Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Halogen-involving weak interactions manifested in the crystal structures of silver(I) or gold(I) 4-halogenated-3,5-diphenylpyrazolato trimers

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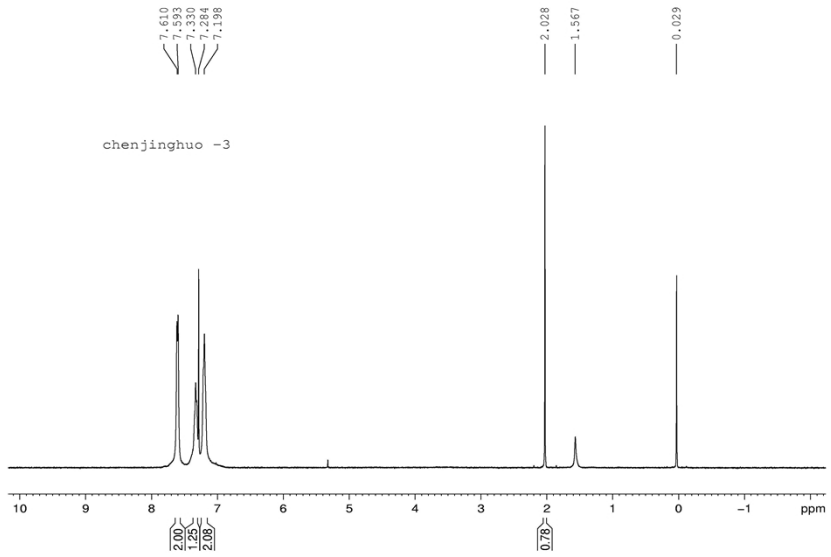

Figure S1a. ^{1}H NMR spectrum of $[Ag(ClPh_2pz)]_3 \cdot CH_3CN$ (**1**) in $CDCl_3$.

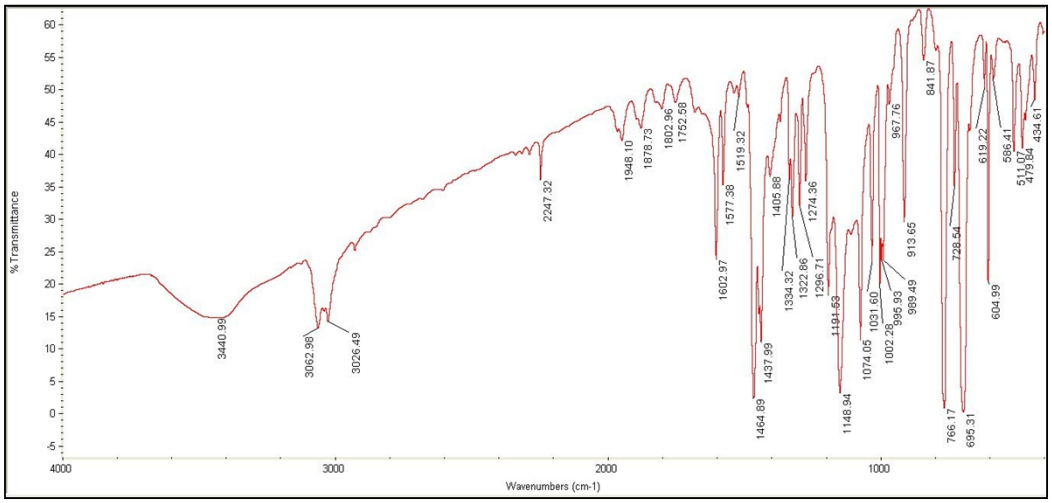

Figure S1b. IR spectrum of $[Ag(ClPh_2pz)]_3$-CH_3CN (**1**) in KBr pellet.

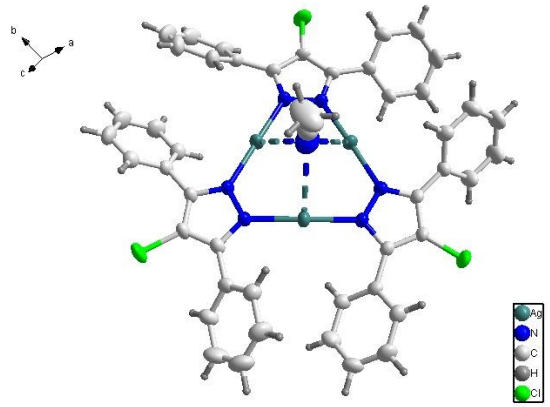

Figure S1c. The asymmetric unit of $[Ag(ClPh_2pz)]_3 \cdot CH_3CN$ (**1**).

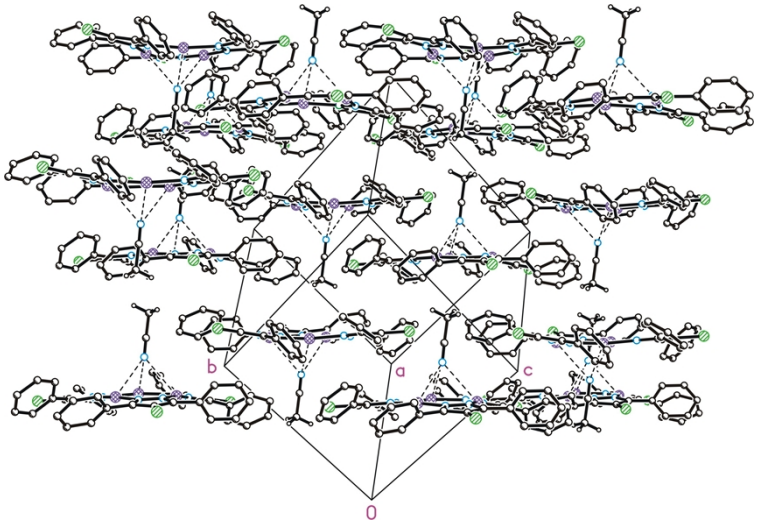

Figure S1d. Packing diagram of $[Ag(ClPh_2pz)]_3 \cdot CH_3CN$ (**1**).

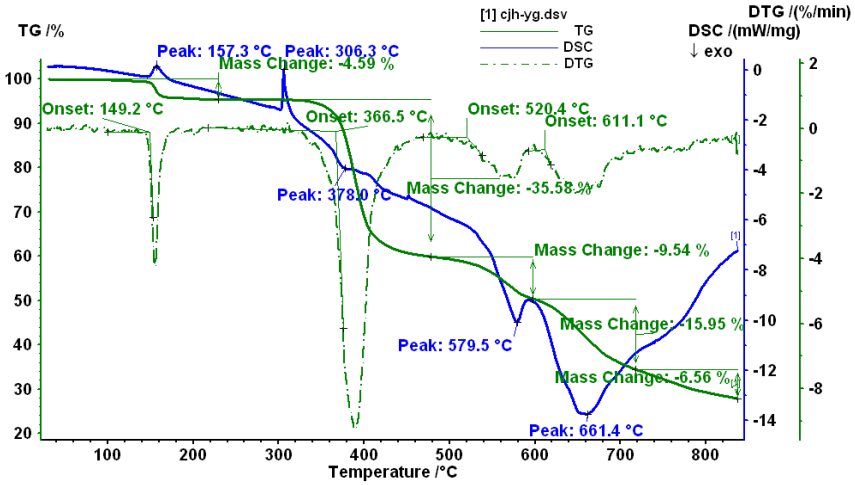

Figure S1f. TG-DSC curves of $[Ag(ClPh_2pz)]_3 \cdot CH_3CN$ (**1**).

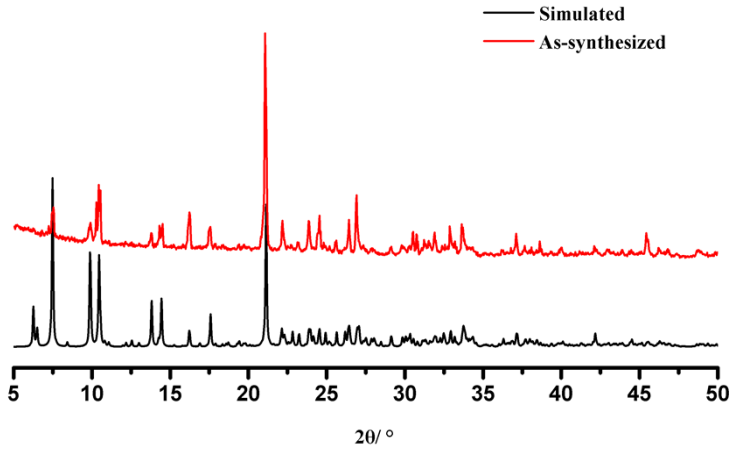

Figure S1g. The PXRD patterns of $[Ag(ClPh_2pz)]_3 \cdot CH_3CN$ (**1**) obtained from the as-synthesized sample (red line) and the simulation based on the crystal data (black line).

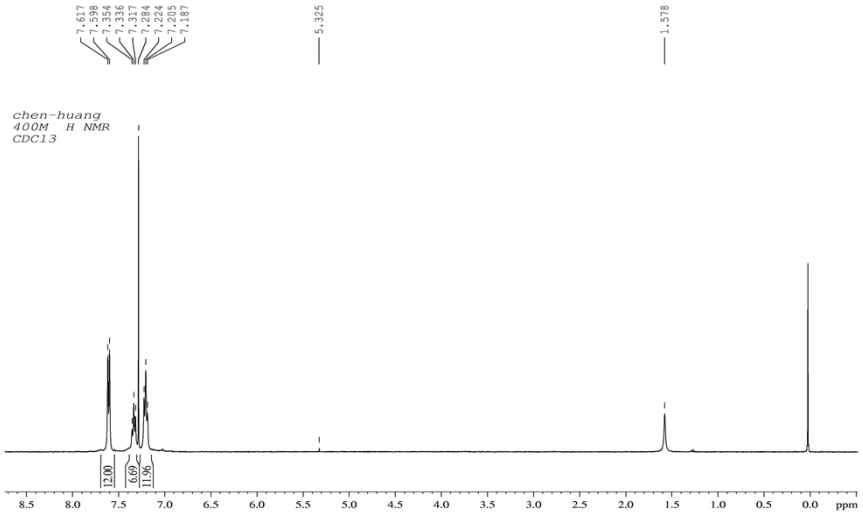

Figure S2a. ^{1}H NMR spectrum of $[Ag(ClPh_2pz)]_3{\cdot}2CH_2Cl_2$ (**2**) in $CDCl_3$.

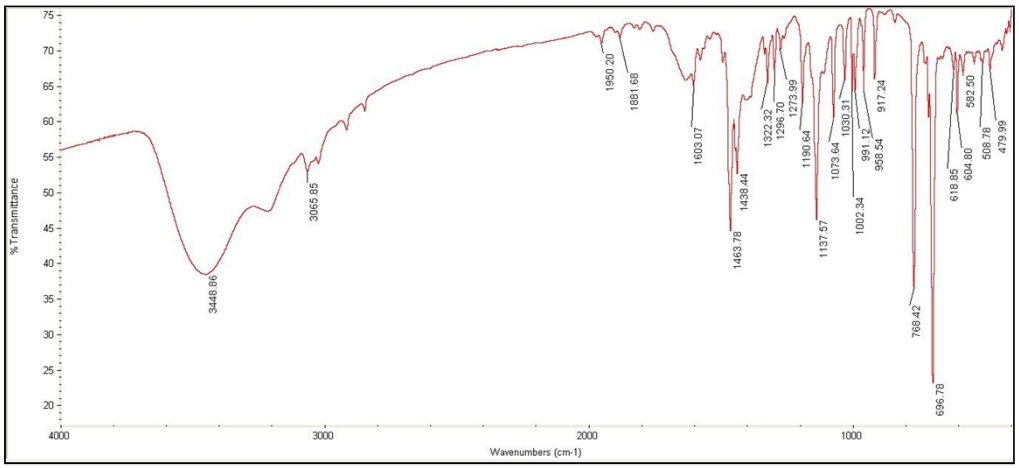

Figure S2b. IR spectrum of $[Ag(ClPh_2pz)]_3{\cdot}2CH_2Cl_2$ (**2**) in KBr pellet.

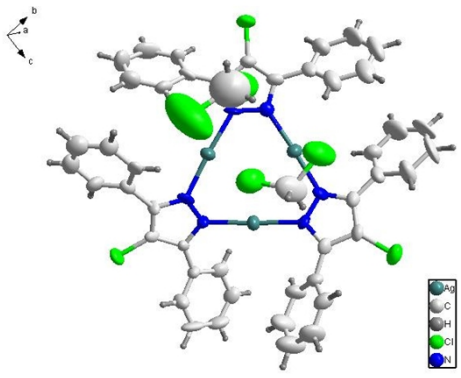

Figure S2c. The asymmetric unit of $[Ag(ClPh_2pz)]_3 \cdot 2CH_2Cl_2$ (**2**).

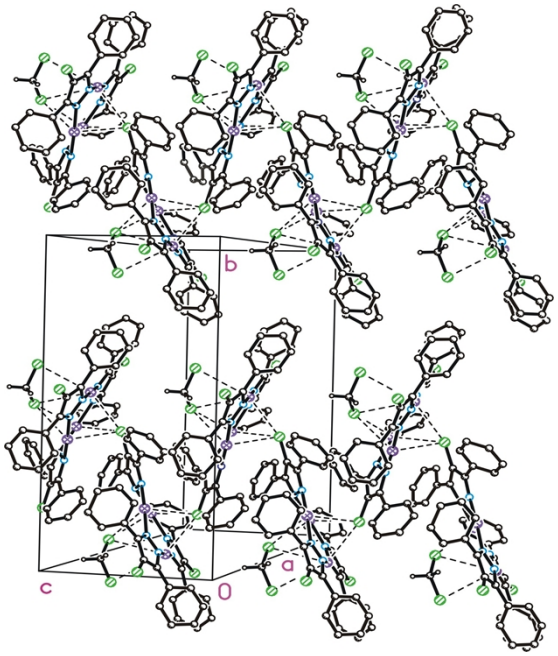

Figure S2d. Packing diagram of $[Ag(ClPh_2pz)]_3 \cdot 2CH_2Cl_2$ (**2**).

