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SUPPLEMENTARY INFORMATION

Low temperature isolation of a dinuclear silver complex of the *cyclo*-tetraphosphane [ClP(μ-PMes*)]$_2$

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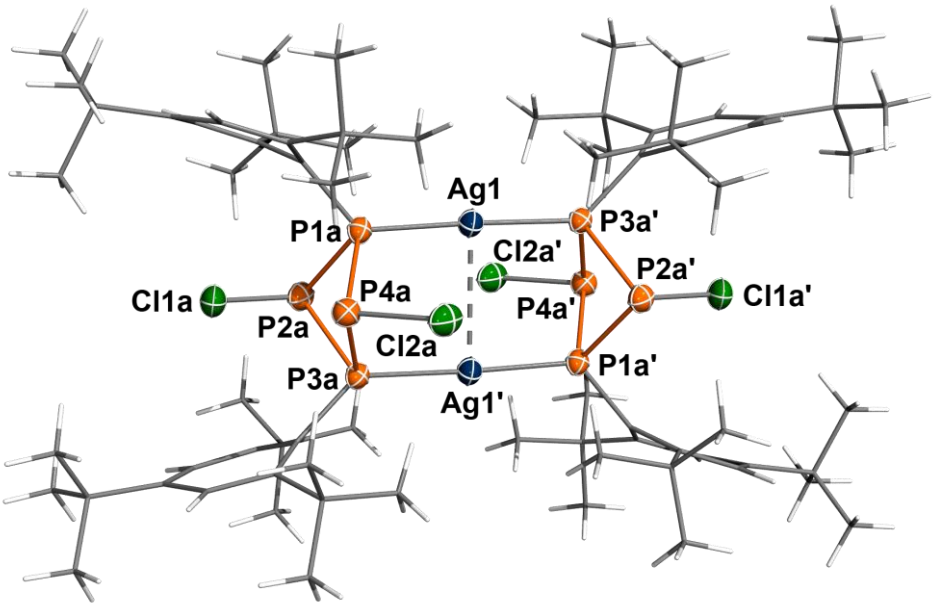


This file includes:

1 Experimental

General Information. All manipulations were carried out under oxygen- and moisture-free conditions under argon using standard Schlenk or Drybox techniques.

Solvents and reactants were obtained from commercial sources or were synthesized. Dichloromethane (CH_2Cl_2) was purified according to a literature procedure,[1] dried over P_4O_{10}, stored over CaH_2 and freshly distilled prior to use. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were dried over Na/benzophenone and freshly distilled prior to use. *n*-Pentane and *n*-hexane were dried over Na/benzophenone/tetraglyme (tetraglyme = $Me(OCH_2CH_2)_3OMe$) and freshly distilled prior to use. Fluorobenzene (PhF) was dried over CaH_2, freshly distilled and degassed prior to use. Deuterated dichloromethane (CD_2Cl_2) and PCl_3 (Merck, for synthesis) were dried over P_4O_{10}, freshly distilled and degassed. $LiAlH_4$ (abcr, 95 %), $MgSO_4$ (dried, 99 %, Grüssing) and *n*-Butyllithium (Acros, 2.5 mol/L in hexanes) were used without further purification. Mes*H and Mes*Br were prepared according to literature procedures.[2,3] $Ag[Al(OR^F)_4]$ (R^F = $CH(CF_3)_2$) was prepared analogously to $Ag[Al(OC(CF_3)_3)_4]$.[4]

NMR spectra were obtained on a Bruker AVANCE 250, 300 or 500 MHz spectrometer and were referenced internally to the deuterated solvent (^{13}C: CD_2Cl_2 δ_{ref} = 54.0 ppm), to protic impurities in the deuterated solvent (^{1}H: $CHDCl_2$ δ_{ref} = 5.31 ppm) or externally (^{31}P: 85% H_3PO_4 δ_{ref} = 0 ppm; ^{19}F: $CFCl_3$ δ_{ref} = 0 ppm). All measurements were carried at room temperature unless denoted otherwise. For NMR spectra simulation, the calculated and experimental ^{31}P NMR spectra were transferred to gNMR.[5] The full lineshape iteration procedure of gNMR was applied to match the calculated to the experimental spectrum. The signs of $^{n}J(^{31}P,^{31}P)$ coupling constants were derived from the calculated spectra (see Computational Details, p. 20).

IR spectra of crystalline samples were recorded on a Nicolet 380 FT-IR spectrometer with a Smart Orbit ATR unit at ambient temperature.

Raman spectra of crystalline samples were recorded using a LabRAM HR 800 Horiba Jobin YVON Raman spectrometer equipped with an Olympus BX41 microscope with variable lenses. The samples were excited by an infrared laser (785 nm, 100 mW) or a red laser (633 nm, 17 mW). All measurements were carried out at ambient temperature unless stated otherwise.

Elemental analyses were obtained using a Thermoquest Flash EA 1112 CHNS analyzer.

Melting points (uncorrected) were determined using a Stanford Research Systems EZ Melt at a heating rate of 20 °C/min.

Mass spectra were recorded on a Finnigan MAT 95-XP (Thermo Electron) using crystalline samples.

2 Structure Elucidation

X-Ray Structure Determination: X-Ray quality crystals were selected in Fomblin Y LVAC 06/6 perfluoroether (Aldrich) at 220 K. The samples were cooled to 173(2) K during measurement. The data were collected on a Bruker Apex Kappa II CCD diffractometer using graphite monochromated Mo K_α radiation (λ = 0.71073 Å). The structures were solved by direct methods (SHELXS-2013)[6] and refined by full matrix least squares procedures (SHELXL-2013).[7] Semi-empirical absorption corrections were applied (SADABS).[8] All non-hydrogen atoms were refined anisotropically, hydrogen atoms were included in the refinement at calculated positions using a riding model.

Disordered groups or molecules were split into two or more parts. The occupancy of each part was refined freely; the geometries of corresponding parts were restrained to be similar within a standard deviation of 0.01 for 1,2-distances or 0.02 for 1,3-distances, respectively. In **3**$[Al(OR^F)_4]_2 \cdot 6.8\ CH_2Cl_2$, the central P_4Cl_2 scaffold of the cation was found to be disordered with respect to the Cl positions and was split in

two parts (0.956/0.044). The ADP's of corresponding atoms in A and B part were equalized. Both *p*-*t*-Bu groups were split in two parts each (0.641/0.359 and 0.774/0.226). The ADP's of the respective atoms were restrained to be similar by application of a rigid bond model (SIMU/DELU). All four $OCH(CF_3)_2$ groups of the anion were found to be disordered and were split in two parts each. Again, the ADP's were restrained by a rigid bond model. Additionally, the ADP's of corresponding oxygen and α-carbon atoms in A and B part were made equal. The solvent CH_2Cl_2 molecules were split in two, three or four parts, respectively. A rigid bond model was assumed. The molecules on the fourfold disordered position were refined with fixed 1,2- and 1,3-distances. Further refinement details can be found in the CIF file.

Table S1: Crystallographic details of **3**$[Al(OR^F)_4]_2$·6.8 CH_2Cl_2.

Compound	**3[Al(OR^F)$_4$]$_2$**·6.8 CH_2Cl_2
Chem. formula	$[C_{72}H_{116}P_8Cl_4Ag_2]$ $[C_{12}H_4O_4F_{24}Al]_2$·6.8 CH_2Cl_2
Formula weight [g/mol]	3554.52
Colour	colourless
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	13.6865(7)
b [Å]	20.7791(12)
c [Å]	27.4127(14)
α [°]	90
β [°]	102.717(3)
γ [°]	90
V [Å^3]	7604.7(7)
Z	2
$\rho_{calc.}$ [g/cm^3]	1.552
μ [mm^{-1}]	0.774
T [K]	173(2)
Measured reflections	82352
Independent reflections	14940
Reflections with $I > 2\sigma(I)$	9819
R_{int}	0.0683
F(000)	3579
$R_1(R[F^2>2\sigma(F^2)])$	0.0557
w$R_2(F^2)$	0.1461
GooF	1.100
No. of Parameters	1422
CCDC #	1417701

Scheme S1. Numbering scheme of $3[Al(OR^F)_4]_2 \cdot 6.8\ CH_2Cl_2$.

