033	-2.30439	-1.44255
C	0	-0.70016	-2.64055	-3.19558
H	0	4.66209	-0.62959	3.09223
H	0	3.37302	0.41886	3.68565
H	0	3.32163	-1.32769	4.00228
H	0	4.27519	-2.1441	1.06171
H	0	2.95457	-2.97647	1.89221
H	0	2.67292	-2.23746	0.31446
H	0	0.23117	-3.28925	4.52918
H	0	0.34511	-3.40239	2.76392
H	0	1.78305	-3.01305	3.73968
H	0	-1.56363	-1.58574	4.5652
H	0	-1.47485	-0.13117	3.55979
H	0	-1.66469	-1.73209	2.80219
H	0	-4.87757	-2.44463	-1.1901
H	0	-3.65605	-2.75341	-2.42536
H	0	-3.21264	-2.84839	-0.71332
H	0	-5.00443	-0.28991	0.03527
H	0	-3.41393	-0.62834	0.73653
H	0	-3.71126	0.91558	-0.08557
H	0	-0.21505	-2.96577	-4.12299
H	0	-0.00044	-2.77507	-2.36766
H	0	-1.54328	-3.30954	-3.00727
H	0	-1.69755	-1.42258	-5.42046
H	0	-3.07363	-1.54178	-4.32461
H	0	-2.36294	0.0429	-4.70086
H	0	3.14408	0.0191	1.24396
H	0	1.14813	1.25659	4.48448
H	0	0.50548	3.61337	4.82829
H	0	-0.3597	4.94163	2.90945
H	0	-0.49237	3.94415	0.6707
H	0	0.51391	3.91756	-1.35534
H	0	-0.9868	5.09102	-2.90685
H	0	-2.95617	3.9145	-3.87861
H	0	-3.33154	1.5344	-3.35249
H	0	-0.25742	-0.57716	-3.57576
H	0	0.79167	-0.8516	4.40923
H	0	-4.03982	-0.31847	-2.25081
H	0	2.65601	2.8536	0.53108
H	0	4.95171	2.85555	-0.35089
H	0	5.60111	1.28149	-2.16498
H	0	3.89758	-0.2748	-3.09806
H	0	1.5969	-0.25195	-2.23939

Etot : -2471.08251428 ua Erep : 5115.6207790892 Hartrees
Etot (ZPE) : -2470.440663 ua G (ZPE) : -2470.513099 ua

• **IIc**

B	0	-1.43268	-0.10415	2.31466
C	0	-1.31652	0.8841	3.63582
C	0	-0.5222	2.03674	3.46413
C	0	-0.35412	3.02689	4.4261
C	0	-0.98478	2.90405	5.65551
C	0	-1.76002	1.77554	5.88721
C	0	-1.93868	0.77153	4.91674
P	0	-2.92255	-0.67514	5.51977
Au	0	-3.8812	-1.7885	3.72041
P	0	-4.28294	-2.2086	1.46371
C	0	-3.23338	-3.47829	0.58219
C	0	-3.65666	-3.6816	-0.8741
C	0	-2.74908	0.22224	1.3516
C	0	-2.70849	1.55803	0.8955
C	0	-3.54602	2.07733	-0.08216
C	0	-4.48317	1.25174	-0.69327
C	0	-4.60302	-0.05514	-0.24408
C	0	-3.79222	-0.56793	0.78703
Cl	0	-1.10194	-1.9331	2.84976
C	0	-6.07453	-2.49047	1.02837
C	0	-6.95576	-1.41674	1.67438
C	0	-6.52133	-3.88491	1.48224
C	0	-1.66414	-1.7264	6.42886
C	0	-1.2334	-1.15162	7.7792
C	0	-4.17737	-0.01994	6.73697
C	0	-5.09511	0.98783	6.03878
C	0	-2.08418	-3.1951	6.52803
C	0	-4.98714	-1.17092	7.34176
C	0	-3.08274	-4.79108	1.35336
H	0	-0.4131	-1.75335	8.18566
H	0	-0.87166	-0.12347	7.69171
H	0	-2.04637	-1.17385	8.51336
H	0	-1.25428	-3.7859	6.93168
H	0	-2.94322	-3.34041	7.18973
H	0	-2.33957	-3.60011	5.5445
H	0	-5.75916	-0.76554	8.00525
H	0	-5.4872	-1.7551	6.56142
H	0	-4.36862	-1.85118	7.9326
H	0	-5.83065	1.37634	6.75198
H	0	-4.54071	1.83362	5.62502
H	0	-5.64044	0.50866	5.21821
H	0	-7.59616	-3.99808	1.3023
H	0	-6.0124	-4.68721	0.94317
H	0	-6.34656	-4.02702	2.5544
H	0	-8.00353	-1.58792	1.40276
H	0	-6.87646	-1.46474	2.76611
H	0	-6.68266	-0.40647	1.36157
H	0	-2.3328	-5.41796	0.85855
H	0	-2.7422	-4.60879	2.37626
H	0	-4.01283	-5.36505	1.39732
H	0	-2.91339	-4.30192	-1.38658
H	0	-4.62117	-4.19419	-0.95659
H	0	-3.71975	-2.73267	-1.41532
H	0	-0.81427	-1.67227	5.73739
H	0	-2.2386	1.68172	6.85627
H	0	-0.87425	3.66001	6.42784
H	0	0.27473	3.88646	4.20918
H	0	0.00652	2.14587	2.5235
H	0	-1.9552	2.21727	1.31392
H	0	-3.44782	3.11794	-0.37972
H	0	-5.12301	1.61853	-1.49086
H	0	-5.36126	-0.68444	-0.69972
H	0	-2.25715	-2.98026	0.59301
H	0	-3.64174	0.48249	7.55108
H	0	-6.17597	-2.43728	-0.06253
Cl	0	0.04808	0.18233	1.12442