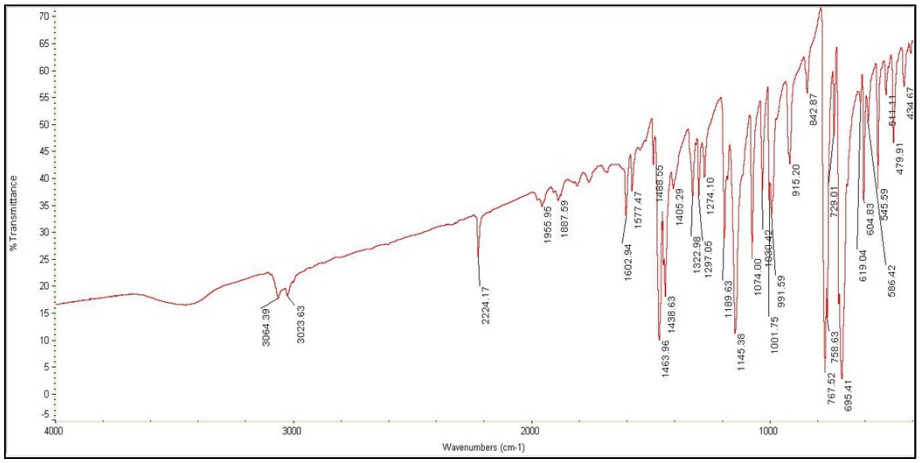

Figure S3a. IR spectrum of $[Ag(ClPh_2pz)]_3 \cdot PhCN$ (**3**) in KBr pellet.

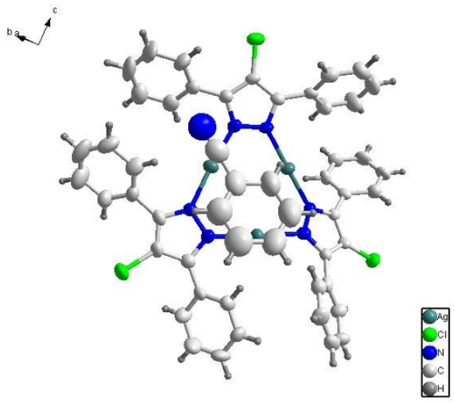

Figure S3b. The asymmetric unit of $[Ag(ClPh_2pz)]_3 \cdot PhCN$ (**3**).

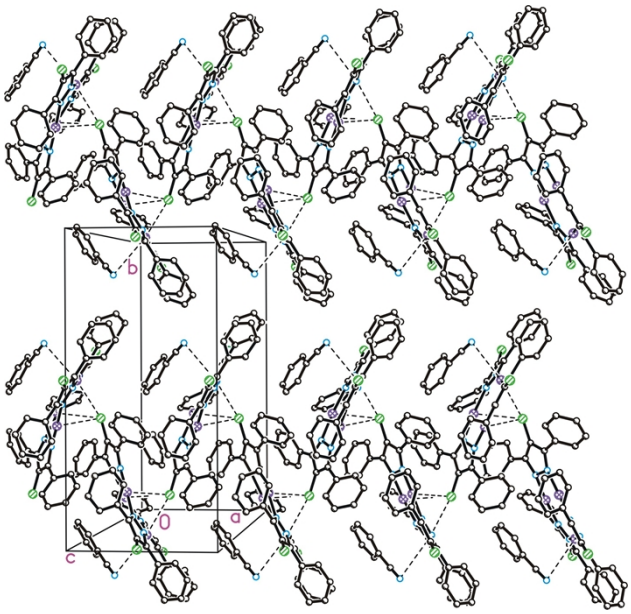

Figure S3c. Packing diagram of $[Ag(ClPh_2pz)]_3 \cdot PhCN$ (**3**).

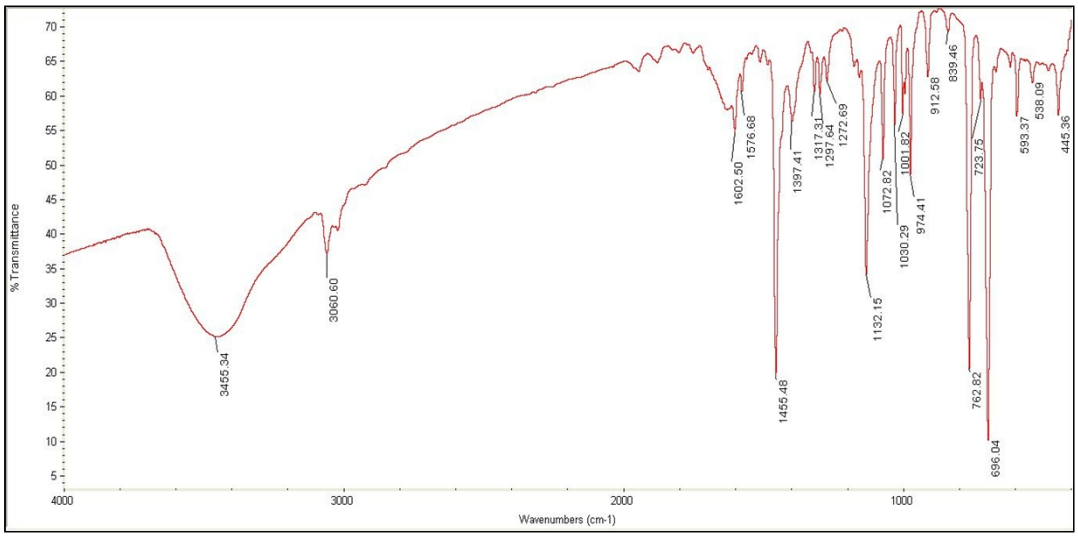

Figure S4a. IR spectrum of $[Ag(IPh_2pz)]_3$ (**4**) in KBr pellet.

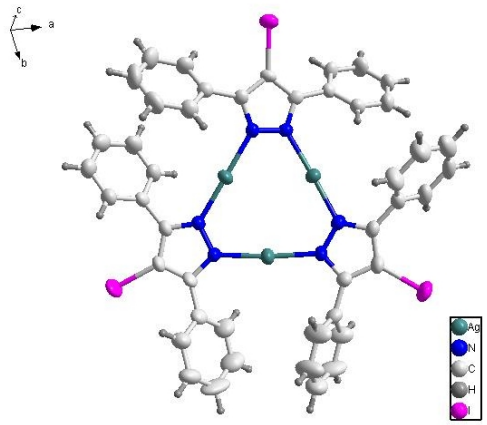

Figure S4b. The asymmetric unit of $[Ag(IPh_2pz)]_3$ (**4**).

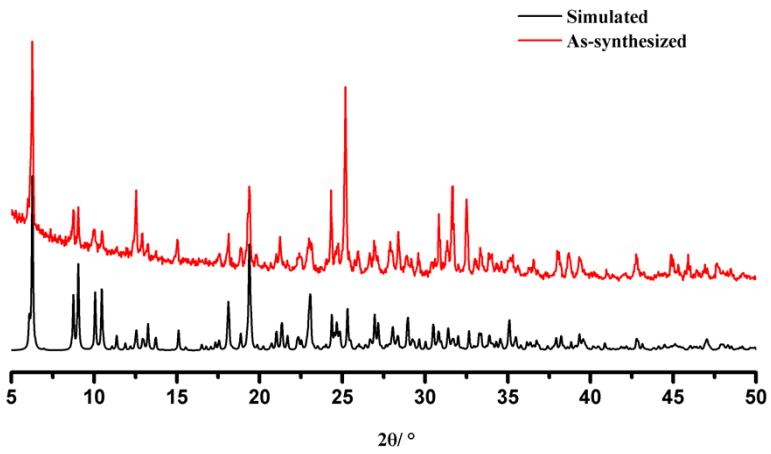

Figure S4c. The PXRD patterns of $[Ag(IPh_2pz)]_3$ (**4**) obtained from the as-synthesized sample

(red line) and the simulation based on the crystal data (black line).

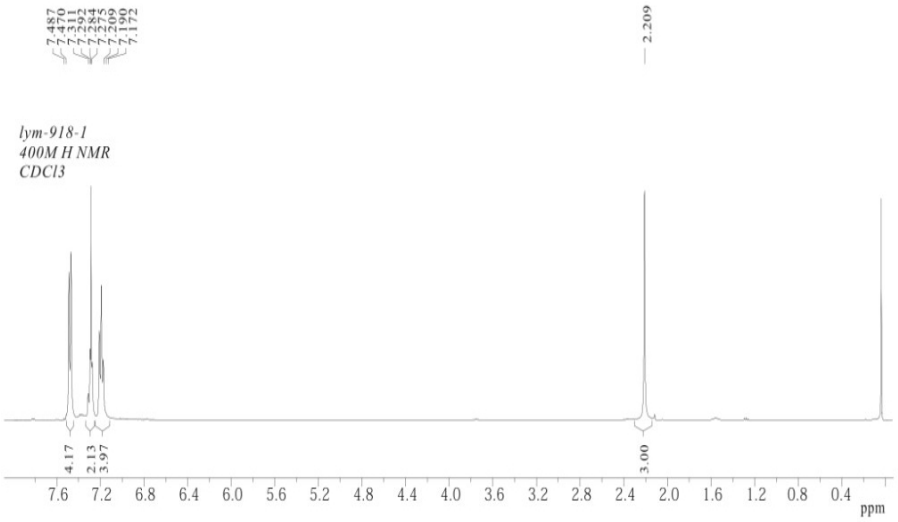

Figure S5a. ^{1}H NMR spectrum of $[Ag(MePh_2pz)]_3 \cdot 1/2CHCl_3$ (**5**) in $CDCl_3$.

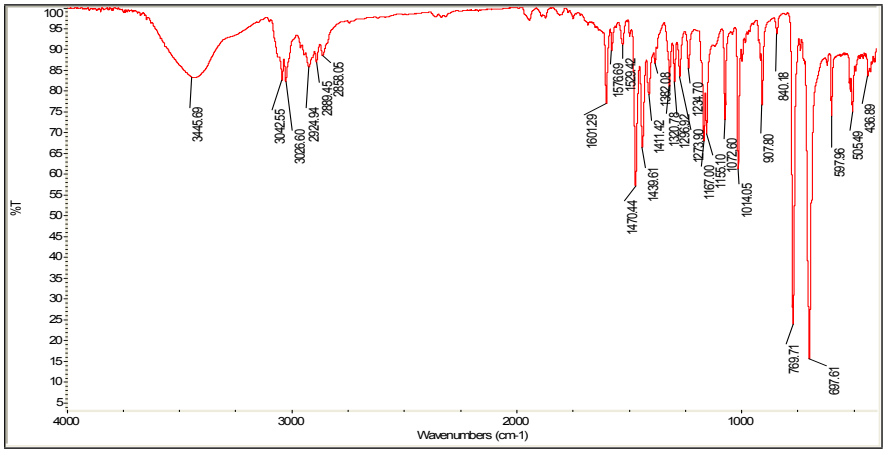

Figure S5b. IR spectra of $[Ag(MePh_2pz)]_3 \cdot 1/2CHCl_3$ (**5**) in KBr pellet.

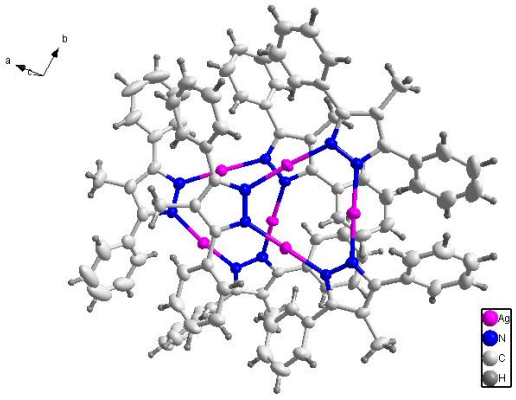

Figure S5c. The asymmetric unit of $[Ag(MePh_2pz)]_3 \cdot 1/2CHCl_3$ (**5**).

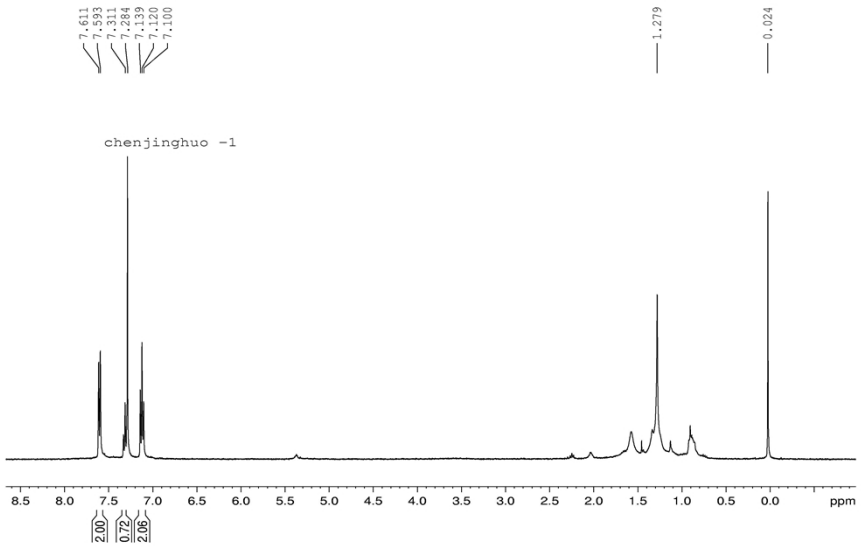

Figure S6a. ^1H NMR spectrum of $[Au(ClPh_2pz)]_3 \cdot CH_2Cl_2$ (**6**) in $CDCl_3$.