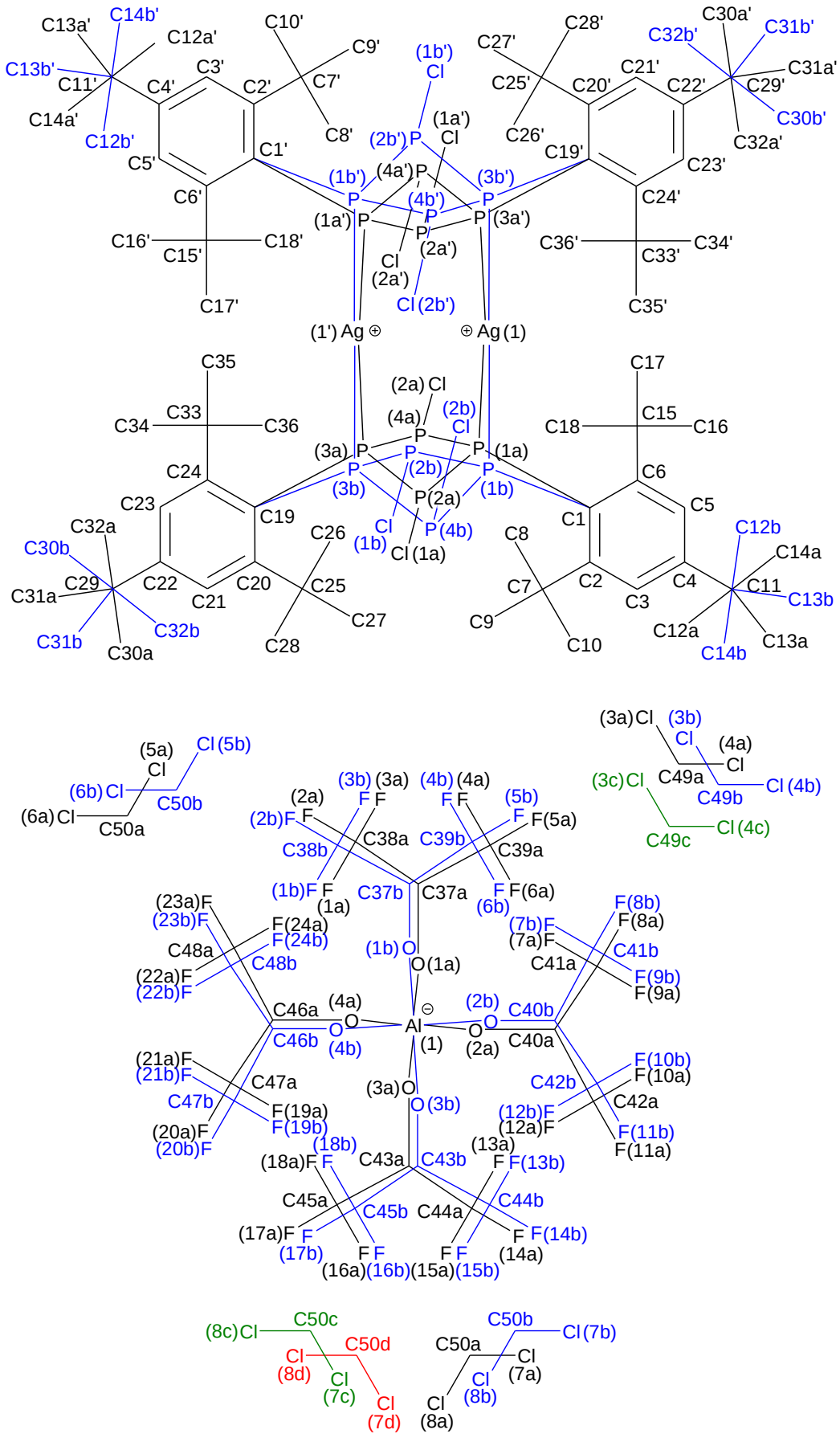


Table S2: Selected bond lengths (Å), angles (°) and dihedral angles (°) of $3[Al(OR^F)_4]_2 \cdot 6.8\ CH_2Cl_2$.

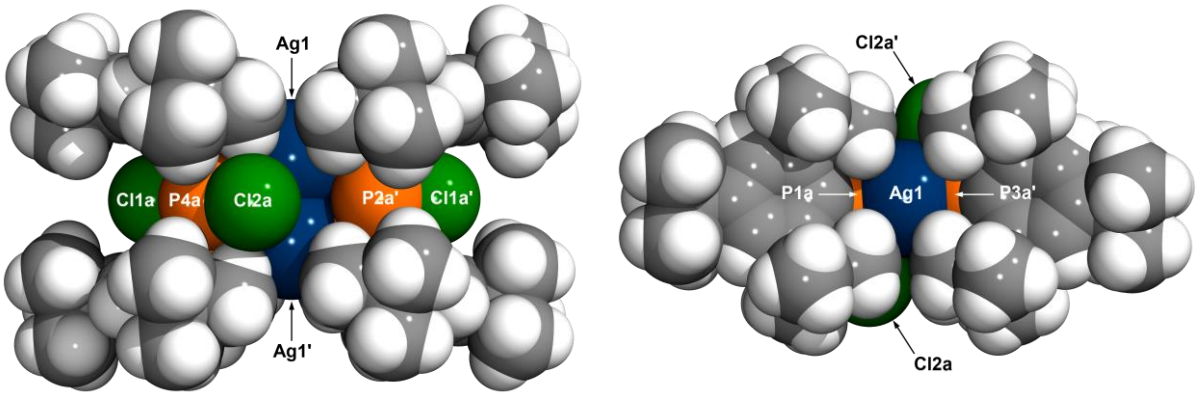
P1A–C1	1.826(5)	P1B–C1	1.89(3)
P1A–Ag1	2.394(2)	P1B–Ag1	2.46(3)
P1A–P2A	2.235(2)	P1B–P2B	2.24(1)
P1A–P4A	2.242(2)	P1B–P4B	2.24(1)
P2A–Cl1A	2.059(2)	P2B–Cl1B	2.06(1)
P2A–P3A	2.232(2)	P2B–P3B	2.23(1)
P3A–C19	1.830(5)	P3B–C19	1.76(4)
P3A–Ag1^{i}	2.391(2)	P3B–Ag1^{i}	2.39(4)
P3A–P4A	2.252(2)	P3B–P4B	2.26(1)
P4A–Cl2A	2.069(2)	P4B–Cl2B	2.06(1)
Ag1–Ag1^{i}	3.0511(7)	Al1–O1A	1.70(1)
C1–P1A–P2A	100.7(2)	C1–P1B–P2B	101(1)
C1–P1A–P4A	111.0(2)	C1–P1B–P4B	116(2)
C1–P1A–Ag1	132.1(2)	C1–P1B–Ag1	125(1)
P2A–P1A–P4A	84.39(6)	P2B–P1B–P4B	84.5(6)
P2A–P1A–Ag1	109.95(7)	P2B–P1B–Ag1	110(1)
P4A–P1A–Ag1	107.96(7)	P4B–P1B–Ag1	111(1)
Cl1A–P2A–P1A	99.39(8)	Cl1B–P2B–P1B	99.0(9)
Cl1A–P2A–P3A	99.47(8)	Cl1B–P2B–P3B	99.1(9)
P3A–P2A–P1A	83.17(6)	P3B–P2B–P1B	82.9(7)
C19–P3A–P2A	103.9(2)	C19–P3B–P2B	98(1)
C19–P3A–P4A	109.6(2)	C19–P3B–P4B	111(2)
C19–P3A–Ag1^{i}	127.4(2)	C19–P3B–Ag1^{i}	131(1)
P2A–P3A–Ag1^{i}	111.58(7)	P2B–P3B–Ag1^{i}	113(2)
P4A–P3A–Ag1^{i}	111.43(8)	P4B–P3B–Ag1^{i}	109(1)
P2A–P3A–P4A	84.23(6)	P2B–P3B–P4B	84.3(6)
Cl2A–P4A–P1A	99.83(7)	Cl2B–P4B–P1B	99.8(9)
Cl2A–P4A–P3A	101.00(8)	Cl2B–P4B–P3B	100.9(9)
P1A–P4A–P3A	82.56(6)	P1B–P4B–P3B	82.2(7)
P3A^{i}–Ag1–P1A	177.52(5)	P3B^{i}–Ag1–P1B	175.7(8)
P1A–Ag1–Ag1^{i}	90.68(4)	P1B–Ag1–Ag1^{i}	87.8(6)
P3A^{i}–Ag1–Ag1^{i}	87.24(4)	P3B^{i}–Ag1–Ag1^{i}	89.9(7)

Table S2 continued.