Etot : = -2699.67951821 ua Erep : 4407.0462099386 Hartrees
Etot (ZPE) : -2699.127062 ua G (ZPE) : -2699.193786 ua

• **II'c**

P	0	-3.71725	-2.04305	1.06231
Au	0	-2.77742	-2.28288	3.23162
Cl	0	-3.25058	-4.74452	3.61963
Cl	0	-4.67558	0.01734	4.00231
B	0	-2.92394	-0.03185	3.26251
C	0	-2.99339	0.51759	1.74867
C	0	-3.60877	-0.25146	0.7353
C	0	-3.99166	0.32225	-0.48252
C	0	-3.67947	1.65006	-0.76171
C	0	-2.95927	2.38921	0.17297
C	0	-2.63108	1.83074	1.40678
C	0	-2.49216	-2.79596	-0.1514
C	0	-2.89156	-2.67338	-1.62419
P	0	-1.14616	-1.95088	4.89584
C	0	-1.44012	-2.7054	6.57104
C	0	-2.86921	-2.36135	7.00759
C	0	-1.94339	0.61983	4.36122
C	0	-2.0056	1.99884	4.64045
C	0	-1.24066	2.58364	5.6436
C	0	-0.3992	1.79943	6.43218
C	0	-0.34635	0.42884	6.21222
C	0	-1.10222	-0.15251	5.18246
C	0	0.53524	-2.42259	4.22163
C	0	1.69175	-2.19848	5.19933
C	0	0.56789	-3.83058	3.61758
C	0	-1.19434	-4.21521	6.62118
C	0	-5.43823	-2.60406	0.62883
C	0	-6.45994	-1.92764	1.5467
C	0	-5.58119	-4.12851	0.66573
C	0	-2.09414	-4.23704	0.18631
H	0	2.6362	-2.45617	4.7072
H	0	1.76455	-1.15718	5.52147
H	0	1.60463	-2.83398	6.08656
H	0	1.48862	-3.94921	3.03545
H	0	0.56061	-4.60683	4.38644
H	0	-0.28405	-4.01822	2.9604
H	0	-1.48037	-4.58741	7.6114
H	0	-1.79856	-4.73634	5.87255
H	0	-0.14283	-4.47223	6.4683
H	0	-3.02544	-2.70039	8.0375
H	0	-3.07093	-1.2872	6.96964
H	0	-3.59758	-2.8701	6.36856
H	0	-6.63186	-4.39331	0.50296
H	0	-4.99515	-4.6197	-0.11478
H	0	-5.26922	-4.53495	1.63287
H	0	-7.47014	-2.19772	1.21957
H	0	-6.33709	-2.26089	2.58084
H	0	-6.37466	-0.83844	1.5354
H	0	-1.19594	-4.49914	-0.38435
H	0	-1.89204	-4.38337	1.24918
H	0	-2.87615	-4.94914	-0.08875
H	0	-2.10102	-3.10862	-2.24578
H	0	-3.8128	-3.22326	-1.8436
H	0	-3.01902	-1.63606	-1.93928
H	0	0.63509	-1.69983	3.39968
H	0	0.27152	-0.18668	6.85964
H	0	0.18947	2.24813	7.22721
H	0	-1.31903	3.6517	5.82902
H	0	-2.70694	2.62114	4.09311
H	0	-2.09253	2.44001	2.1245
H	0	-2.669	3.41265	-0.04993
H	0	-3.97364	2.09206	-1.70937
H	0	-4.52794	-0.26323	-1.22401
H	0	-1.61815	-2.15292	0.02292
H	0	-0.73288	-2.20031	7.24348
H	0	-5.60207	-2.24959	-0.39924