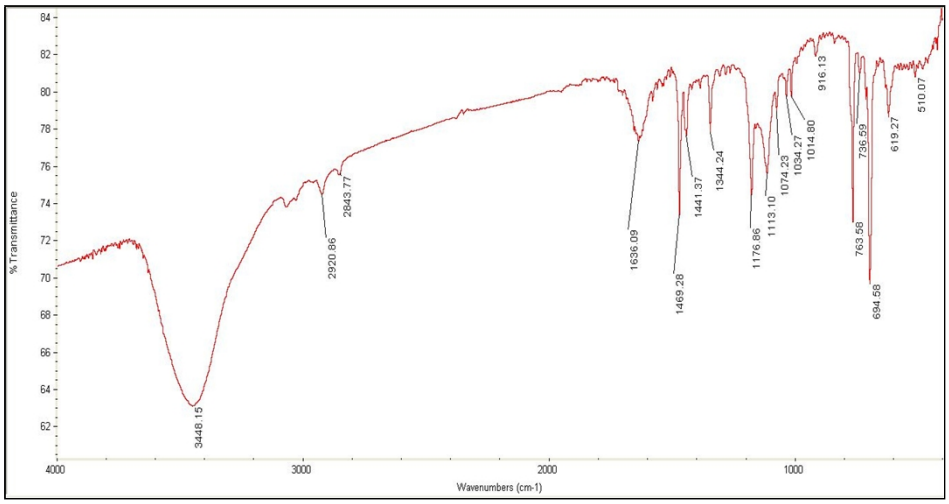

Figure S6b. IR spectrum of $[Au(ClPh_2pz)]_3 \cdot CH_2Cl_2$ (**6**) in KBr pellet.

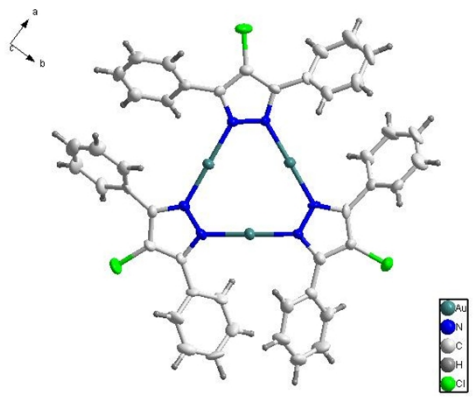

Figure S6c. The asymmetric unit of $[Au(ClPh_2pz)]_3 \cdot CH_2Cl_2$ (**6**).

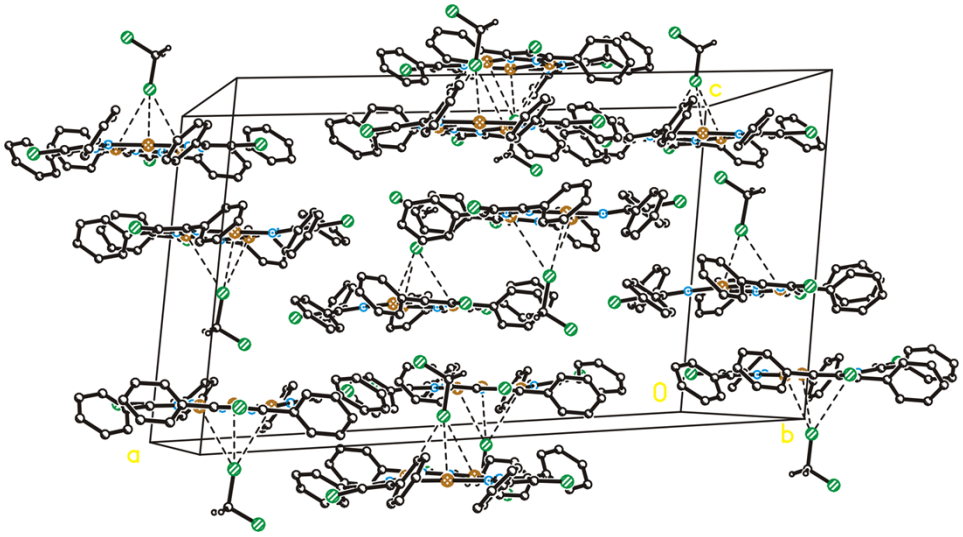

Figure S6d. Packing diagram of $[Au(ClPh_2pz)]_3 \cdot CH_2Cl_2$ (**6**).

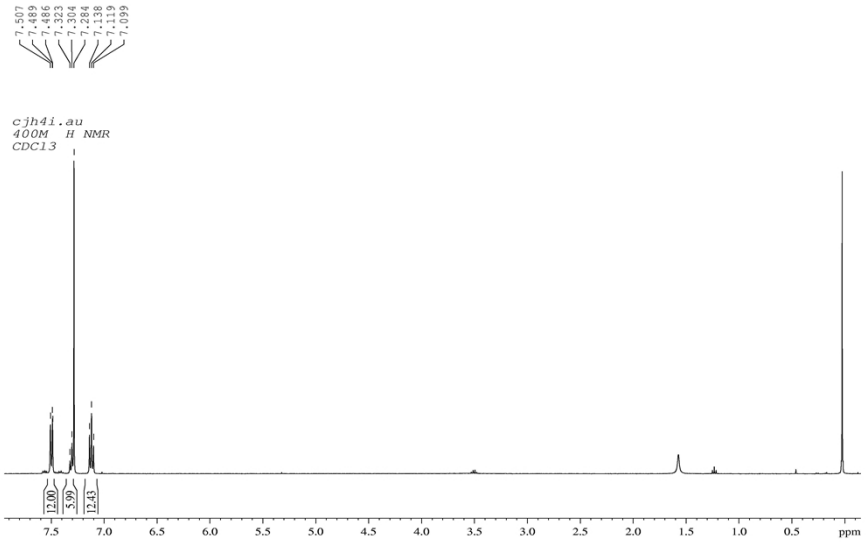

Figure S7a. ^1H NMR spectrum of $[Au(IPh_2pz)]_3$ (**7**) in $CDCl_3$.

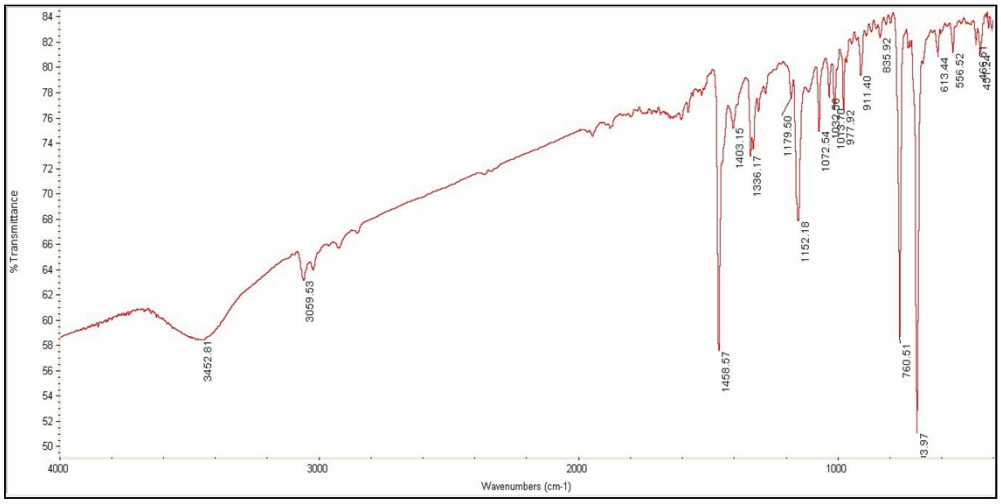

Figure S7b. IR spectrum of $[Au(IPh_2pz)]_3$ (**7**) in KBr pellet.

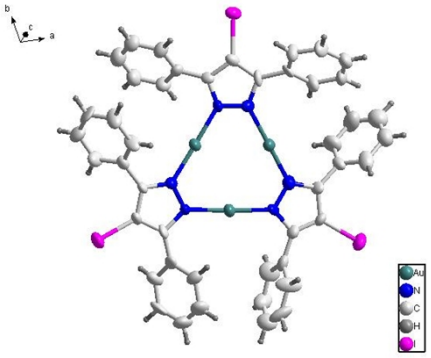

Figure S7c. The asymmetric unit of $[Au(IPh_2pz)]_3$ (**7**).

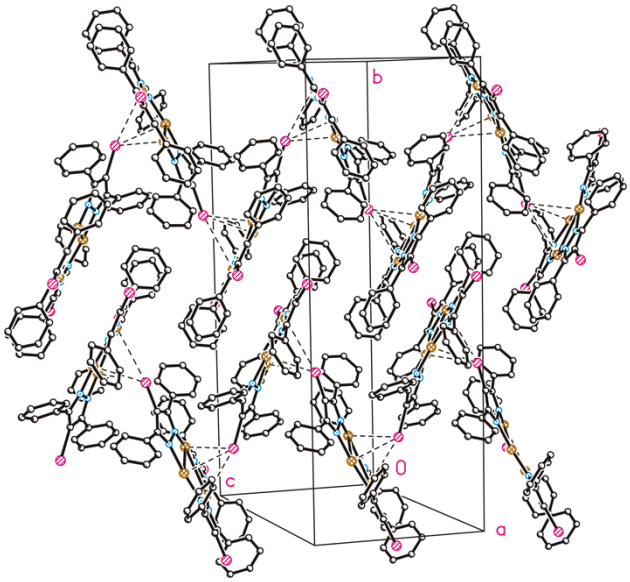

Figure S7d Packing diagram of $[Au(IPh_2pz)]_3$ (**7**).

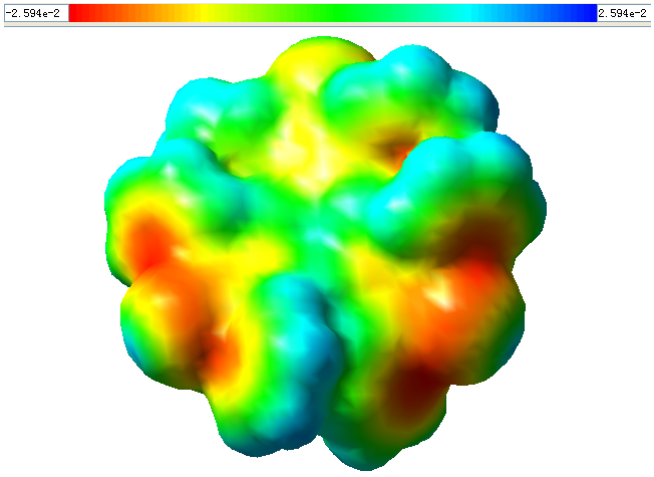

Figure S8a. Top view of MEP surface of $[Ag(IPh_2pz)]_3$. MEP color scale is such that the electron density increases from blue → green → yellow → orange → red.

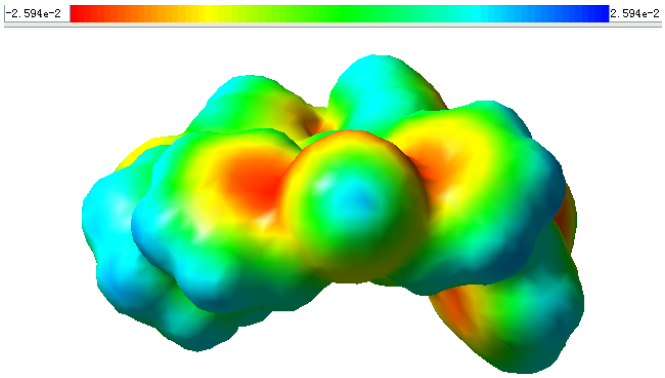

Figure S8b. Side view of MEP surface of $[Ag(IPh_2pz)]_3$.

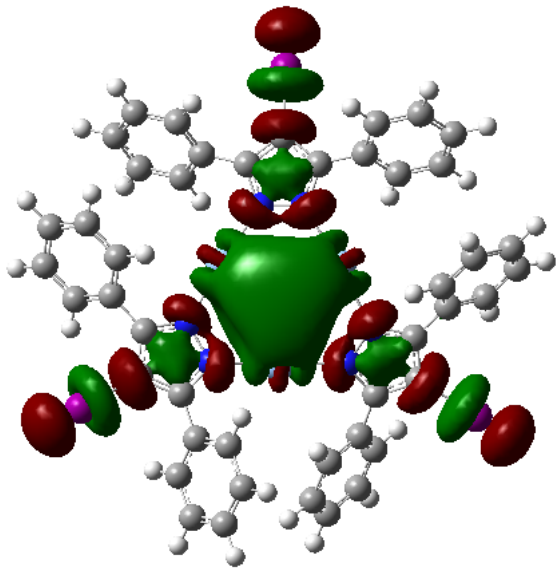

Figure S8c. Top view of LUMO of $[Ag(IPh_2pz)]_3$.

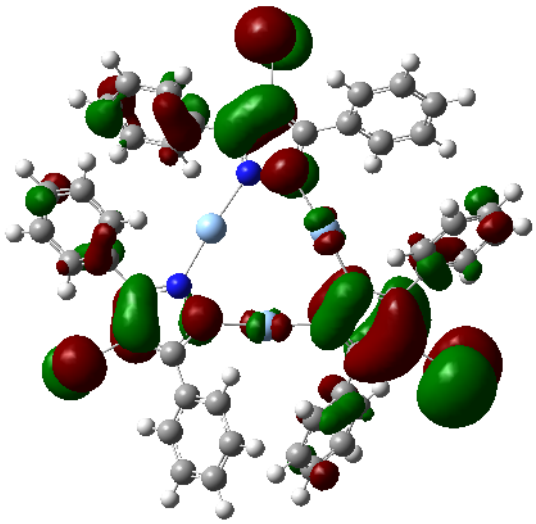

Figure S8d. Top view of HOMO of $[Ag(IPh_2pz)]_3$.