C2–C1–P1A	119.1(3)	C20–C19–P3A	119.1(3)
C6–C1–P1A	118.7(3)	C24–C19–P3A	118.7(3)
C2–C1–P1B	129.5(9)	C20–C19–P3B	111(1)
C6–C1–P1B	106.9(9)	C24–C19–P3B	128(1)
C6–C1–C2	119.5(4)	C24–C19–C20	119.3(4)
C3–C2–C1	117.1(4)	C21–C20–C19	116.9(4)
C1–C2–C7	124.9(4)	C19–C20–C25	125.8(4)
C5–C6–C1	116.7(4)	C23–C24–C19	117.4(4)
C1–C6–C15	126.6(4)	C19–C24–C33	125.4(4)
O4A–Al1–O1A	109(1)	O1A–Al1–O2A	103.1(9)
O4A–Al1–O2A	115(2)	O1A–Al1–O3A	115.8(7)
O4A–Al1–O3A	107(1)	O3A–Al1–O2A	107(1)
C37A–O1A–Al1	132.2(9)	C43A–O3A–Al1	128(2)
C40A–O2A–Al1	139(3)	C46A–O4A–Al1	138(2)
P1A–P2A–P4A–P3A	−126.41(9)	P2A–P1A–P3A–P4A	−127.06(9)
Ag1–P1A–C1–C2	−108.9(3)	Ag1–P1B–C1–C2	−93(1)
Ag1–P1A–C1–C6	89.6(4)	Ag1–P1B–C1–C6	111(1)
P1A–C1–C2–C3	−141.6(4)	P1B–C1–C2–C3	−134(1)
P1A–C1–C2–C7	46.9(6)	P1B–C1–C2–C7	54(1)
P1A–C1–C6–C5	143.2(4)	P1B–C1–C6–C5	141.1(8)
P1A–C1–C6–C15	−44.6(6)	P1B–C1–C6–C15	−46.6(9)
$Ag1^{i}$–P3A–C19–C20	−96.5(4)	$Ag1^{i}$–P3B–C19–C20	−111(2)
$Ag1^{i}$–P3A–C19–C24	102.9(4)	$Ag1^{i}$–P3B–C19–C24	86(2)
P3A–C19–C20–C21	−142.9(4)	P3B–C19–C20–C21	−147.1(9)
P3A–C19–C20–C25	44.4(6)	P3B–C19–C20–C25	40(1)
P3A–C19–C24–C23	142.2(4)	P3B–C19–C24–C23	144(1)
P3A–C19–C24–C33	−45.1(6)	P3B–C19–C24–C33	−44(1)

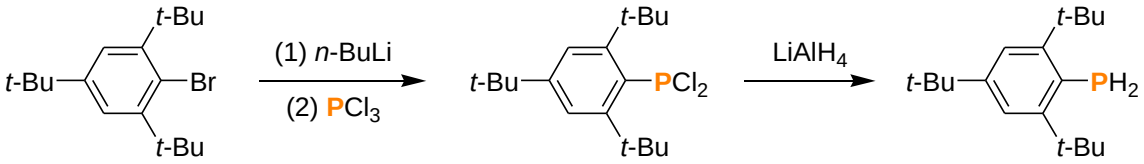
Symmetry code: (i) $-x+1, -y+1, -z+1$.

Figure S1. Space-filling representations of $\mathbf{3}^{+}$ (left: side view; right: top view).



3 Syntheses of Starting Materials

3.1 2,4,6-Tri-*tert*-butylphenylphosphane

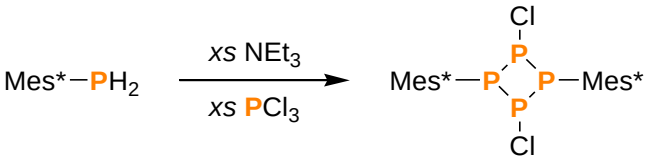


Mes^*PH_2 is prepared according to a modified literature procedure.[3] A solution of *n*-butyllithium (2.5 M in hexanes, 48 mL, 120 mmol) is added dropwise to a stirred solution of Mes*Br (32.6 g, 100 mmol) in THF (400 mL) at −80 °C over a period of 15 minutes. After stirring at −80 °C for one hour, PCl_3 (27.5 g, 200 mmol) is added over a period of two minutes, whereupon the solution turns yellow. The reaction vessel is warmed to ambient temperature over a period of one hour and heated to a brief reflux afterwards (ca. 10 min), resulting in the precipitation of a white solid. After cooling to ambient temperature, the solvent and excess PCl_3 are removed *in vacuo*. The resulting solid is extracted with Et_2O (400 mL); the insoluble residue is separated by filtration. The filtrate is added to $LiAlH_4$ (4.56 g, 120 mmol) at −80 °C and stirred overnight at ambient temperature. After cooling to −20 °C, excess hydrides are destroyed by *slowly* adding aqueous HCl (1 mol/L, 100 mL). Caution: Vigorous H_2 gas evolution is possible! *n*-Pentane (100 mL) is added, the slightly yellow organic layer is separated and subsequently washed with distilled water. The organic phase is dried over $MgSO_4$. After separating the inorganic solids by filtration, the solvents are evaporated. The crude product is recrystallized from boiling ethanol, yielding colourless needles of Mes^*PH_2, which are washed with cold ethanol and subsequently dried *in vacuo*. Yield: 19.29 g (69 mmol, 69 %).

Mp. 175 °C. CHN calc. (found) in %: C 77.65 (77.71), H 11.22 (11.07). $^{31}P\{^1H\}$-NMR (CD_2Cl_2, 121.5 MHz): δ = −130.9 (s). ^1H-NMR (CD_2Cl_2, 300.1 MHz): δ = 1.29 (s, 9 H,

p-*t*-Bu), 1.55 (s, 18 H, *o*-*t*-Bu), 4.20 (d, $^{1}J(^{1}H,^{31}P)$ = 210 Hz, 2 H, P*H*$_2$), 7.41 (d, $^{4}J(^{1}H,^{31}P)$ = 2.5 Hz, 2 H, *m*-H). $^{13}C\{^{1}H\}$-NMR (CD_2Cl_2, 75.5 MHz): δ = 31.6 (s, *p*-C(CH_3)$_3$), 32.8 (d, $^{4}J(^{13}C,^{31}P)$ = 7.2 Hz, *o*-C(CH_3)$_3$), 35.3 (s, *p*-*C*(CH_3)$_3$), 38.4 (s, *o*-*C*(CH_3)$_3$), 122.6 (d, $^{3}J(^{13}C,^{31}P)$ = 2.8 Hz, *m*-C), 149.6 (s, *p*-C), 154.7 (d, $^{2}J(^{13}C,^{31}P)$ = 7.2 Hz, *o*-C), *ipso*-C not observed. IR (ATR, 32 scans, cm^{-1}): $\tilde{\nu}$ = 3102 (w), 2958 (s), 2904 (m), 2868 (m), 2743 (w), 2711 (w), 2350 (w), 2283 (w), 1765 (w), 1597 (m), 1547 (w), 1533 (w), 1473 (m), 1461 (m), 1410 (m), 1394 (m), 1361 (s), 1283 (w), 1238 (m), 1213 (m), 1189 (m), 1128 (w), 1106 (m), 1027 (w), 924 (w), 746 (w), 731 (m), 715 (w), 646 (w), 614 (w), 596 (w), 584 (w), 549 (w). Raman (785 nm, 4 scans, 40 s, cm^{-1}): $\tilde{\nu}$ = 3110 (1), 2965 (8), 2926 (7), 2904 (8), 2878 (4), 2780 (1), 2708 (1), 2408 (2), 2351 (2), 2285 (3), 1600 (8), 1462 (6), 1449 (7), 1396 (4), 1363 (4), 1285 (5), 1243 (5), 1204 (6), 1193 (6), 1178 (4), 1163 (4), 1130 (6), 1110 (3), 1048 (6), 1028 (3), 925 (8), 907 (3), 889 (2), 821 (10), 774 (2), 746 (3), 732 (5), 639 (2), 597 (2), 569 (10), 491 (3), 410 (5), 335 (4), 313 (4), 271 (10), 248 (8).