Etot : = -2699.69373331 ua Erep : 4411.1104633013 Hartrees.
Etot (ZPE) : -2699.141604 ua G (ZPE) : -2699.209710 ua

• **IId**

P	1.43568	0.20941	3.76542
Al	-1.94214	-0.00285	1.9178
C	-2.84132	1.85632	1.87572
P	-2.43695	2.76113	4.56282
C	-3.0269	-1.25665	0.7434
Cl	-2.1606	-0.96127	3.94881
C	0.02558	-0.05113	1.28655
Au	-0.42851	1.51183	4.4286
C	1.06276	-1.64326	5.92411
C	0.08051	-0.22724	-0.11306
C	1.29389	0.00017	1.91626
C	2.49114	-0.13052	1.19816
C	2.48416	-0.28816	-0.1839
C	1.26281	-0.32997	-0.84366
C	3.10848	1.03296	4.12271
C	3.15937	2.39832	3.43828
C	-3.08215	2.88785	2.81653
C	-3.82305	4.03416	2.49614
C	-4.33438	4.22239	1.21644
C	-4.10742	3.24348	0.25762
C	-3.39221	2.09706	0.59851
C	-3.83914	1.91537	5.53965
C	-5.05045	2.82586	5.71665
C	1.43682	-1.57128	4.44603
C	2.72647	-2.31745	4.11598
C	-2.18886	4.53048	5.20732
C	-1.1787	5.26024	4.32238
C	3.34513	1.15734	5.62708
C	-1.73623	4.52158	6.66713
C	-3.3558	1.29374	6.84687
H	2.61984	-3.37117	4.39672
H	2.95428	-2.28364	3.04655
H	3.58463	-1.91877	4.66849
H	0.91532	-2.69158	6.20685
H	1.84164	-1.23467	6.57481
H	0.12825	-1.11102	6.12102
H	4.28772	1.68681	5.80562
H	2.54351	1.72839	6.10819
H	3.41437	0.18472	6.12002
H	4.13307	2.86716	3.61983
H	3.01166	2.32523	2.3581
H	2.38398	3.05949	3.84035
H	-1.52102	5.54698	6.98816
H	-2.49749	4.11945	7.33994
H	-0.82161	3.9319	6.79355
H	-1.06218	6.29264	4.67086
H	-0.19894	4.77293	4.37344
H	-1.48742	5.28632	3.27453
H	-4.16196	0.6901	7.27856
H	-2.5009	0.63444	6.67527
H	-3.07399	2.04542	7.59011
H	-5.87708	2.25321	6.15167
H	-4.8407	3.66111	6.39431
H	-5.39786	3.23068	4.76153
H	0.61222	-2.00601	3.86937
H	3.44804	-0.10429	1.71227
H	3.42014	-0.38013	-0.72802
H	1.22427	-0.45479	-1.92289
H	-0.84856	-0.31104	-0.66714
H	-3.27851	1.34121	-0.1717
H	-4.49459	3.36129	-0.75134
H	-4.90112	5.11898	0.98079
H	-4.00249	4.80002	3.24556
H	-4.0991	1.09867	4.85619
H	3.88143	0.38135	3.6989
H	-3.16133	5.03306	5.14358
C	-3.23077	-1.13961	-0.64849
C	-3.99566	-2.04309	-1.38618
C	-4.60185	-3.124	-0.75111
C	-4.42853	-3.28019	0.6212
C	-3.65933	-2.36556	1.34256
H	-2.78442	-0.31618	-1.20637
H	-4.11714	-1.90072	-2.45783
H	-5.19993	-3.83291	-1.31845
H	-4.89363	-4.11789	1.1365
H	-3.55021	-2.52494	2.41215

Etot -2688.65141375 ua Erep : 5170.5241381770 Hartrees
Etot (ZPE) : -2688.015339 ua G (ZPE) : -2688.090578ua