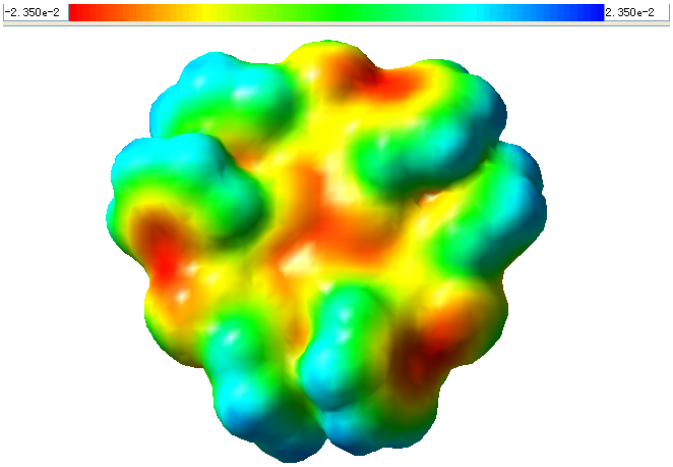

Figure S9a Top view of MEP surface of $[Au(ClPh_2pz)]_3$.

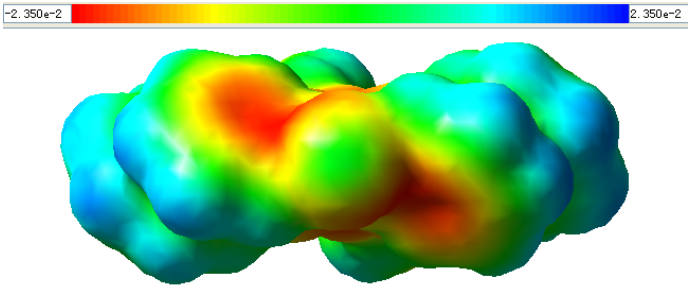

Figure S9b. Side view of MEP surface of $[Au(ClPh_2pz)]_3$.

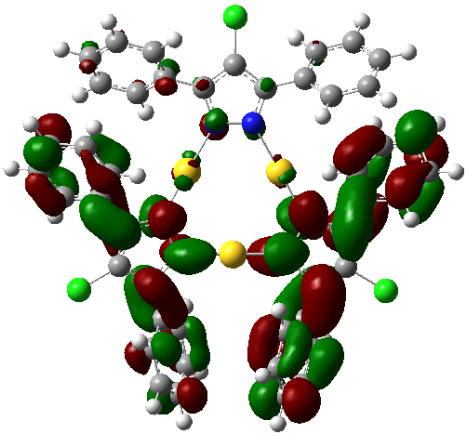

Figure S9c. Top view of LUMO of $[Au(ClPh_2pz)]_3$.

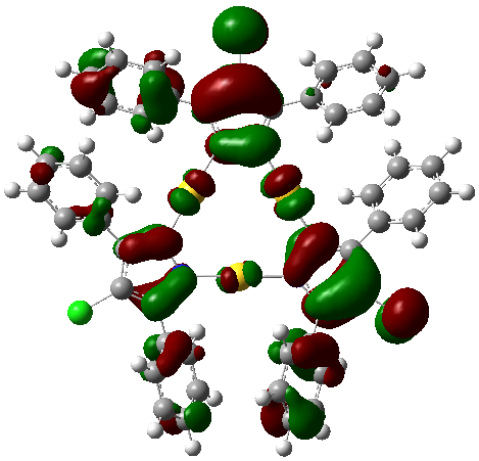

Figure S9d. Side view of HOMO of $[Au(ClPh_2pz)]_3$.

Table S1. Selected bond distances (Å) and bond angles(º).

1			
Ag(1)-N(1)	2.078(2)	Ag(2)-N(3)	2.0914(22)
Ag(1)-N(6)	2.0770(22)	Ag(3)-N(4)	2.0922(25)
Ag(2)-N(2)	2.0849(22)	Ag(3)-N(5)	2.0957(24)
Ag(1)···Ag(2)	3.4195(11)	Ag(1)···N(7)	3.0030(44)
Ag(2)···Ag(3)	3.4852(12)	Ag(3)···N(7)	2.9760(43)
Ag(1)···Ag(3)	3.4711(13)	Ag(2)···N(7)	2.9391(52)
N(1)-Ag(1)-N(6)	175.77(10)	N(2)-Ag(2)-N(3)	173.65(10)
N(4)-Ag(3)-N(5)	173.84(10)		
2			
Ag(1)-N(1)	2.083(11)	Ag(2)-N(3)	2.084(12)
Ag(1)-N(6)	2.091(10)	Ag(3)-N(4)	2.094(11)
Ag(2)-N(2)	2.087(13)	Ag(3)-N(5)	2.113(11)
Ag(1)···Ag(2)	3.5493(16)	Ag(1)···Cl(5)	3.4000(58)
Ag(2)···Ag(3)	3.4813(15)	Ag(2)···Cl(5)	3.4782(68)
Ag(1)···Ag(3)	3.4694(17)	Ag(3)···Cl(7)	3.4342(65)
N(1)-Ag(1)-N(6)	175.9(5)	N(4)-Ag(3)-N(5)	175.5(4)
N(3)-Ag(2)-N(2)	177.8(5)		
3			
Ag(1)-N(1)	2.101(5)	Ag(2)-N(3)	2.088(5)
Ag(1)-N(6)	2.107(5)	Ag(3)-N(4)	2.087(5)
Ag(2)-N(2)	2.090(5)	Ag(3)-N(5)	2.082(5)
Ag(1)···Ag(2)	3.4082(9)	Ag(1)···Cl(1a)	3.4405(18)
Ag(2)···Ag(3)	3.4707(9)	Ag(2)···Cl(1a)	3.4399(18)
Ag(1)···Ag(3)	3.6077(8)	Ag(3)···Cl(1a)	3.1850(17)
N(1)-Ag(1)-N(6)	174.80(19)	N(3)-Ag(2)-N(2)	178.13(19)
N(5)-Ag(3)-N(4)	175.43(19)		

4			
Ag(1)-N(1)	2.081(6)	Ag(2)-N(3)	2.079(5)
Ag(1)-N(6)	2.093(5)	Ag(3)-N(4)	2.088(5)
Ag(2)-N(2)	2.074(5)	Ag(3)-N(5)	2.090(5)
Ag(1)···Ag(2)	3.5957(11)	Ag(1)···I(2a)	3.389(1)
Ag(2)···Ag(3)	3.4763(10)	Ag(2)···I(2a)	3.8178(10)
Ag(1)···Ag(3)	3.4144(12)	Ag(3)···I(2a)	3.6357(13)
N(1)-Ag(1)-N(6)	173.6(2)	N(4)-Ag(3)-N(5)	174.8(2)
N(2)-Ag(2)-N(3)	174.7(2)		
5			
Ag(1)-N(1)	2.087(3)	Ag(4)-N(7)	2.082(3)
Ag(1)-N(6)	2.089(3)	Ag(4)-N(12)	2.092(3)
Ag(2)-N(2)	2.068(3)	Ag(5)-N(8)	2.076(3)
Ag(2)-N(3)	2.059(3)	Ag(5)-N(9)	2.084(3)
Ag(3)-N(4)	2.071(3)	Ag(6)-N(10)	2.073(3)
Ag(3)-N(5)	2.090(3)	Ag(6)-N(11)	2.067(3)
Ag(1)···Ag(2)	3.3683(4)	Ag(4)···Ag(5)	3.4501(1)
Ag(2)···Ag(3)	3.4075(1)	Ag(5)···Ag(6)	3.3417(4)
Ag(1)···Ag(3)	3.5718(1)	Ag(4)···Ag(6)	3.5728(1)
N(1)-Ag(1)-N(6)	175.77(10)	N(7)-Ag(4)-N(12)	173.934(3)
N(2)-Ag(2)-N(3)	173.65(10)	N(8)-Ag(5)-N(9)	175.948(3)
N(4)-Ag(3)-N(5)	173.84(10)	N(10)-Ag(6)-N(11)	174.601(3)
6			
Au(1)-N(1)	2.006(7)	Au(2)-N(3)	2.009(6)
Au(1)-N(6)	2.007(7)	Au(3)-N(4)	1.997(7)
Au(2)-N(2)	1.999(6)	Au(3)-N(5)	2.006(7)
Au(1)···Au(2)	3.3396(5)	Au(1)···Cl(4)	3.5898(35)
Au(2)···Au(3)	3.3642(5)	Au(3)···Cl(4)	3.5948(31)

Au(1)···Au(3)	3.3862(4)	Au(2)···Cl(4)	3.5692(34)
N(1)-Au(1)-N(6)	178.2(3)	N(4)-Au(3)-N(5)	179.2(3)
N(2)-Au(2)-N(3)	179.2(3)		
7			
Au(1)-N(1)	2.045(13)	Au(1)-N(6)	2.003(15)
Au(2)-N(2)	2.034(13)	Au(2)-N(3)	2.025(14)
Au(3)-N(4)	2.015(13)	Au(3)-N(5)	2.015(15)
Au(1)···Au(2)	3.3471(13)	Au(1)···I(1a)	3.4975(16)
Au(2)···Au(3)	3.3658(11)	Au(2)···I(1a)	3.8369(20)
Au(1)···Au(3)	3.4547(12)	Au(3)···I(1a)	4.0349(16)
N(1)-Au(1)-N(6)	175.4(6)	N(4)-Au(3)-N(5)	177.7(5)
N(2)-Au(2)-N(3)	178.0(6)		

Symmetry codes:

3 a) 0.5+*x*, 0.5-*y*, *z*

4 a) *x*, 0.5-*y*, -0.5+*z*

7 a) *x*, 0.5-*y*, -0.5+*z*

Table S2. Composition analysis on the LUMO of $[Ag(ClPh_2pz)]_3$.*

	C	C^2	
Ag 1S	0.22283	4.96532E-02	4.297%
2S	-0.11394	1.29823E-02	1.123%
3S	0.18237	3.32588E-02	2.878%
4PX	-0.05404	2.92032E-03	0.253%
4PY	-0.00392	1.53664E-05	0.001%
4PZ	-0.00007	4.90000E-09	0.000%
5PX	0.16114	2.59661E-02	2.247%
5PY	0.01114	1.24100E-04	0.011%
5PZ	0.00016	2.56000E-08	0.000%
6PX	0.03536	1.25033E-03	0.108%
6PY	0.00236	5.56960E-06	0.000%
6PZ	0.00033	1.08900E-07	0.000%
7D 0	-0.08096	6.55452E-03	0.567%
7D+1	-0.00261	6.81210E-06	0.001%
7D-1	0.03518	1.23763E-03	0.107%
7D+2	-0.20106	4.04251E-02	3.498%
7D-2	-0.02912	8.47974E-04	0.073%
8D 0	-0.017	2.89000E-04	0.025%
8D+1	-0.00066	4.35600E-07	0.000%
8D-1	0.00839	7.03921E-05	0.006%
8D+2	-0.04895	2.39610E-03	0.207%
8D-2	-0.00716	5.12656E-05	0.004%
sum			15.407%
Ag 1S	0.22162	4.91154E-02	4.250%
2S	-0.11334	1.28460E-02	1.112%
3S	0.18166	3.30004E-02	2.856%
4PX	0.03035	9.21123E-04	0.080%
4PY	-0.04496	2.02140E-03	0.175%
4PZ	0.00001	1.00000E-10	0.000%
5PX	-0.09112	8.30285E-03	0.718%
5PY	0.13423	1.80177E-02	1.559%
5PZ	0.0001	1.00000E-08	0.000%
6PX	-0.02002	4.00800E-04	0.035%