3.2 Synthesis of [ClP(μ-PMes*)]$_2$ (1)



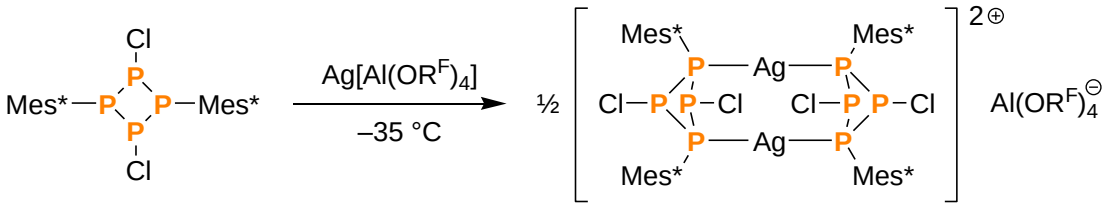
PCl_3 (7.7 g, 56 mmol) is added to a solution of Mes*PH_2 (7.9 g, 28.4 mmol) and NEt_3 (14.2 g, 140 mmol) in Et_2O (150 mL) at −80 °C. The reaction mixture is warmed to ambient temperature and stirred for 18 hours. Afterwards, all volatile components are removed *in vacuo*. The solid residue is thoroughly dried *in vacuo* at 50 °C for at least one hour and is then extracted with *n*-pentane. The suspension is filtered over a glass sinter frit yielding a clear, dark red filtrate. This extraction procedure is repeated two or three times by back-condensation of the solvent. Subsequently, the solvent is evaporated and the solid residue is solved in CH_2Cl_2. The solution is kept at 5 °C overnight, whereupon it turns yellow. Again, the solvent is removed *in vacuo*. The solid residue is crystallized from PhF at ambient temperature, yielding block-shaped,

slightly yellowish crystals. The supernatant is separated using a syringe and concentrated, yielding another crop of product. To remove adhering impurities, the product is re-crystallized from PhF (15 mL) and dried *in vacuo*, resulting in pure [ClP(μ-PMes*)]$_2$ (**1**). Total yield: 4.42 g (6.4 mmol, 45 %).

Mp. 154 °C. CHN calc. (found) in %: C 63.06 (64.06), H 8.53 (8.28). $^{31}P\{^1H\}$ NMR (CD_2Cl_2, 121.5 MHz): δ = −8.1 (t, $^1J(^{31}P,^{31}P)$ = 218 Hz, 2 P, *P*Mes*), 131.3 (t, $^1J(^{31}P,^{31}P)$ = 218 Hz, 2 P, *P*Cl). ^1H NMR (CD_2Cl_2, 300.1 MHz): δ = 1.29 (s, 18 H, *p*-*t*-Bu), 1.40 (s, 36 H, *o*-*t*-Bu), 7.28 (m, 4 H, *m*-H). $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 75.5 MHz): δ = 31.5 (s, *p*-C(CH_3)$_3$), 34.1 (m, *o*-C(CH_3)$_3$), 35.2 (s, *p*-*C*(CH_3)$_3$) 39.6 (s, *o*-*C*(CH_3)$_3$), 123.9 (s, *m*-C), 151.2 (s, *p*-C), 157.8 (m, *o*-C), 163.5 (d, $^1J(^{13}C,^{31}P)$ = 245 Hz, *i*-C). IR (ATR, 32 scans, cm^{-1}): $\tilde{\nu}$ = 2954 (s), 2902 (m), 2864 (m), 2743 (w), 2713 (w), 1592 (m), 1581 (m), 1521 (w), 1493 (m), 1474 (s), 1461 (s), 1441 (m), 1391 (s), 1361 (s), 1278 (w), 1235 (m), 1212 (s), 1178 (m), 1152 (m), 1122 (m), 1064 (m), 1020 (m), 947 (w), 932 (w), 920 (m), 893 (m), 875 (s), 830 (w), 804 (m), 753 (s), 740 (s), 714 (w), 684 (m), 650 (m), 646 (m), 637 (m), 597 (m), 581 (m), 574 (m), 546 (w), 539 (w). Raman (633 nm, 30 s, 4 scans, cm^{-1}): $\tilde{\nu}$ = 3086 (1), 3067 (2), 2969 (4), 2962 (4), 2922 (4), 2902 (5), 2864 (2), 2781 (1), 2709 (1), 1590 (5), 1579 (3), 1458 (2), 1444 (2), 1384 (2), 1359 (1), 1281 (4), 1239 (2), 1204 (3), 1172 (4), 1151 (2), 1122 (5), 1008 (10), 931 (2), 920 (3), 891 (1), 876 (1), 819 (6), 803 (3), 772 (1), 748 (2), 642 (1), 596 (3), 580 (3), 564 (6), 516 (3), 488 (4), 461 (6), 445 (8), 435 (8), 400 (4), 385 (2), 360 (1), 322 (2), 298 (2), 254 (4), 232 (4), 172 (3), 163 (4). MS (CI positive, *iso*-butane, m/z): 685 $[M+H]^+$, 649 $[M-Cl]^+$, 627 $[M-t\text{-}Bu]^+$, 557 $[M-t\text{-}Bu-Cl_2]^+$, 343 $[MesPPCl+H]^+$.

4 Syntheses of Compounds

4.1 Synthesis of {[ClP(μ-PMes*)]$_2$Ag}$_2$[Al(OCH(CF$_3$)$_2$)$_4$]$_2$ (3[Al(OR^F)$_4$]$_2$)



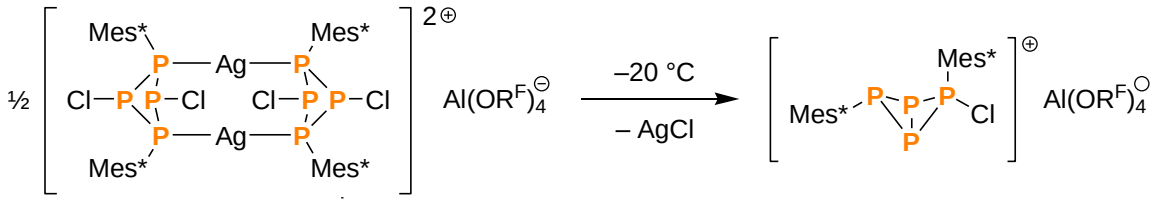
CH_2Cl_2 (4 mL) is added to a mixture of [ClP(μ-PMes*)]$_2$ (**1**, 171 mg, 0.25 mmol) and Ag[Al(OCH(CF$_3$)$_2$)$_4$] (201 mg, 0.25 mmol) at −80 °C. The mixture is stirred and warmed to −35 °C over a period of 1.5 hours, whereupon all solids slowly dissolve until a clear yellow solution is obtained. The solution is concentrated and slowly cooled to −80 °C, yielding colourless crystals of {[ClP(μ-PMes*)]$_2$Ag}$_2$[Al(OCH(CF$_3$)$_2$)$_4$]$_2$·6.8 CH_2Cl_2 (**3**[Al(OR^F)$_4$]$_2$·6.8 CH_2Cl_2). Upon drying in vacuo at −50 °C, *ca.* 6 molecules of CH_2Cl_2 are removed. Yield: 106 mg (0.035 mmol, 28 %).