• **II'd**

C	0	-1.86621	-1.82619	3.47914
P	0	-3.47243	2.25303	1.25481
P	0	-3.49216	-2.46423	1.30802
C	0	-1.8465	1.65057	3.43655
C	0	0.16655	-0.12453	1.50505
Cl	0	-5.51365	-0.12084	-0.77465
Au	0	-3.63025	-0.10869	0.96418
Al	0	-1.56059	-0.10106	2.50597
C	0	-1.22664	-2.1312	4.69367
C	0	-1.40884	-3.34945	5.34492
C	0	-2.2345	-4.31918	4.77989
C	0	-2.87075	-4.06204	3.56901
C	0	-2.69367	-2.82707	2.92577
C	0	-2.40723	-3.28456	0.02622
C	0	-2.69928	-2.79457	-1.39519
C	0	-5.1525	-3.31562	1.39443
C	0	-5.8339	-3.54513	0.04398
C	0	-6.0586	-2.53167	2.35028
C	0	-2.66622	2.64561	2.86164
C	0	-2.82962	3.89734	3.47558
C	0	-2.18646	4.17786	4.67753
C	0	-1.36777	3.2144	5.26306
C	0	-1.19981	1.97887	4.64122
C	0	-5.12586	3.11877	1.32839
C	0	-5.8135	3.3189	-0.02357
C	0	-2.38735	3.03955	-0.04829
C	0	-2.68324	2.51517	-1.45652
C	0	-2.34626	4.5676	0.01969
C	0	-2.36925	-4.81051	0.13185
C	0	-6.03213	2.36707	2.30963
H	0	-1.6279	-5.20473	-0.57193
H	0	-2.08373	-5.14562	1.1329
H	0	-3.3325	-5.26301	-0.12333
H	0	-1.92442	-3.17288	-2.07121
H	0	-3.66684	-3.13981	-1.76587
H	0	-2.7013	-1.70294	-1.4546
H	0	-6.807	-4.01798	0.22054
H	0	-6.00121	-2.60061	-0.48011
H	0	-5.26092	-4.21367	-0.60352
H	0	-6.98771	-3.08885	2.51332
H	0	-5.59006	-2.36657	3.32541
H	0	-6.31892	-1.56209	1.91451
H	0	-6.78051	3.80652	0.14616
H	0	-5.23781	3.96383	-0.69227
H	0	-5.99357	2.36271	-0.52156
H	0	-6.95799	2.93317	2.45984
H	0	-6.2989	1.38648	1.90331
H	0	-5.56069	2.22784	3.28737
H	0	-1.9109	2.87776	-2.14395
H	0	-2.68407	1.42247	-1.48902
H	0	-3.65245	2.85008	-1.83237
H	0	-1.60694	4.94307	-0.69638
H	0	-3.30971	5.01561	-0.24259
H	0	-2.05608	4.92665	1.01106
H	0	-1.41851	-2.89925	0.30844
H	0	-3.50608	-4.83214	3.14103
H	0	-2.38389	-5.27329	5.27783
H	0	-0.9098	-3.54416	6.29093
H	0	-0.56907	-1.39525	5.15332
H	0	-0.54761	1.24802	5.11641
H	0	-0.86323	3.42734	6.20219
H	0	-2.32515	5.14513	5.15265
H	0	-3.46001	4.66252	3.03169
H	0	-1.39876	2.65961	0.24151
H	0	-4.93589	-4.29432	1.84181
H	0	-4.8989	4.10713	1.74868
C	0	0.82202	-1.32807	1.17937
C	0	2.04374	-1.35236	0.50594
C	0	2.65858	-0.15679	0.13789
C	0	2.05137	1.05505	0.46293
C	0	0.82972	1.06234	1.13676
H	0	0.38142	-2.27724	1.48215
H	0	2.52011	-2.30233	0.2747
H	0	3.61026	-0.16924	-0.38723
H	0	2.53358	1.99314	0.19784
H	0	0.39535	2.02448	1.40568

Etot : -2688.64492973 ua Erep : 5259.9320157602 Hartrees
Etot (ZPE) : -2688.007744 ua G (ZPE) : -2688.083514 ua

Results of the NBO analyses:

• II’a

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
137. LP (5)Au 6	/140. LP*(2)Al 8	19.05	0.43	0.084

• II’b

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
140. LP (5)Au 1	/148. LP*(1) B 11	32.84	0.32	0.102

• II’c

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u	F(i,j) a.u.
127. LP (5)Au 2	/135. LP*(1) B 5	75.19	0.27	0.144

• II’d

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
150. LP (5)Au 7	/153. LP*(2)Al 8	9.85	0.49	0.065