6PY	0.02948	8.69070E-04	0.075%
6PZ	-0.00112	1.25440E-06	0.000%
7D 0	-0.08091	6.54643E-03	0.566%
7D+1	-0.02854	8.14532E-04	0.070%
7D-1	-0.01948	3.79470E-04	0.033%
7D+2	0.07561	5.71687E-03	0.495%
7D-2	0.18871	3.56115E-02	3.081%
8D 0	-0.01714	2.93780E-04	0.025%
8D+1	-0.00682	4.65124E-05	0.004%
8D-1	-0.00465	2.16225E-05	0.002%
8D+2	0.01841	3.38928E-04	0.029%
8D-2	0.04578	2.09581E-03	0.181%
sum			15.347%
Ag 1S	0.22418	5.02567E-02	4.349%
2S	-0.11461	1.31355E-02	1.137%
3S	0.18344	3.36502E-02	2.912%
4PX	0.02374	5.63588E-04	0.049%
4PY	0.04889	2.39023E-03	0.207%
4PZ	-0.0002	4.00000E-08	0.000%
5PX	-0.07031	4.94350E-03	0.428%
5PY	-0.14539	2.11383E-02	1.829%
5PZ	0.0007	4.90000E-07	0.000%
6PX	-0.01589	2.52492E-04	0.022%
6PY	-0.03218	1.03555E-03	0.090%
6PZ	0.00089	7.92100E-07	0.082%
7D 0	-0.08109	6.57559E-03	0.569%
7D+1	0.03266	1.06668E-03	0.092%
7D-1	-0.01598	2.55360E-04	0.022%
7D+2	0.12575	1.58131E-02	1.368%
7D-2	-0.15968	2.54977E-02	2.206%
8D 0	-0.0169	2.85610E-04	0.025%
8D+1	0.00781	6.09961E-05	0.005%
8D-1	-0.00386	1.48996E-05	0.001%
8D+2	0.03076	9.46178E-04	0.082%
8D-2	-0.03901	1.52178E-03	0.132%
sum			15.606%
N 1S	0.0275	7.56250E-04	0.065%
2S	-0.06218	3.86635E-03	0.335%
2PX	0.01986	3.94420E-04	0.034%
2PY	-0.10679	1.14041E-02	0.987%
2PZ	0.03454	1.19301E-03	0.103%
3S	-0.16796	2.82106E-02	2.441%
3PX	0.00739	5.46121E-05	0.005%
3PY	-0.10539	1.11071E-02	0.961%
3PZ	0.03397	1.15396E-03	0.100%
4D 0	-0.00417	1.73889E-05	0.002%
4D+1	-0.00115	1.32250E-06	0.000%
4D-1	-0.00066	4.35600E-07	0.000%
4D+2	-0.01234	1.52276E-04	0.013%
4D-2	-0.00006	3.60000E-09	0.000%
sum			5.046%
N 1S	0.02747	7.54601E-04	0.065%
2S	-0.06211	3.85765E-03	0.334%
2PX	-0.09603	9.22176E-03	0.798%
2PY	-0.05064	2.56441E-03	0.222%
2PZ	-0.03475	1.20756E-03	0.104%
3S	-0.16812	2.82643E-02	2.446%
3PX	-0.08691	7.55335E-03	0.654%
3PY	-0.0597	3.56409E-03	0.308%
3PZ	-0.034	1.15600E-03	0.100%
4D 0	-0.00416	1.73056E-05	0.001%
4D+1	-0.0002	4.00000E-08	0.000%
4D-1	0.00132	1.74240E-06	0.000%
4D+2	0.00293	8.58490E-06	0.001%
4D-2	0.01198	1.43520E-04	0.012%
sum			5.046%
N 1S	0.02744	7.52954E-04	0.065%
2S	-0.06204	3.84896E-03	0.333%
2PX	0.0826	6.82276E-03	0.590%
2PY	0.07007	4.90980E-03	0.425%
2PZ	0.03533	1.24821E-03	0.108%
3S	-0.16813	2.82677E-02	2.446%
3PX	0.08746	7.64925E-03	0.662%
3PY	0.05802	3.36632E-03	0.291%
3PZ	0.03454	1.19301E-03	0.103%
4D 0	-0.00416	1.73056E-05	0.001%
4D+1	0.00123	1.51290E-06	0.000%
4D-1	-0.00067	4.48900E-07	0.000%
4D+2	0.00614	3.76996E-05	0.003%
4D-2	0.0107	1.14490E-04	0.010%
sum			5.039%
N 1S	0.02755	7.59003E-04	0.066%
2S	-0.06233	3.88503E-03	0.336%
2PX	0.09202	8.46768E-03	0.733%
2PY	-0.05777	3.33737E-03	0.289%

	2PZ	-0.03505	1.22850E-03	0.106%
	3S	-0.16814	2.82711E-02	2.446%
	3PX	0.09528	9.07828E-03	0.786%
	3PY	-0.0459	2.10681E-03	0.182%
	3PZ	-0.03446	1.18749E-03	0.103%
	4D 0	-0.00419	1.75561E-05	0.002%
	4D+1	-0.0011	1.21000E-06	0.000%
	4D-1	-0.00082	6.72400E-07	0.000%
	4D+2	0.00893	7.97449E-05	0.007%
	4D-2	-0.00852	7.25904E-05	0.006%
sum				5.061%
N	1S	0.02758	7.60656E-04	0.066%
	2S	-0.0624	3.89376E-03	0.337%
	2PX	-0.10249	1.05042E-02	0.909%
	2PY	0.037	1.36900E-03	0.118%
	2PZ	0.03517	1.23693E-03	0.107%
	3S	-0.16847	2.83821E-02	2.456%
	3PX	-0.09475	8.97756E-03	0.777%
	3PY	0.04701	2.20994E-03	0.191%
	3PZ	0.03452	1.19163E-03	0.103%
	4D 0	-0.00419	1.75561E-05	0.002%
	4D+1	0.00009	8.10000E-09	0.000%
	4D-1	0.00132	1.74240E-06	0.000%
	4D+2	0.00617	3.80689E-05	0.003%
	4D-2	-0.01071	1.14704E-04	0.010%
sum				5.079%
N	1S	0.02746	7.54052E-04	0.065%
	2S	-0.06211	3.85765E-03	0.334%
	2PX	0.00426	1.81476E-05	0.002%
	2PY	0.10826	1.17202E-02	1.014%
	2PZ	-0.03571	1.27520E-03	0.110%
	3S	-0.16788	2.81837E-02	2.439%
	3PX	-0.00794	6.30436E-05	0.005%
	3PY	0.1047	1.09621E-02	0.949%
	3PZ	-0.03524	1.24186E-03	0.107%
	4D 0	-0.00415	1.72225E-05	0.001%
	4D+1	0.00125	1.56250E-06	0.000%
	4D-1	-0.00056	3.13600E-07	0.000%
	4D+2	-0.01187	1.40897E-04	0.012%
	4D-2	-0.00342	1.16964E-05	0.001%
sum				5.040%
C	1S	0.00349	1.21801E-05	0.001%
	2S	-0.00821	6.74041E-05	0.006%
	2PX	0.01003	1.00601E-04	0.009%
	2PY	-0.00306	9.36360E-06	0.001%
	2PZ	-0.00569	3.23761E-05	0.003%
	3S	-0.01979	3.91644E-04	0.034%
	3PX	0.02575	6.63063E-04	0.057%
	3PY	-0.01548	2.39630E-04	0.021%
	3PZ	-0.00669	4.47561E-05	0.004%
	4D 0	-0.00111	1.23210E-06	0.000%
	4D+1	-0.00006	3.60000E-09	0.000%
	4D-1	-0.00021	4.41000E-08	0.000%
	4D+2	0.00115	1.32250E-06	0.000%
	4D-2	-0.00025	6.25000E-08	0.000%
sum				0.135%
H	1S	-0.00315	9.92250E-06	0.001%
	2S	0.01585	2.51223E-04	0.022%
	3PX	0.00006	3.60000E-09	0.000%
	3PY	0.0009	8.10000E-07	0.000%
	3PZ	-0.00004	1.60000E-09	0.000%
sum				0.023%
C	1S	-0.00111	1.23210E-06	0.000%
	2S	0.00459	2.10681E-05	0.002%
	2PX	-0.00102	1.04040E-06	0.000%
	2PY	0.00736	5.41696E-05	0.005%
	2PZ	-0.00639	4.08321E-05	0.004%
	3S	-0.01577	2.48693E-04	0.022%
	3PX	0.01077	1.15993E-04	0.010%
	3PY	0.00307	9.42490E-06	0.001%
	3PZ	-0.00219	4.79610E-06	0.000%
	4D 0	-0.00021	4.41000E-08	0.000%
	4D+1	0.00019	3.61000E-08	0.000%
	4D-1	-0.00044	1.93600E-07	0.000%
	4D+2	-0.00072	5.18400E-07	0.000%
	4D-2	0.00051	2.60100E-07	0.000%
sum				0.043%
H	1S	-0.00112	1.25440E-06	0.000%
	2S	-0.00314	9.85960E-06	0.001%
	3PX	-0.00007	4.90000E-09	0.000%
	3PY	0.00038	1.44400E-07	0.000%
	3PZ	-0.00017	2.89000E-08	0.000%
sum				0.001%
C	1S	-0.00016	2.56000E-08	0.000%
	2S	0.00011	1.21000E-08	0.000%
	2PX	-0.00767	5.88289E-05	0.005%
	2PY	-0.00788	6.20944E-05	0.005%

2PZ	0.00881	7.76161E-05	0.007%
3S	0.00733	5.37289E-05	0.005%
3PX	-0.01613	2.60177E-04	0.023%
3PY	-0.0054	2.91600E-05	0.003%
3PZ	0.00847	7.17409E-05	0.006%
4D 0	-0.00029	8.41000E-08	0.000%
4D+1	0.00012	1.44000E-08	0.000%
4D-1	-0.0002	4.00000E-08	0.000%
4D+2	-0.0003	9.00000E-08	0.000%
4D-2	-0.00019	3.61000E-08	0.000%
sum			0.053%
H 1S	0.00141	1.98810E-06	0.000%
2S	0.00403	1.62409E-05	0.001%
3PX	-0.00028	7.84000E-08	0.000%
3PY	-0.00029	8.41000E-08	0.000%
3PZ	0.00031	9.61000E-08	0.000%
sum			0.002%
C 1S	-0.0002	4.00000E-08	0.000%
2S	0.00165	2.72250E-06	0.000%
2PX	-0.00059	3.48100E-07	0.000%
2PY	0.00189	3.57210E-06	0.000%
2PZ	-0.0025	6.25000E-06	0.001%
3S	-0.01497	2.24101E-04	0.019%
3PX	0.0045	2.02500E-05	0.002%
3PY	-0.00588	3.45744E-05	0.003%
3PZ	-0.00438	1.91844E-05	0.002%
4D 0	0.00081	6.56100E-07	0.000%
4D+1	0.00032	1.02400E-07	0.000%
4D-1	-0.00065	4.22500E-07	0.000%
4D+2	-0.00047	2.20900E-07	0.000%
4D-2	-0.00009	8.10000E-09	0.000%
sum			0.027%
H 1S	-0.00114	1.29960E-06	0.000%
2S	-0.00526	2.76676E-05	0.002%
3PX	-0.00008	6.40000E-09	0.000%
3PY	0.00011	1.21000E-08	0.000%
3PZ	-0.00009	8.10000E-09	0.000%
sum			0.003%
C 1S	0.00033	1.08900E-07	0.000%
2S	-0.00122	1.48840E-06	0.000%
2PX	0.00593	3.51649E-05	0.003%
2PY	0.00288	8.29440E-06	0.001%
2PZ	-0.01037	1.07537E-04	0.009%
3S	0.01628	2.65038E-04	0.023%
3PX	0.01645	2.70603E-04	0.023%
3PY	-0.00199	3.96010E-06	0.000%
3PZ	-0.01037	1.07537E-04	0.009%
4D 0	-0.00004	1.60000E-09	0.000%
4D+1	-0.0006	3.60000E-07	0.000%
4D-1	-0.00003	9.00000E-10	0.000%
4D+2	0.00041	1.68100E-07	0.000%
4D-2	-0.00067	4.48900E-07	0.000%
sum			0.069%
H 1S	-0.00063	3.96900E-07	0.000%
2S	-0.00939	8.81721E-05	0.008%
3PX	0.00016	2.56000E-08	0.000%
3PY	0.00014	1.96000E-08	0.000%
3PZ	-0.0003	9.00000E-08	0.000%
sum			0.008%
C 1S	-0.00527	2.77729E-05	0.002%
2S	0.01036	1.07330E-04	0.009%
2PX	-0.02329	5.42424E-04	0.047%
2PY	0.00789	6.22521E-05	0.005%
2PZ	0.00578	3.34084E-05	0.003%
3S	0.04734	2.24108E-03	0.194%
3PX	-0.02667	7.11289E-04	0.062%
3PY	0.01881	3.53816E-04	0.031%
3PZ	0.01068	1.14062E-04	0.010%
4D 0	0.00026	6.76000E-08	0.000%
4D+1	-0.00125	1.56250E-06	0.000%
4D-1	0.0006	3.60000E-07	0.000%
4D+2	0.0002	4.00000E-08	0.000%
4D-2	-0.00072	5.18400E-07	0.000%
sum			0.363%
C 1S	-0.00432	1.86624E-05	0.002%
2S	0.01604	2.57282E-04	0.022%
2PX	-0.00111	1.23210E-06	0.000%
2PY	0.02882	8.30592E-04	0.072%
2PZ	0.01947	3.79081E-04	0.033%
3S	-0.04577	2.09489E-03	0.181%
3PX	-0.01989	3.95612E-04	0.034%
3PY	0.00021	4.41000E-08	0.000%
3PZ	0.01676	2.80898E-04	0.024%
4D 0	0.00116	1.34560E-06	0.000%
4D+1	0.00014	1.96000E-08	0.000%
4D-1	-0.00305	9.30250E-06	0.001%
4D+2	-0.00107	1.14490E-06	0.000%