CHN calc. (found) in % (dried substance): C 38.05 (37.58), H 4.15 (4.01). $^{31}P\{^1H\}$ NMR (CD_2Cl_2, 121.5 MHz, 213 K): δ = 16.8 (m, $^1J(^{31}P,^{31}P)$ = −248 Hz, $^1J(^{31}P,^{31}P)$ = −215 Hz, $^1J(^{31}P,^{107}Ag)$ = −468 Hz, $^3J(^{31}P,^{107}Ag)$ ≈ +6 Hz, 4 P, *P*Ag), 122.1 (m, $^1J(^{31}P,^{31}P)$ = −248 Hz, $^2J(^{31}P,^{31}P)$ ≈ −12 Hz, $^2J(^{31}P,^{107}Ag)$ ≈ −3 Hz, 2 P, *P*Cl$_{eq.}$), 126.9 (m, $^1J(^{31}P,^{31}P)$ = −215 Hz, $^2J(^{31}P,^{31}P)$ ≈ −12 Hz, $^2J(^{31}P,^{107}Ag)$ ≈ −45 Hz, 2 P, *P*Cl$_{ax.}$). For further details, see Table S3. ^1H NMR (CD_2Cl_2, 300.1 MHz, 213 K): δ = 1.17 (s, 36 H, *p*-*t*-Bu), 1.47 (s, 36 H, *o*-*t*-Bu), 1.50 (s, 36 H, *o*-*t*-Bu), 4.44 (sept, $^3J(^1H,^{19}F)$ = 5.8 Hz, 8 H, C*H*(CF$_3$)$_2$), 5.32 (s, 2 H, C*H*$_2$Cl$_2$), 7.37 (s, broad, 8 H, *m*-H). $^{19}F\{^1H\}$ NMR (CD_2Cl_2, 282.4 MHz, 213 K): δ = −77.2 (s, C*F*$_3$). Raman (633 nm, 40 s, 6 scans, 193 K, cm^{-1}): $\tilde{\nu}$ = 3072 (1), 3062 (1), 2972 (4), 2933 (3), 2911 (4), 2873 (2), 2788 (1), 2716 (1), 1582 (9), 1531 (1), 1464 (2), 1441 (2), 1385 (2), 1364 (1), 1309 (1), 1284 (3), 1258 (1), 1241 (2), 1204 (2), 1185 (2), 1174 (2), 1130 (10), 1102 (1), 1018 (8), 1007 (7), 935 (2), 927 (2), 894 (1), 882 (2), 856

(3), 840 (1), 818 (6), 808 (5), 773 (1), 761 (3), 746 (4), 739 (9), 705 (5), 685 (1), 650 (1), 637 (1), 603 (3), 563 (8), 534 (2), 514 (2), 493 (5), 464 (4), 450 (2), 428 (4), 393 (5), 358 (3), 330 (3), 306 (3), 285 (4), 261 (3), 236 (2), 212 (1), 185 (2), 182 (2), 162 (4), 137 (4), 102 (8).

The crystallization method described above yielded crystals suitable for single crystal X-ray diffraction analysis.

4.2 Decomposition of 3[Al(OR^F)$_4$]$_2$

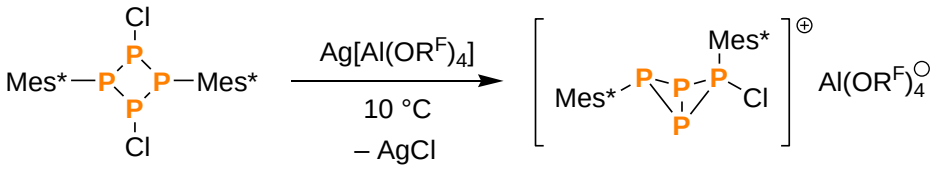


3[Al(OR^F)$_4$]$_2$ (20 mg) is dissolved in CD_2Cl_2 (0.5 mL) at −60 °C in an NMR tube. The sample is slowly warmed to +25 °C, which results in precipitation of AgCl and formation of the bicyclic cation [Mes*P$_4$(Cl)Mes*]$^+$ (**4**). The reaction is observed by NMR spectroscopy.

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 121.5 MHz): δ = −225.1 (dd, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^1J(^{31}P,^{31}P)$ = −187 Hz, 2 P, *endo-exo*-**4**$^+$, bridgehead-P), −214.6 (dd, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^1J(^{31}P,^{31}P)$ = −198 Hz, 1 P, *exo-exo*-**4**$^+$, bridgehead-P), −123.4 (td, $^1J(^{31}P,^{31}P)$ = −187 Hz, $^2J(^{31}P,^{31}P)$ = +99 Hz, 1 P, *endo-exo*-**4**$^+$, PMes*), −89.5 (td, $^1J(^{31}P,^{31}P)$ = −198 Hz, $^2J(^{31}P,^{31}P)$ = +135 Hz, 1 P, *exo-exo*-**4**$^+$, PMes*), +9.0 (td, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^2J(^{31}P,^{31}P)$ = +99 Hz, 1 P, *endo-exo*-**4**$^+$, P(Cl)Mes*), +51.2 (td, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^2J(^{31}P,^{31}P)$ = +135 Hz, 1 P, *exo-exo*-**4**$^+$, P(Cl)Mes*). ^1H NMR (CD_2Cl_2, 300.1 MHz): δ = 1.20 (s, 9 H, *p-t*-Bu, *exo-exo*-**4**$^+$), 1.22 (s, 9 H, *p-t*-Bu, *endo-exo*-**4**$^+$), 1.29 (s, 9 H, *p-t*-Bu, *exo-exo*-**4**$^+$), 1.36 (s, 9 H, *p-t*-Bu, *endo-exo*-**4**$^+$), 1.50 (s, 18 H, *o-t*-Bu, *endo-exo*-**4**$^+$), 1.68 (s, 18 H, *o-t*-Bu, *exo-exo*-**4**$^+$), 1.69 (s, 18 H, *o-t*-Bu, *exo-exo*-**4**$^+$), 1.72 (s, 18 H, *o-t*-Bu, *endo-exo*-**4**$^+$), 4.44 (sept, $^3J(^1H,^{19}F)$ = 5.8 Hz, C*H*(CF$_3$)$_2$), 7.24 (d $^4J(^1H,^{31}P)$ = 2 Hz, 2 H, *m*-H, *endo-*

exo-**4**$^+$), 7.28 (d $^4J(^1H,^{31}P)$ = 2 Hz, 2 H, *m*-H, *exo-exo*-**4**$^+$), 7.56 (d $^4J(^1H,^{31}P)$ = 9 Hz, 2 H, *m*-H, *exo-exo*-**4**$^+$), 7.58 (d $^4J(^1H,^{31}P)$ = 9 Hz, 2 H, *m*-H, *endo-exo*-**4**$^+$).

4.3 Synthesis of [Mes*P$_4$(Cl)Mes*][Al(OR$_F$)$_4$] (4[Al(OR$_F$)$_4$])



A mixture of [ClP(μ-PMes*)]$_2$ (**1**, 171 mg, 0.25 mmol) and Ag[Al(OCH(CF$_3$)$_2$)$_4$] (201 mg, 0.25 mmol) is solved in CH_2Cl_2 (5 mL) at −60 °C and slowly warmed to 10 °C over a period of five hours. The mixture in then re-cooled to −30 °C and the colourless precipitate is filtered off at that temperature, yielding a clear solution of *exo-exo*- and *endo-exo*-[Mes*P$_4$(Cl)Mes*][Al(OR^F)$_4$] (**4**[Al(OR^F)$_4$]) in a 1:5 ratio.

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 202.5 MHz, 300 K): δ = −224.9 (dd, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^1J(^{31}P,^{31}P)$ = −192 Hz, 2 P, *endo-exo*-**4**$^+$, bridgehead-P), −214.5 (dd, $^1J(^{31}P,^{31}P)$ = −305 Hz, $^1J(^{31}P,^{31}P)$ = −198 Hz, 1 P, *exo-exo*-**4**$^+$, bridgehead-P), −123.5 (td, $^1J(^{31}P,^{31}P)$ = −192 Hz, $^2J(^{31}P,^{31}P)$ = +101 Hz, 1 P, *endo-exo*-**4**$^+$, PMes*), −89.5 (td, $^1J(^{31}P,^{31}P)$ = −198 Hz, $^2J(^{31}P,^{31}P)$ = +137 Hz, 1 P, *exo-exo*-**4**$^+$, PMes*), +9.1 (td, $^1J(^{31}P,^{31}P)$ = −302 Hz, $^2J(^{31}P,^{31}P)$ = +101 Hz, 1 P, *endo-exo*-**4**$^+$, P(Cl)Mes*), +51.2 (td, $^1J(^{31}P,^{31}P)$ = −305 Hz, $^2J(^{31}P,^{31}P)$ = +137 Hz, 1 P, *exo-exo*-**4**$^+$, P(Cl)Mes*). ^1H NMR (CD_2Cl_2, 500.1 MHz): δ = 1.21 (s, 9 H, *p-t*-Bu, *exo-exo*-**4**$^+$), 1.23 (s, 9 H, *p-t*-Bu, *endo-exo*-**4**$^+$), 1.30 (s, 9 H, *p-t*-Bu, *exo-exo*-**4**$^+$), 1.37 (s, 9 H, *p-t*-Bu, *endo-exo*-**4**$^+$), 1.51 (s, 18 H, *o-t*-Bu, *endo-exo*-**4**$^+$), 1.68 (s, 18 H, *o-t*-Bu, *exo-exo*-**4**$^+$), 1.70 (s, 18 H, *o-t*-Bu, *exo-exo*-**4**$^+$), 1.73 (s, 18 H, *o-t*-Bu, *endo-exo*-**4**$^+$), 4.42 (sept, $^3J(^1H,^{19}F)$ = 6 Hz, C*H*(CF$_3$)$_2$), 7.26 (d $^4J(^1H,^{31}P)$ = 2 Hz, 2 H, *m*-H, *endo-exo*-**4**$^+$), 7.29 (d $^4J(^1H,^{31}P)$ = 2 Hz, 2 H, *m*-H, *exo-exo*-**4**$^+$), 7.57 (d $^4J(^1H,^{31}P)$ = 9 Hz, 2 H, *m*-H, *exo-exo*-**4**$^+$), 7.59 (d $^4J(^1H,^{31}P)$ = 9 Hz, 2 H, *m*-H, *endo-exo*-**4**$^+$).