	4D-2	-0.00916	8.39056E-05	0.007%
sum				0.377%
C	1S	0.02433	5.91949E-04	0.051%
	2S	-0.04998	2.49800E-03	0.216%
	2PX	0.00803	6.44809E-05	0.006%
	2PY	0.0166	2.75560E-04	0.024%
	2PZ	0.00034	1.15600E-07	0.000%
	3S	-0.16388	2.68567E-02	2.324%
	3PX	0.03334	1.11156E-03	0.096%
	3PY	0.06879	4.73206E-03	0.409%
	3PZ	0.00025	6.25000E-08	0.000%
	4D 0	-0.00151	2.28010E-06	0.000%
	4D+1	0.00133	1.76890E-06	0.000%
	4D-1	-0.00068	4.62400E-07	0.000%
	4D+2	-0.00452	2.04304E-05	0.002%
	4D-2	0.00574	3.29476E-05	0.003%
sum				3.131%
C	1S	-0.00434	1.88356E-05	0.002%
	2S	0.01608	2.58566E-04	0.022%
	2PX	0.02339	5.47092E-04	0.047%
	2PY	0.01692	2.86286E-04	0.025%
	2PZ	-0.01979	3.91644E-04	0.034%
	3S	-0.04538	2.05934E-03	0.178%
	3PX	0.01218	1.48352E-04	0.013%
	3PY	-0.0155	2.40250E-04	0.021%
	3PZ	-0.01708	2.91726E-04	0.025%
	4D 0	0.00115	1.32250E-06	0.000%
	4D+1	0.00246	6.05160E-06	0.001%
	4D-1	0.00177	3.13290E-06	0.000%
	4D+2	0.00917	8.40889E-05	0.007%
	4D-2	-0.00108	1.16640E-06	0.000%
sum				0.375%
C	1S	-0.00526	2.76676E-05	0.002%
	2S	0.01034	1.06916E-04	0.009%
	2PX	0.0206	4.24360E-04	0.037%
	2PY	-0.01355	1.83603E-04	0.016%
	2PZ	-0.00595	3.54025E-05	0.003%
	3S	0.04727	2.23445E-03	0.193%
	3PX	0.03074	9.44948E-04	0.082%
	3PY	-0.00927	8.59329E-05	0.007%
	3PZ	-0.01096	1.20122E-04	0.010%
	4D 0	0.00026	6.76000E-08	0.000%
	4D+1	-0.00125	1.56250E-06	0.000%
	4D-1	0.00062	3.84400E-07	0.000%
	4D+2	0.00064	4.09600E-07	0.000%
	4D-2	-0.00036	1.29600E-07	0.000%
sum				0.360%
C	1S	0.00033	1.08900E-07	0.000%
	2S	-0.0012	1.44000E-06	0.000%
	2PX	-0.00136	1.84960E-06	0.000%
	2PY	0.00645	4.16025E-05	0.004%
	2PZ	0.01034	1.06916E-04	0.009%
	3S	0.01603	2.56961E-04	0.022%
	3PX	-0.01161	1.34792E-04	0.012%
	3PY	0.01156	1.33634E-04	0.012%
	3PZ	0.0105	1.10250E-04	0.010%
	4D 0	-0.00003	9.00000E-10	0.000%
	4D+1	-0.00036	1.29600E-07	0.000%
	4D-1	0.0005	2.50000E-07	0.000%
	4D+2	0.00055	3.02500E-07	0.000%
	4D-2	-0.00057	3.24900E-07	0.000%
sum				0.068%
H	1S	-0.00064	4.09600E-07	0.000%
	2S	-0.00947	8.96809E-05	0.008%
	3PX	0.00001	1.00000E-10	0.000%
	3PY	0.00021	4.41000E-08	0.000%
	3PZ	0.0003	9.00000E-08	0.000%
sum				0.008%
C	1S	-0.0002	4.00000E-08	0.000%
	2S	0.00163	2.65690E-06	0.000%
	2PX	0.00186	3.45960E-06	0.000%
	2PY	0.00082	6.72400E-07	0.000%
	2PZ	0.0026	6.76000E-06	0.001%
	3S	-0.01478	2.18448E-04	0.019%
	3PX	-0.00726	5.27076E-05	0.005%
	3PY	0.00007	4.90000E-09	0.000%
	3PZ	0.00451	2.03401E-05	0.002%
	4D 0	0.00081	6.56100E-07	0.000%
	4D+1	0.00071	5.04100E-07	0.000%
	4D-1	0.00015	2.25000E-08	0.000%
	4D+2	0.0002	4.00000E-08	0.000%
	4D-2	0.00044	1.93600E-07	0.000%
sum				0.027%
H	1S	-0.00113	1.27690E-06	0.000%
	2S	-0.00522	2.72484E-05	0.002%
	3PX	0.00014	1.96000E-08	0.000%
	3PY	0.00002	4.00000E-10	0.000%

	3PZ	0.00009	8.10000E-09	0.000%
sum				0.002%
C	1S	-0.00017	2.89000E-08	0.000%
	2S	0.00014	1.96000E-08	0.000%
	2PX	-0.00148	2.19040E-06	0.000%
	2PY	-0.01096	1.20122E-04	0.010%
	2PZ	-0.0089	7.92100E-05	0.007%
	3S	0.00715	5.11225E-05	0.004%
	3PX	0.00553	3.05809E-05	0.003%
	3PY	-0.01612	2.59854E-04	0.022%
	3PZ	-0.00859	7.37881E-05	0.006%
	4D 0	-0.00028	7.84000E-08	0.000%
	4D+1	0.00023	5.29000E-08	0.000%
	4D-1	0.00003	9.00000E-10	0.000%
	4D+2	0.00026	6.76000E-08	0.000%
	4D-2	0.00024	5.76000E-08	0.000%
sum				0.053%
H	1S	0.00141	1.98810E-06	0.000%
	2S	0.00391	1.52881E-05	0.001%
	3PX	-0.00005	2.50000E-09	0.000%
	3PY	-0.0004	1.60000E-07	0.000%
	3PZ	-0.00031	9.61000E-08	0.000%
sum				0.002%
C	1S	-0.0011	1.21000E-06	0.000%
	2S	0.00457	2.08849E-05	0.002%
	2PX	0.00641	4.10881E-05	0.004%
	2PY	0.0037	1.36900E-05	0.001%
	2PZ	0.00633	4.00689E-05	0.003%
	3S	-0.01551	2.40560E-04	0.021%
	3PX	-0.00424	1.79776E-05	0.002%
	3PY	0.01015	1.03023E-04	0.009%
	3PZ	0.00235	5.52250E-06	0.000%
	4D 0	-0.00021	4.41000E-08	0.000%
	4D+1	0.00047	2.20900E-07	0.000%
	4D-1	0.00013	1.69000E-08	0.000%
	4D+2	-0.00033	1.08900E-07	0.000%
	4D-2	0.00083	6.88900E-07	0.000%
sum				0.042%
H	1S	-0.00113	1.27690E-06	0.000%
	2S	-0.00311	9.67210E-06	0.001%
	3PX	0.00034	1.15600E-07	0.000%
	3PY	0.00018	3.24000E-08	0.000%
	3PZ	0.00016	2.56000E-08	0.000%
sum				0.001%
C	1S	0.0035	1.22500E-05	0.001%
	2S	-0.0082	6.72400E-05	0.006%
	2PX	-0.00855	7.31025E-05	0.006%
	2PY	0.00612	3.74544E-05	0.003%
	2PZ	0.00575	3.30625E-05	0.003%
	3S	-0.01993	3.97205E-04	0.034%
	3PX	-0.02773	7.68953E-04	0.067%
	3PY	0.01096	1.20122E-04	0.010%
	3PZ	0.00651	4.23801E-05	0.004%
	4D 0	-0.00111	1.23210E-06	0.000%
	4D+1	0.00012	1.44000E-08	0.000%
	4D-1	0.00019	3.61000E-08	0.000%
	4D+2	-0.00004	1.60000E-09	0.000%
	4D-2	-0.00117	1.36890E-06	0.000%
sum				0.135%
H	1S	-0.00315	9.92250E-06	0.001%
	2S	0.01518	2.30432E-04	0.020%
	3PX	0.00066	4.35600E-07	0.000%
	3PY	0.00061	3.72100E-07	0.000%
	3PZ	0.00003	9.00000E-10	0.000%
sum				0.021%
C	1S	0.00351	1.23201E-05	0.001%
	2S	-0.00826	6.82276E-05	0.006%
	2PX	-0.00751	5.64001E-05	0.005%
	2PY	-0.0077	5.92900E-05	0.005%
	2PZ	-0.00584	3.41056E-05	0.003%
	3S	-0.01971	3.88484E-04	0.034%
	3PX	-0.02556	6.53314E-04	0.057%
	3PY	-0.01509	2.27708E-04	0.020%
	3PZ	-0.00666	4.43556E-05	0.004%
	4D 0	-0.00114	1.29960E-06	0.000%
	4D+1	-0.00015	2.25000E-08	0.000%
	4D-1	0.00014	1.96000E-08	0.000%
	4D+2	-0.00039	1.52100E-07	0.000%
	4D-2	0.00112	1.25440E-06	0.000%
sum				0.134%
H	1S	-0.00319	1.01761E-05	0.001%
	2S	0.01488	2.21414E-04	0.019%
	3PX	0.00074	5.47600E-07	0.000%
	3PY	-0.00052	2.70400E-07	0.000%
	3PZ	-0.00003	9.00000E-10	0.000%
sum				0.020%
C	1S	-0.00111	1.23210E-06	0.000%

2S	0.00457	2.08849E-05	0.002%
2PX	0.00691	4.77481E-05	0.004%
2PY	-0.0029	8.41000E-06	0.001%
2PZ	-0.00637	4.05769E-05	0.004%
3S	-0.01532	2.34702E-04	0.020%
3PX	-0.00258	6.65640E-06	0.001%
3PY	-0.01083	1.17289E-04	0.010%
3PZ	-0.00225	5.06250E-06	0.000%
4D 0	-0.00023	5.29000E-08	0.000%
4D+1	-0.00049	2.40100E-07	0.000%
4D-1	0.00005	2.50000E-09	0.000%
4D+2	-0.00007	4.90000E-09	0.000%
4D-2	-0.00093	8.64900E-07	0.000%
sum			0.042%
H 1S	-0.00116	1.34560E-06	0.000%
2S	-0.00328	1.07584E-05	0.001%
3PX	0.00037	1.36900E-07	0.000%
3PY	-0.00014	1.96000E-08	0.000%
3PZ	-0.00016	2.56000E-08	0.000%
sum			0.001%
C 1S	-0.00017	2.89000E-08	0.000%
2S	0.00013	1.69000E-08	0.000%
2PX	-0.0031	9.61000E-06	0.001%
2PY	0.01113	1.23877E-04	0.011%
2PZ	0.00912	8.31744E-05	0.007%
3S	0.00717	5.14089E-05	0.004%
3PX	0.00312	9.73440E-06	0.001%
3PY	0.01724	2.97218E-04	0.026%
3PZ	0.00883	7.79689E-05	0.007%
4D 0	-0.00028	7.84000E-08	0.000%
4D+1	-0.00023	5.29000E-08	0.000%
4D-1	-0.00001	1.00000E-10	0.000%
4D+2	0.00032	1.02400E-07	0.000%
4D-2	-0.00017	2.89000E-08	0.000%
sum			0.057%
H 1S	0.00139	1.93210E-06	0.000%
2S	0.00392	1.53664E-05	0.001%
3PX	-0.00011	1.21000E-08	0.000%
3PY	0.0004	1.60000E-07	0.000%
3PZ	0.00031	9.61000E-08	0.000%
sum			0.002%
C 1S	-0.00019	3.61000E-08	0.000%
2S	0.00161	2.59210E-06	0.000%
2PX	0.00196	3.84160E-06	0.000%
2PY	-0.00073	5.32900E-07	0.000%
2PZ	-0.00271	7.34410E-06	0.001%
3S	-0.01487	2.21117E-04	0.019%
3PX	-0.00719	5.16961E-05	0.004%
3PY	-0.00143	2.04490E-06	0.000%
3PZ	-0.00456	2.07936E-05	0.002%
4D 0	0.00084	7.05600E-07	0.000%
4D+1	-0.00074	5.47600E-07	0.000%
4D-1	0.00007	4.90000E-09	0.000%
4D+2	0.00034	1.15600E-07	0.000%
4D-2	-0.00038	1.44400E-07	0.000%
sum			0.027%
H 1S	-0.00112	1.25440E-06	0.000%
2S	-0.00516	2.66256E-05	0.002%
3PX	0.00014	1.96000E-08	0.000%
3PY	0	0.00000E+00	0.000%
3PZ	-0.0001	1.00000E-08	0.000%
sum			0.002%
C 1S	0.0003	9.00000E-08	0.000%
2S	-0.00113	1.27690E-06	0.000%
2PX	-0.00026	6.76000E-08	0.000%
2PY	-0.00699	4.88601E-05	0.004%
2PZ	-0.0105	1.10250E-04	0.010%
3S	0.01601	2.56320E-04	0.022%
3PX	-0.00994	9.88036E-05	0.009%
3PY	-0.01354	1.83332E-04	0.016%
3PZ	-0.01069	1.14276E-04	0.010%
4D 0	-0.00003	9.00000E-10	0.000%
4D+1	0.0003	9.00000E-08	0.000%
4D-1	0.00056	3.13600E-07	0.000%
4D+2	0.00035	1.22500E-07	0.000%
4D-2	0.00073	5.32900E-07	0.000%
sum			0.070%
H 1S	-0.00064	4.09600E-07	0.000%
2S	-0.0095	9.02500E-05	0.008%
3PX	0.00005	2.50000E-09	0.000%
3PY	-0.00022	4.84000E-08	0.000%
3PZ	-0.00031	9.61000E-08	0.000%
sum			0.008%
C 1S	-0.00527	2.77729E-05	0.002%
2S	0.01034	1.06916E-04	0.009%
2PX	0.01839	3.38192E-04	0.029%
2PY	0.01681	2.82576E-04	0.024%

	2PZ	0.00605	3.66025E-05	0.003%
	3S	0.0476	2.26576E-03	0.196%
	3PX	0.02901	8.41580E-04	0.073%
	3PY	0.01436	2.06210E-04	0.018%
	3PZ	0.01079	1.16424E-04	0.010%
	4D 0	0.00023	5.29000E-08	0.000%
	4D+1	0.0012	1.44000E-06	0.000%
	4D-1	0.00081	6.56100E-07	0.000%
	4D+2	0.0005	2.50000E-07	0.000%
	4D-2	0.00055	3.02500E-07	0.000%
sum				0.366%
C	1S	-0.00433	1.87489E-05	0.002%
	2S	0.01606	2.57924E-04	0.022%
	2PX	0.02562	6.56384E-04	0.057%
	2PY	-0.01319	1.73976E-04	0.015%
	2PZ	0.02061	4.24772E-04	0.037%
	3S	-0.04532	2.05390E-03	0.178%
	3PX	0.01035	1.07123E-04	0.009%
	3PY	0.01739	3.02412E-04	0.026%
	3PZ	0.01769	3.12936E-04	0.027%
	4D 0	0.00113	1.27690E-06	0.000%
	4D+1	-0.00275	7.56250E-06	0.001%
	4D-1	0.00148	2.19040E-06	0.000%
	4D+2	0.0085	7.22500E-05	0.006%
	4D-2	0.00358	1.28164E-05	0.001%
sum				0.381%
C	1S	0.0244	5.95360E-04	0.052%
	2S	-0.05011	2.51101E-03	0.217%
	2PX	0.01021	1.04244E-04	0.009%
	2PY	-0.01532	2.34702E-04	0.020%
	2PZ	-0.00037	1.36900E-07	0.000%
	3S	-0.16479	2.71557E-02	2.350%
	3PX	0.04247	1.80370E-03	0.156%
	3PY	-0.06321	3.99550E-03	0.346%
	3PZ	0	0.00000E+00	0.000%
	4D 0	-0.00148	2.19040E-06	0.000%
	4D+1	-0.00123	1.51290E-06	0.000%
	4D-1	-0.00093	8.64900E-07	0.000%
	4D+2	-0.00271	7.34410E-06	0.001%
	4D-2	-0.00681	4.63761E-05	0.004%
sum				3.155%
C	1S	-0.00439	1.92721E-05	0.002%
	2S	0.0162	2.62440E-04	0.023%
	2PX	0.00298	8.88040E-06	0.001%
	2PY	-0.02908	8.45646E-04	0.073%
	2PZ	-0.01992	3.96806E-04	0.034%
	3S	-0.04528	2.05028E-03	0.177%
	3PX	-0.02008	4.03206E-04	0.035%
	3PY	-0.00341	1.16281E-05	0.001%
	3PZ	-0.01734	3.00676E-04	0.026%
	4D 0	0.0012	1.44000E-06	0.000%
	4D+1	0.00026	6.76000E-08	0.000%
	4D-1	-0.00309	9.54810E-06	0.001%
	4D+2	-0.00361	1.30321E-05	0.001%
	4D-2	0.0085	7.22500E-05	0.006%
sum				0.380%
C	1S	-0.00527	2.77729E-05	0.002%
	2S	0.01032	1.06502E-04	0.009%
	2PX	-0.02219	4.92396E-04	0.043%
	2PY	-0.01092	1.19246E-04	0.010%
	2PZ	-0.00613	3.75769E-05	0.003%
	3S	0.04775	2.28006E-03	0.197%
	3PX	-0.02398	5.75040E-04	0.050%
	3PY	-0.02233	4.98629E-04	0.043%
	3PZ	-0.01109	1.22988E-04	0.011%
	4D 0	0.00024	5.76000E-08	0.000%
	4D+1	0.00118	1.39240E-06	0.000%
	4D-1	0.00079	6.24100E-07	0.000%
	4D+2	-0.00001	1.00000E-10	0.000%
	4D-2	0.00075	5.62500E-07	0.000%
sum				0.369%
C	1S	0.00031	9.61000E-08	0.000%
	2S	-0.00118	1.39240E-06	0.000%
	2PX	0.00631	3.98161E-05	0.003%
	2PY	-0.00213	4.53690E-06	0.000%
	2PZ	0.01053	1.10881E-04	0.010%
	3S	0.01661	2.75892E-04	0.024%
	3PX	0.01617	2.61469E-04	0.023%
	3PY	0.00439	1.92721E-05	0.002%
	3PZ	0.01057	1.11725E-04	0.010%
	4D 0	-0.00002	4.00000E-10	0.000%
	4D+1	0.00061	3.72100E-07	0.000%
	4D-1	0.00008	6.40000E-09	0.000%
	4D+2	0.00023	5.29000E-08	0.000%
	4D-2	0.00077	5.92900E-07	0.000%
sum				0.071%
H	1S	-0.00061	3.72100E-07	0.000%

2S	-0.00946	8.94916E-05	0.008%
3PX	0.00018	3.24000E-08	0.000%
3PY	-0.00012	1.44000E-08	0.000%
3PZ	0.00031	9.61000E-08	0.000%
sum			0.008%
C 1S	-0.00018	3.24000E-08	0.000%
2S	0.00162	2.62440E-06	0.000%
2PX	-0.00011	1.21000E-08	0.000%
2PY	-0.00204	4.16160E-06	0.000%
2PZ	0.0027	7.29000E-06	0.001%
3S	-0.01526	2.32868E-04	0.020%
3PX	0.00397	1.57609E-05	0.001%
3PY	0.00642	4.12164E-05	0.004%
3PZ	0.00459	2.10681E-05	0.002%
4D 0	0.00084	7.05600E-07	0.000%
4D+1	-0.00024	5.76000E-08	0.000%
4D-1	-0.0007	4.90000E-07	0.000%
4D+2	-0.00049	2.40100E-07	0.000%
4D-2	-0.00004	1.60000E-09	0.000%
sum			0.028%
H 1S	-0.00113	1.27690E-06	0.000%
2S	-0.00521	2.71441E-05	0.002%
3PX	-0.00005	2.50000E-09	0.000%
3PY	-0.00013	1.69000E-08	0.000%
3PZ	0.0001	1.00000E-08	0.000%
sum			0.002%
C 1S	-0.00017	2.89000E-08	0.000%
2S	0.00011	1.21000E-08	0.000%
2PX	-0.0089	7.92100E-05	0.007%
2PY	0.00687	4.71969E-05	0.004%
2PZ	-0.00917	8.40889E-05	0.007%
3S	0.00732	5.35824E-05	0.005%
3PX	-0.01699	2.88660E-04	0.025%
3PY	0.00325	1.05625E-05	0.001%
3PZ	-0.00893	7.97449E-05	0.007%
4D 0	-0.00027	7.29000E-08	0.000%
4D+1	-0.00009	8.10000E-09	0.000%
4D-1	-0.00022	4.84000E-08	0.000%
4D+2	-0.00034	1.15600E-07	0.000%
4D-2	0.00011	1.21000E-08	0.000%
sum			0.056%
H 1S	0.00141	1.98810E-06	0.000%
2S	0.00402	1.61604E-05	0.001%
3PX	-0.00032	1.02400E-07	0.000%
3PY	0.00025	6.25000E-08	0.000%
3PZ	-0.00032	1.02400E-07	0.000%
sum			0.002%
C 1S	-0.00111	1.23210E-06	0.000%
2S	0.00458	2.09764E-05	0.002%
2PX	-0.00008	6.40000E-09	0.000%
2PY	-0.00739	5.46121E-05	0.005%
2PZ	0.00639	4.08321E-05	0.004%
3S	-0.0158	2.49640E-04	0.022%
3PX	0.01103	1.21661E-04	0.011%
3PY	-0.00153	2.34090E-06	0.000%
3PZ	0.00231	5.33610E-06	0.000%
4D 0	-0.00021	4.41000E-08	0.000%
4D+1	-0.00013	1.69000E-08	0.000%
4D-1	-0.00049	2.40100E-07	0.000%
4D+2	-0.00057	3.24900E-07	0.000%
4D-2	-0.00071	5.04100E-07	0.000%
sum			0.043%
H 1S	-0.00115	1.32250E-06	0.000%
2S	-0.00311	9.67210E-06	0.001%
3PX	-0.00002	4.00000E-10	0.000%
3PY	-0.00039	1.52100E-07	0.000%
3PZ	0.00017	2.89000E-08	0.000%
sum			0.001%
C 1S	0.00354	1.25316E-05	0.001%
2S	-0.00829	6.87241E-05	0.006%
2PX	0.00976	9.52576E-05	0.008%
2PY	0.00435	1.89225E-05	0.002%
2PZ	0.00594	3.52836E-05	0.003%
3S	-0.02022	4.08848E-04	0.035%
3PX	0.02367	5.60269E-04	0.048%
3PY	0.01886	3.55700E-04	0.031%
3PZ	0.00687	4.71969E-05	0.004%
4D 0	-0.00112	1.25440E-06	0.000%
4D+1	0.00011	1.21000E-08	0.000%
4D-1	-0.0002	4.00000E-08	0.000%
4D+2	0.00105	1.10250E-06	0.000%
4D-2	0.00054	2.91600E-07	0.000%
sum			0.139%
H 1S	-0.00317	1.00489E-05	0.001%
2S	0.01577	2.48693E-04	0.022%
3PX	0.0002	4.00000E-08	0.000%
3PY	-0.00089	7.92100E-07	0.000%

	3PZ	0.00005	2.50000E-09	0.000%
sum				0.022%
C	1S	0.00353	1.24609E-05	0.001%
	2S	-0.00824	6.78976E-05	0.006%
	2PX	-0.0025	6.25000E-06	0.001%
	2PY	0.01032	1.06502E-04	0.009%
	2PZ	-0.00581	3.37561E-05	0.003%
	3S	-0.02012	4.04814E-04	0.035%
	3PX	0.00006	3.60000E-09	0.000%
	3PY	0.02993	8.95805E-04	0.078%
	3PZ	-0.0064	4.09600E-05	0.004%
	4D 0	-0.00112	1.25440E-06	0.000%
	4D+1	0.00021	4.41000E-08	0.000%
	4D-1	0.00006	3.60000E-09	0.000%
	4D+2	-0.00077	5.92900E-07	0.000%
	4D-2	-0.00088	7.74400E-07	0.000%
sum				0.136%
H	1S	-0.00319	1.01761E-05	0.001%
	2S	0.01506	2.26804E-04	0.020%
	3PX	-0.00083	6.88900E-07	0.000%
	3PY	-0.00039	1.52100E-07	0.000%
	3PZ	-0.00003	9.00000E-10	0.000%
sum				0.021%
C	1S	-0.0011	1.21000E-06	0.000%
	2S	0.00455	2.07025E-05	0.002%
	2PX	-0.00572	3.27184E-05	0.003%
	2PY	-0.00461	2.12521E-05	0.002%
	2PZ	-0.00627	3.93129E-05	0.003%
	3S	-0.01551	2.40560E-04	0.021%
	3PX	-0.00775	6.00625E-05	0.005%
	3PY	0.00769	5.91361E-05	0.005%
	3PZ	-0.00222	4.92840E-06	0.000%
	4D 0	-0.00021	4.41000E-08	0.000%
	4D+1	0.00029	8.41000E-08	0.000%
	4D-1	0.00039	1.52100E-07	0.000%
	4D+2	0.00082	6.72400E-07	0.000%
	4D-2	0.00037	1.36900E-07	0.000%
sum				0.042%
H	1S	-0.00113	1.27690E-06	0.000%
	2S	-0.00309	9.54810E-06	0.001%
	3PX	-0.00029	8.41000E-08	0.000%
	3PY	-0.00025	6.25000E-08	0.000%
	3PZ	-0.00016	2.56000E-08	0.000%
sum				0.001%
C	1S	-0.00016	2.56000E-08	0.000%
	2S	0.00012	1.44000E-08	0.000%
	2PX	0.0108	1.16640E-04	0.010%
	2PY	-0.00275	7.56250E-06	0.001%
	2PZ	0.00888	7.88544E-05	0.007%
	3S	0.0071	5.04100E-05	0.004%
	3PX	0.013	1.69000E-04	0.015%
	3PY	-0.0112	1.25440E-04	0.011%
	3PZ	0.00851	7.24201E-05	0.006%
	4D 0	-0.00027	7.29000E-08	0.000%
	4D+1	0.00011	1.21000E-08	0.000%
	4D-1	0.0002	4.00000E-08	0.000%
	4D+2	-0.00003	9.00000E-10	0.000%
	4D-2	0.00036	1.29600E-07	0.000%
sum				0.054%
H	1S	0.00141	1.98810E-06	0.000%
	2S	0.00399	1.59201E-05	0.001%
	3PX	0.00039	1.52100E-07	0.000%
	3PY	-0.0001	1.00000E-08	0.000%
	3PZ	0.00031	9.61000E-08	0.000%
sum				0.002%
C	1S	-0.0002	4.00000E-08	0.000%
	2S	0.00163	2.65690E-06	0.000%
	2PX	-0.00158	2.49640E-06	0.000%
	2PY	-0.00136	1.84960E-06	0.000%
	2PZ	-0.00272	7.39840E-06	0.001%
	3S	-0.01482	2.19632E-04	0.019%
	3PX	0.0025	6.25000E-06	0.001%
	3PY	0.00684	4.67856E-05	0.004%
	3PZ	-0.00461	2.12521E-05	0.002%
	4D 0	0.00082	6.72400E-07	0.000%
	4D+1	0.00041	1.68100E-07	0.000%
	4D-1	0.0006	3.60000E-07	0.000%
	4D+2	0.00016	2.56000E-08	0.000%
	4D-2	0.00046	2.11600E-07	0.000%
sum				0.027%
H	1S	-0.00113	1.27690E-06	0.000%
	2S	-0.00521	2.71441E-05	0.002%
	3PX	-0.00007	4.90000E-09	0.000%
	3PY	-0.00012	1.44000E-08	0.000%
	3PZ	-0.0001	1.00000E-08	0.000%
sum				0.002%
C	1S	0.00033	1.08900E-07	0.000%