Unfortunately, all attempts to crystallize and subsequently isolate *exo*-*exo*- or *endo*-*exo*-**4**[Al(OR^F)$_4$] remained futile.

5 Additional spectroscopic data

Figure S2. Experimental (up) and simulated (down) ^{31}P NMR spectrum of isolated **3**[Al(OR^F)$_4$]$_2$·CH$_2$Cl$_2$ at −60 °C. Due to the widespread coupling and general low solubility of **3**[Al(OR^F)$_4$]$_2$, the signal-to-noise ratio is rather poor.

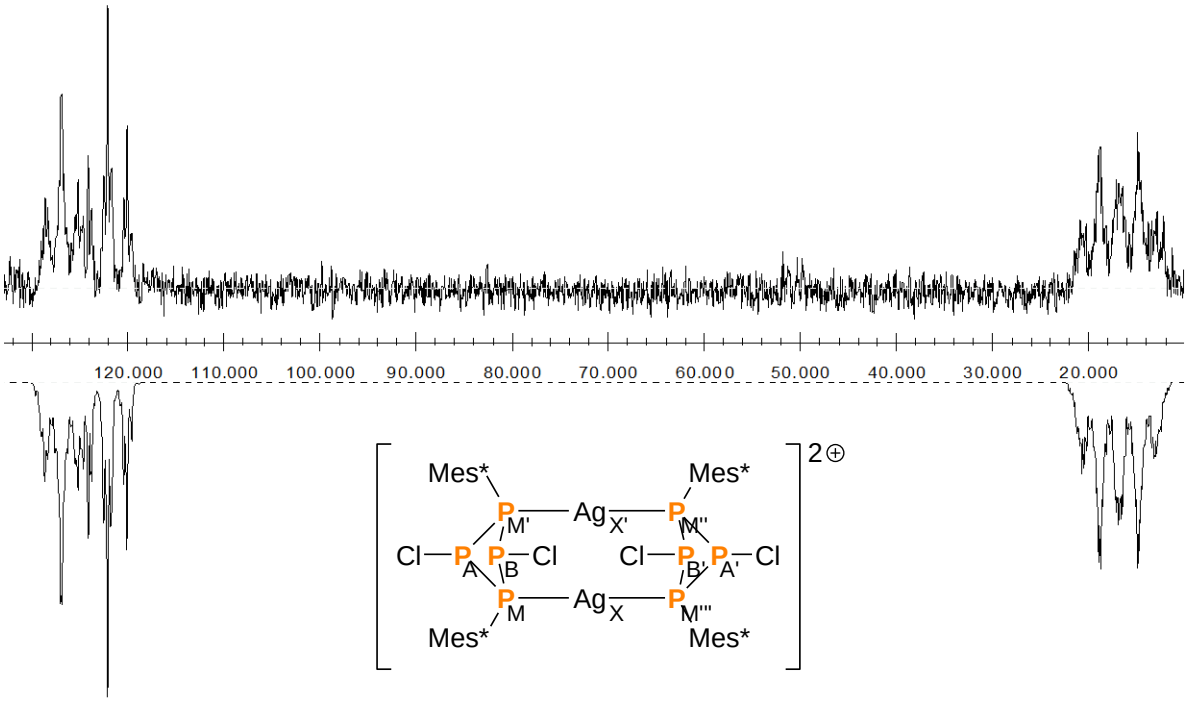


Table S3. ^{31}P NMR data of **3**$^+$ as derived by spectrum simulation. Calculated values (GIAO method) are given in brackets. Values in italics have higher uncertainties due to the low signal to noise ratio.

X	***δ* [ppm]**	***J* [Hz]**			
		P_A	P_B	P_M	P_X
P_A	+126.9 (+138.8)	$J_{AA'}$ = *+1* (+1)			
P_B	+122.1 (+133.4)	J_{AB} = *−12* (−20) $J_{AB'}$ = *+1* (+1)	$J_{BB'}$ = *0* (0)		
P_M	+16.8 (−1.4)	J_{AM} = −215 (−170) $J_{AM'}$ = *+9* (+8)	J_{BM} = −248 (−218) $J_{BM'}$ = *+2* (+2)	$J_{MM'}$ = *+122* (+102) $J_{MM''}$ = *+1* (+1) $J_{MM'''}$ = *+101* (+84)	
Ag_X	–	J_{AX} = *−44* (−33)	J_{BX} = *−3* (−1)	J_{MX} = −468 (−367) $J_{MX'}$ = *+6* (+6)	J_{XX} = *+10* (+10)

Figure S3. Variable temperature *in situ* ^{31}P NMR spectrum of the reaction of **1** and Ag[Al(OR^F)$_4$]. At low temperatures, the formation of two silver complexes is observed, one of which could be isolated and characterized as **3**$^+$. Above −30 °C, the complexes eliminate AgCl, leading to the formation of *exo-exo*- (minor component) and *endo-exo*-**4**$^+$ (major component)

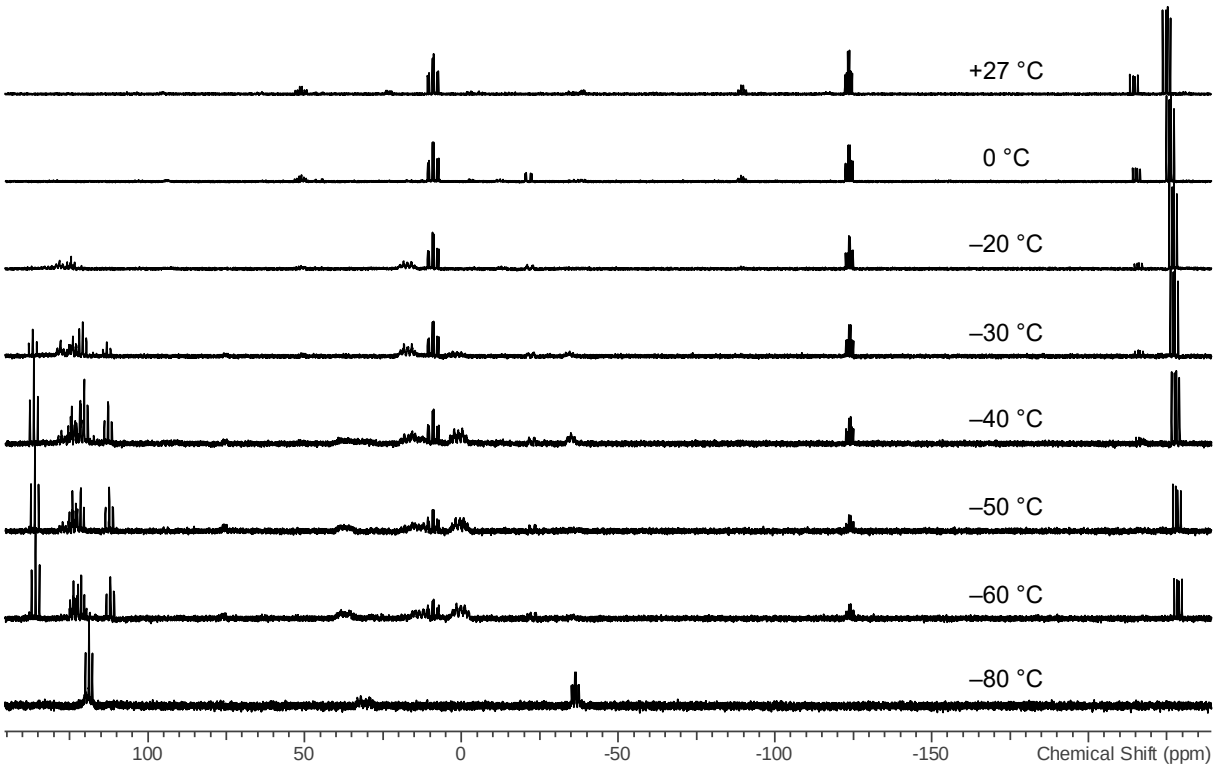


Figure S4. Experimental and calculated Raman spectrum of crystalline **3**[Al(OR^F)$_4$]$_2$·6.8 CH_2Cl_2.