	2S	-0.0012	1.44000E-06	0.000%
	2PX	-0.00549	3.01401E-05	0.003%
	2PY	0.00369	1.36161E-05	0.001%
	2PZ	-0.01031	1.06296E-04	0.009%
	3S	0.01604	2.57282E-04	0.022%
	3PX	-0.00645	4.16025E-05	0.004%
	3PY	0.01513	2.28917E-04	0.020%
	3PZ	-0.0104	1.08160E-04	0.009%
	4D 0	-0.00003	9.00000E-10	0.000%
	4D+1	0.00032	1.02400E-07	0.000%
	4D-1	-0.00052	2.70400E-07	0.000%
	4D+2	-0.0008	6.40000E-07	0.000%
	4D-2	-0.00004	1.60000E-09	0.000%
sum				0.068%
H	1S	-0.00063	3.96900E-07	0.000%
	2S	-0.00939	8.81721E-05	0.008%
	3PX	-0.0002	4.00000E-08	0.000%
	3PY	0.00007	4.90000E-09	0.000%
	3PZ	-0.0003	9.00000E-08	0.000%
sum				0.008%
C	1S	-0.00527	2.77729E-05	0.002%
	2S	0.01036	1.07330E-04	0.009%
	2PX	0.00505	2.55025E-05	0.002%
	2PY	-0.0242	5.85640E-04	0.051%
	2PZ	0.0059	3.48100E-05	0.003%
	3S	0.04735	2.24202E-03	0.194%
	3PX	-0.00264	6.96960E-06	0.001%
	3PY	-0.03202	1.02528E-03	0.089%
	3PZ	0.01089	1.18592E-04	0.010%
	4D 0	0.00024	5.76000E-08	0.000%
	4D+1	0.00011	1.21000E-08	0.000%
	4D-1	-0.00139	1.93210E-06	0.000%
	4D+2	-0.00072	5.18400E-07	0.000%
	4D-2	0.00018	3.24000E-08	0.000%
sum				0.361%
C	1S	-0.0044	1.93600E-05	0.002%
	2S	0.0162	2.62440E-04	0.023%
	2PX	-0.02455	6.02703E-04	0.052%
	2PY	-0.01561	2.43672E-04	0.021%
	2PZ	0.01967	3.86909E-04	0.033%
	3S	-0.04497	2.02230E-03	0.175%
	3PX	0.00976	9.52576E-05	0.008%
	3PY	-0.0172	2.95840E-04	0.026%
	3PZ	0.01693	2.86625E-04	0.025%
	4D 0	0.00116	1.34560E-06	0.000%
	4D+1	0.00261	6.81210E-06	0.001%
	4D-1	0.00167	2.78890E-06	0.000%
	4D+2	-0.00739	5.46121E-05	0.005%
	4D-2	0.00553	3.05809E-05	0.003%
sum				0.373%
C	1S	0.02436	5.93410E-04	0.051%
	2S	-0.05005	2.50500E-03	0.217%
	2PX	-0.01842	3.39296E-04	0.029%
	2PY	-0.00139	1.93210E-06	0.000%
	2PZ	-0.00028	7.84000E-08	0.000%
	3S	-0.1642	2.69616E-02	2.333%
	3PX	-0.07618	5.80339E-03	0.502%
	3PY	-0.00555	3.08025E-05	0.003%
	3PZ	-0.00021	4.41000E-08	0.000%
	4D 0	-0.00149	2.22010E-06	0.000%
	4D+1	-0.00013	1.69000E-08	0.000%
	4D-1	0.00145	2.10250E-06	0.000%
	4D+2	0.00725	5.25625E-05	0.005%
	4D-2	0.00104	1.08160E-06	0.000%
sum				3.141%
C	1S	-0.00433	1.87489E-05	0.002%
	2S	0.01606	2.57924E-04	0.022%
	2PX	-0.02634	6.93796E-04	0.060%
	2PY	0.01184	1.40186E-04	0.012%
	2PZ	-0.0194	3.76360E-04	0.033%
	3S	-0.04562	2.08118E-03	0.180%
	3PX	0.00706	4.98436E-05	0.004%
	3PY	0.01889	3.56832E-04	0.031%
	3PZ	-0.01657	2.74565E-04	0.024%
	4D 0	0.00118	1.39240E-06	0.000%
	4D+1	-0.00283	8.00890E-06	0.001%
	4D-1	0.0013	1.69000E-06	0.000%
	4D+2	-0.00552	3.04704E-05	0.003%
	4D-2	-0.00737	5.43169E-05	0.005%
sum				0.376%
C	1S	-0.00528	2.78784E-05	0.002%
	2S	0.01038	1.07744E-04	0.009%
	2PX	0.00137	1.87690E-06	0.000%
	2PY	0.02465	6.07623E-04	0.053%
	2PZ	-0.00568	3.22624E-05	0.003%
	3S	0.04773	2.27815E-03	0.197%
	3PX	-0.00742	5.50564E-05	0.005%

	3PY	0.03184	1.01379E-03	0.088%
	3PZ	-0.01045	1.09203E-04	0.009%
	4D 0	0.00023	5.29000E-08	0.000%
	4D+1	0.00009	8.10000E-09	0.000%
	4D-1	-0.00138	1.90440E-06	0.000%
	4D+2	-0.00067	4.48900E-07	0.000%
	4D-2	-0.00038	1.44400E-07	0.000%
sum				0.367%
C	1S	0.00034	1.15600E-07	0.000%
	2S	-0.00122	1.48840E-06	0.000%
	2PX	-0.00488	2.38144E-05	0.002%
	2PY	-0.00455	2.07025E-05	0.002%
	2PZ	0.01042	1.08576E-04	0.009%
	3S	0.01606	2.57924E-04	0.022%
	3PX	-0.00423	1.78929E-05	0.002%
	3PY	-0.0161	2.59210E-04	0.022%
	3PZ	0.01037	1.07537E-04	0.009%
	4D 0	-0.00004	1.60000E-09	0.000%
	4D+1	-0.00024	5.76000E-08	0.000%
	4D-1	-0.00055	3.02500E-07	0.000%
	4D+2	-0.00078	6.08400E-07	0.000%
	4D-2	-0.00019	3.61000E-08	0.000%
sum				0.069%
H	1S	-0.00062	3.84400E-07	0.000%
	2S	-0.00935	8.74225E-05	0.008%
	3PX	-0.00019	3.61000E-08	0.000%
	3PY	-0.0001	1.00000E-08	0.000%
	3PZ	0.0003	9.00000E-08	0.000%
sum				0.008%
C	1S	-0.0002	4.00000E-08	0.000%
	2S	0.00164	2.68960E-06	0.000%
	2PX	-0.00162	2.62440E-06	0.000%
	2PY	0.00119	1.41610E-06	0.000%
	2PZ	0.00261	6.81210E-06	0.001%
	3S	-0.01493	2.22905E-04	0.019%
	3PX	0.00364	1.32496E-05	0.001%
	3PY	-0.0064	4.09600E-05	0.004%
	3PZ	0.00442	1.95364E-05	0.002%
	4D 0	0.00083	6.88900E-07	0.000%
	4D+1	-0.00049	2.40100E-07	0.000%
	4D-1	0.00053	2.80900E-07	0.000%
	4D+2	0.00028	7.84000E-08	0.000%
	4D-2	-0.00039	1.52100E-07	0.000%
sum				0.027%
H	1S	-0.00114	1.29960E-06	0.000%
	2S	-0.00524	2.74576E-05	0.002%
	3PX	-0.00008	6.40000E-09	0.000%
	3PY	0.00011	1.21000E-08	0.000%
	3PZ	0.00009	8.10000E-09	0.000%
sum				0.002%
C	1S	-0.00016	2.56000E-08	0.000%
	2S	0.0001	1.00000E-08	0.000%
	2PX	0.01025	1.05063E-04	0.009%
	2PY	0.00431	1.85761E-05	0.002%
	2PZ	-0.00888	7.88544E-05	0.007%
	3S	0.00719	5.16961E-05	0.004%
	3PX	0.01116	1.24546E-04	0.011%
	3PY	0.01306	1.70564E-04	0.015%
	3PZ	-0.00844	7.12336E-05	0.006%
	4D 0	-0.00028	7.84000E-08	0.000%
	4D+1	-0.00014	1.96000E-08	0.000%
	4D-1	0.00019	3.61000E-08	0.000%
	4D+2	0.00008	6.40000E-09	0.000%
	4D-2	-0.00034	1.15600E-07	0.000%
sum				0.054%
H	1S	0.00141	1.98810E-06	0.000%
	2S	0.00406	1.64836E-05	0.001%
	3PX	0.00037	1.36900E-07	0.000%
	3PY	0.00016	2.56000E-08	0.000%
	3PZ	-0.00031	9.61000E-08	0.000%
sum				0.002%
C	1S	-0.0011	1.21000E-06	0.000%
	2S	0.00457	2.08849E-05	0.002%
	2PX	-0.0064	4.09600E-05	0.004%
	2PY	0.00368	1.35424E-05	0.001%
	2PZ	0.00643	4.13449E-05	0.004%
	3S	-0.01578	2.49008E-04	0.022%
	3PX	-0.00672	4.51584E-05	0.004%
	3PY	-0.00885	7.83225E-05	0.007%
	3PZ	0.0022	4.84000E-06	0.000%
	4D 0	-0.0002	4.00000E-08	0.000%
	4D+1	-0.00035	1.22500E-07	0.000%
	4D-1	0.00035	1.22500E-07	0.000%
	4D+2	0.00088	7.74400E-07	0.000%
	4D-2	-0.00012	1.44000E-08	0.000%
sum				0.043%
H	1S	-0.00111	1.23210E-06	0.000%

2S	-0.0031	9.61000E-06	0.001%
3PX	-0.00033	1.08900E-07	0.000%
3PY	0.00021	4.41000E-08	0.000%
3PZ	0.00016	2.56000E-08	0.000%
sum			0.001%
C 1S	0.00352	1.23904E-05	0.001%
2S	-0.00825	6.80625E-05	0.006%
2PX	-0.00087	7.56900E-07	0.000%
2PY	-0.01058	1.11936E-04	0.010%
2PZ	0.00579	3.35241E-05	0.003%
3S	-0.01993	3.97205E-04	0.034%
3PX	0.00463	2.14369E-05	0.002%
3PY	-0.02978	8.86848E-04	0.077%
3PZ	0.00646	4.17316E-05	0.004%
4D 0	-0.00111	1.23210E-06	0.000%
4D+1	-0.00021	4.41000E-08	0.000%
4D-1	0.00004	1.60000E-09	0.000%
4D+2	-0.00099	9.80100E-07	0.000%
4D-2	0.00062	3.84400E-07	0.000%
sum			0.136%
H 1S	-0.00316	9.98560E-06	0.001%
2S	0.01548	2.39630E-04	0.021%
3PX	-0.00088	7.74400E-07	0.000%
3PY	0.00027	7.29000E-08	0.000%
3PZ	0.00003	9.00000E-10	0.000%
Cl 1S	0.00361	1.30321E-05	0.001%
2S	-0.0158	2.49640E-04	0.022%
2PX	-0.01352	1.82790E-04	0.016%
2PY	-0.02789	7.77852E-04	0.067%
2PZ	0.00013	1.69000E-08	0.000%
3S	0.03923	1.53899E-03	0.133%
3PX	0.03705	1.37270E-03	0.119%
3PY	0.07644	5.84307E-03	0.506%
3PZ	-0.00036	1.29600E-07	0.000%
4S	0.07576	5.73958E-03	0.497%
4PX	0.04867	2.36877E-03	0.205%
4PY	0.10049	1.00982E-02	0.874%
4PZ	-0.0004	1.60000E-07	0.000%
5D 0	0.00544	2.95936E-05	0.003%
5D+1	0.00065	4.22500E-07	0.000%
5D-1	-0.00022	4.84000E-08	0.000%
5D+2	0.00528	2.78784E-05	0.002%
5D-2	-0.00669	4.47561E-05	0.004%
sum			2.469%
Cl 1S	0.00361	1.30321E-05	0.001%
2S	-0.01583	2.50589E-04	0.022%
2PX	-0.01742	3.03456E-04	0.026%
2PY	0.0257	6.60490E-04	0.057%
2PZ	-0.0003	9.00000E-08	0.000%
3S	0.03929	1.54370E-03	0.134%
3PX	0.04773	2.27815E-03	0.197%
3PY	-0.07044	4.96179E-03	0.429%
3PZ	0.00082	6.72400E-07	0.000%
4S	0.07579	5.74412E-03	0.497%
4PX	0.06273	3.93505E-03	0.341%
4PY	-0.09253	8.56180E-03	0.741%
4PZ	0.001	1.00000E-06	0.000%
5D 0	0.00545	2.97025E-05	0.003%
5D+1	-0.00068	4.62400E-07	0.000%
5D-1	-0.00024	5.76000E-08	0.000%
5D+2	0.00316	9.98560E-06	0.001%
5D-2	0.00793	6.28849E-05	0.005%
sum			2.454%
Cl 1S	0.00361	1.30321E-05	0.001%
2S	-0.01582	2.50272E-04	0.022%
2PX	0.03095	9.57903E-04	0.083%
2PY	0.00222	4.92840E-06	0.000%
2PZ	-0.00011	1.21000E-08	0.000%
3S	0.03928	1.54292E-03	0.134%
3PX	-0.08484	7.19783E-03	0.623%
3PY	-0.00609	3.70881E-05	0.003%
3PZ	0.0003	9.00000E-08	0.000%
4S	0.07582	5.74867E-03	0.497%
4PX	-0.11149	1.24300E-02	1.076%
4PY	-0.00796	6.33616E-05	0.005%
4PZ	0.00034	1.15600E-07	0.000%
5D 0	0.00545	2.97025E-05	0.003%
5D+1	0.00003	9.00000E-10	0.000%
5D-1	0.00068	4.62400E-07	0.000%
5D+2	-0.00845	7.14025E-05	0.006%
5D-2	-0.00121	1.46410E-06	0.000%
sum			2.453%
Total		1.15565E+00	100.000%

* More than 46 % of the LUMO of $[Au(ClPh_2pz)]_3$ originates from the orbitals of three Ag atoms, to which *s* and *d* orbitals contribute most.