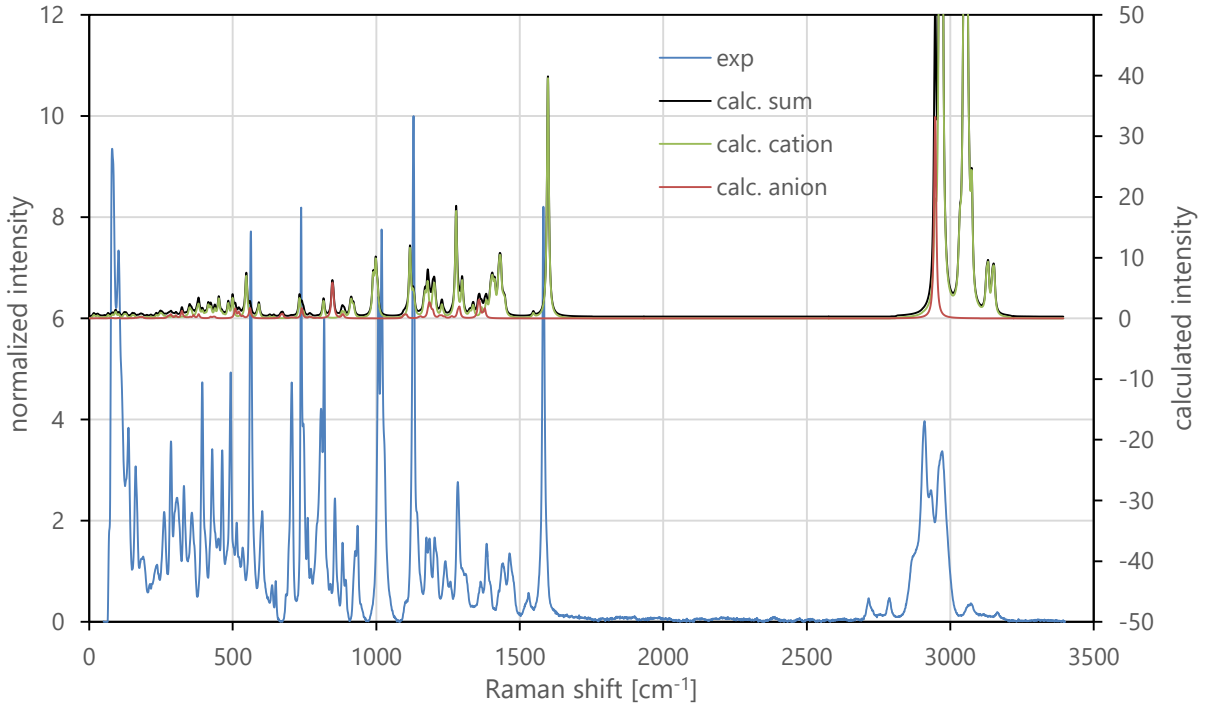
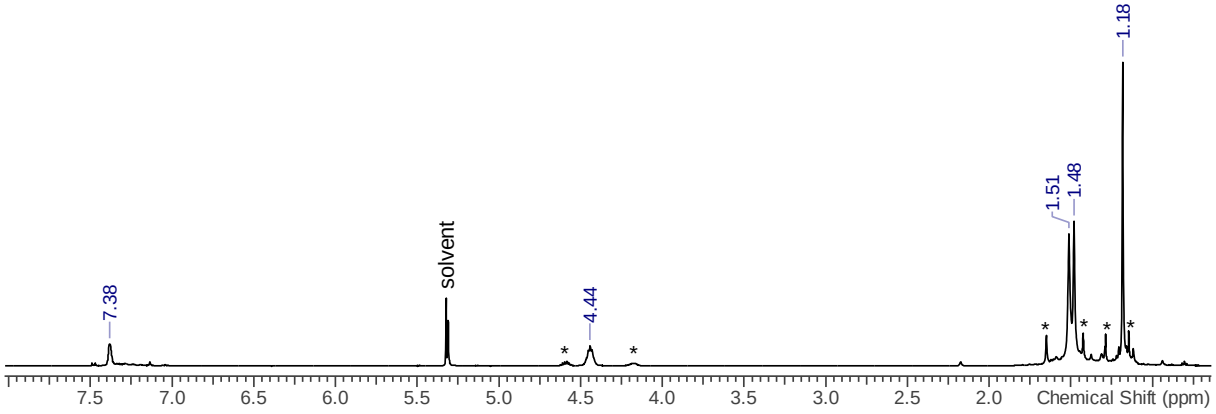


Figure S5. ^{1}H NMR spectrum of isolated **3**$[Al(OR^F)_4]_2 \cdot CH_2Cl_2$ (* = impurities).



6 Computational Details

All computations were carried out using the Gaussian09 program package[9] and the standalone version of NBO 6.0.[10–13] The Kohn-Sham wave function was calculated using the hybrid DFT functional PBE0[14–16], using a cc-pVDZ basis at H, C, F and Al, an aug-cc-pVDZ basis at P and Cl,[17–22] as well as an energy consistent, fully relativistic pseudopotential of the Stuttgart/Cologne group (ECP28MDF)[23] in combination with a suitable aug-cc-pVDZ basis at Ag[24]. P-Ag coupling constants were calculated using a DZP basis at H, C and Cl[25] and an ADZP basis at P[25] and Ag.[26]

All structures were fully optimized and confirmed as minima by frequency analyses. Partial charges were determined by Natural Population analysis using the NBO program. Chemical shifts and coupling constants were derived by the GIAO method.[27–31] The calculated absolute shifts ($\sigma_{calc,X}$) were referenced to the experimental absolute shift of 85 % H_3PO_4 in the gas phase ($\sigma_{ref,1}$ = 328.35 ppm),[32] using PH_3 ($\sigma_{ref,2}$ = 594.45 ppm) as a secondary standard:[33]

$$\begin{aligned} \delta_{calc,X} &= (\sigma_{ref,1} - \sigma_{ref,2}) - (\sigma_{calc,X} - \sigma_{calc,PH_3}) \\ &= \sigma_{calc,PH_3} - \sigma_{calc,X} - 266.1 \text{ ppm} \end{aligned}$$

At the PBE0/aug-cc-pVDZ level of theory, σ_{calc,PH_3} amounts to +633.04 ppm. It should be emphasized that all computations were carried out for single, isolated gas phase molecules. There may well be significant differences between gas phase, solution and solid state data.

6.1 PH_3 (NMR standard)

6.1.1 Optimized structure

Atom	x	y	z
P	0.00000	0.00000	0.13009
H	0.00000	1.20158	-0.65044
H	1.04060	-0.60079	-0.65044
H	-1.04060	-0.60079	-0.65044

6.2 $\{[ClP(\mu\text{-}PMes^*)]_2Ag\}_2^{2+}$ (3^{2+})

6.2.1 Optimized structure

Atom	x	y	z
C	-4.06065	2.27019	-3.85193
C	-4.17850	-2.81922	-3.43146
C	4.18731	2.94444	-3.51501
C	4.00409	-2.56196	-3.89587
C	-3.42871	-5.06144	-2.60717
C	-3.31245	4.59966	-3.31837
C	-8.16586	4.45403	-1.94787
C	3.79971	5.27910	-2.73798
C	-3.34876	3.14111	-2.80635
C	3.63420	-4.96024	-3.33532
C	-3.43627	-3.54624	-2.30085
C	-1.96212	-3.12833	-2.32169
C	-1.88133	2.71160	-2.71681
C	3.56764	3.79069	-2.39537
C	3.43506	-3.51233	-2.83429
C	1.91917	-3.34584	-2.70264
C	2.04703	3.62473	-2.35965
C	-7.68341	-5.94695	-0.35650
C	-5.41399	3.71278	-1.53930
C	-5.44414	-3.91662	-0.87748
C	-4.11804	3.18857	-1.46152
C	8.29402	4.79885	-0.77894
C	-4.15328	-3.39220	-0.93610
C	-7.63061	4.51178	-0.51576
C	-8.43806	-3.55994	-0.56926
C	5.52444	4.01561	-0.85054
C	4.22844	3.51833	-1.02659
C	-7.73117	5.96141	-0.01351
C	-6.18002	4.04176	-0.42406
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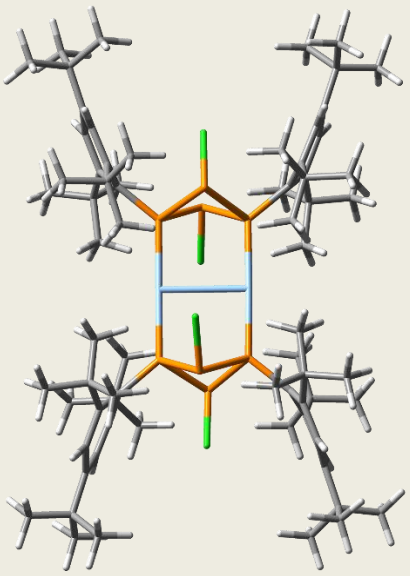
C	-7.61739	-4.54731	0.27644
C	5.46968	-3.88708	-1.42853
C	-8.49741	3.59909	0.36709
C	-6.16498	-4.07448	0.30936
C	7.70843	-5.92126	-0.92418
C	8.45777	-3.52836	-1.07948
C	-3.60129	2.93294	-0.15734



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C	3.59031	2.94404	0.10820
C	8.39478	3.41986	1.29183
C	3.59207	-2.94367	-0.25429
C	-8.23184	-4.61454	1.67609
C	-5.52253	4.01462	0.80874
C	6.17777	-4.06620	-0.23683
C	7.63143	-4.53530	-0.26289
C	-5.45832	-3.87067	1.49219
C	-4.22989	3.52296	0.98063
C	7.63405	5.81179	1.39839
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C	5.38405	3.74185	1.49928
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C	5.45797	-3.88577	0.94157
C	8.23104	-4.62990	1.14156
C	-3.55108	3.82066	2.33595
C	-3.41766	-3.46811	2.88320
C	-2.03069	3.65839	2.28144
C	-3.78292	5.31332	2.65869
C	-1.90246	-3.30058	2.74823
C	-3.61380	-4.90857	3.40716
C	1.96740	-3.07931	2.36215
C	1.84167	2.76026	2.65299
C	3.30651	3.19534	2.75407
C	3.44333	-3.49099	2.35052
C	3.44160	-5.00053	2.68524
C	3.26033	4.66319	3.23717
C	-4.15158	2.99011	3.47743
C	-3.98908	-2.50217	3.92941
C	4.00492	2.34578	3.82588
C	4.18240	-2.74084	3.46812
H	-3.52367	2.32213	-4.81163
H	-3.68545	-3.01965	-4.39523
H	3.73719	3.20369	-4.48569
H	-5.09149	2.60396	-4.03496
H	3.49471	-2.71389	-4.85998
H	-2.91097	-5.24297	-3.56189
H	-5.22156	-3.15331	-3.52020
H	-2.76470	4.64340	-4.27270
H	3.25632	5.52677	-3.66284
H	-4.10299	1.21230	-3.55029
H	5.27073	3.11935	-3.59006
H	3.04419	-5.11057	-4.25250
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H	-4.19085	-1.72836	-3.28435
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H	-1.50355	-3.48456	-3.25616
H	-7.62803	5.14033	-2.62010
H	-1.38876	2.92541	-3.67720
H	-8.11042	3.43775	-2.36834
H	4.04486	1.86420	-3.35914
H	-9.22308	4.75634	-1.95784
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H	1.61861	3.94907	-3.31981

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H         -2.80317        5.25819       -2.59790
H         -5.90964       -4.23474       -1.81094
H         -1.81071       -2.03785       -2.31286
H         -1.74533        1.63290       -2.54626
H          3.42991        5.93616       -1.93638
H         -8.72571       -6.30056       -0.37767
H          8.29906        3.91106       -1.43032
H          1.59417       -2.32364       -2.46113
H          3.29658       -5.69231       -2.58624
H          1.71042        2.58630       -2.22904
H         -8.06799       -3.49340       -1.60351
H          6.04371        4.40505       -1.72422
H         -7.09063       -6.67320        0.22054
H          7.81883        5.62950       -1.32322
H         -1.39911       -3.58664       -1.49179
H         -1.33674        3.27812       -1.94376
H          9.34158        5.08488       -0.60545
H          5.94488       -4.18057       -2.36472
H          1.51163       -4.03369       -1.94517
H          1.60130        4.24202       -1.56387
H         -7.10961        6.63736       -0.62063
H         -9.48847       -3.88581       -0.61401
H          7.34771       -5.90552       -1.96355
H          8.10026       -3.44436       -2.11686
H         -8.77336        6.30954       -0.07846
H         -8.45208        2.55401        0.02272
H         -9.54827        3.92425        0.32713
H          8.75217       -6.27078       -0.94273
H         -8.41494       -2.54884       -0.13345
H          8.40649        2.48656        0.70725
H          9.51015       -3.84870       -1.11745
H         -7.41624        6.06093        1.03620
H          9.43754        3.73789        1.44369
H         -9.28791       -4.91174        1.60027
H          7.11275       -6.66149       -0.36825
H          8.42426       -2.52548       -0.62567
H         -8.18320        3.62371        1.42153
H          7.07091        6.61795        0.90361
H         -7.73227       -5.36001        2.31387
H          8.67169        6.15467        1.53006
H         -6.03503        4.42267        1.67992
H         -8.19917       -3.63958        2.18680
H          7.96929        3.19572        2.28175
H         -5.92991       -4.13666        2.43646
H         -1.59766        4.26314        1.46918
H         -1.49351       -4.00303        2.00513
H         -3.42680        5.95884        1.84173
H          9.28855       -4.92323        1.07089
H          7.20723        5.66407        2.40197
H         -3.27648       -5.65169        2.66886
H          1.40774       -3.55569        1.54020
H          1.30492        3.31358        1.86504
H          5.79700        3.93150        2.49041
H          7.72680       -5.38957        1.75868
H         -4.83853        5.55036        2.84443
```

```
H          2.91997       -5.57741        1.90607
H         -1.58028       -2.28301        2.48474
H          8.19041       -3.66565        1.67179
H          2.76119        5.30664        2.49627
H         -1.69407        2.61846        2.16394
H          5.92073       -4.17573        1.88349
H         -4.65841       -5.13074        3.66083
H          1.81063       -1.98996        2.33280
H          1.71086        1.67873        2.49684
H          4.45585       -5.40915        2.78266
H          4.26178        5.07544        3.41765
H         -4.00846        1.90801        3.33611
H         -1.58978        4.00019        3.22981
H         -5.23434        3.16310        3.56563
H         -1.42386       -3.51526        3.71553
H         -3.22777        5.57747        3.57197
H         -3.87352       -1.44607        3.64199
H         -3.02119       -5.04339        4.32505
H         -5.06354       -2.67840        4.08507
H          1.50949       -3.42033        3.30258
H          1.33677        2.98708        3.60394
H          4.05081        1.28197        3.54643
H          4.19010       -1.65264        3.30229
H          2.92264       -5.16546        3.64228
H          5.03343        2.68319        4.01535
H          2.69863        4.72535        4.18237
H          5.22680       -3.06890        3.56278
H         -3.68805        3.26525        4.43741
H         -3.48248       -2.64135        4.89687
H          3.45616        2.41735        4.77764
H          3.68978       -2.92655        4.43506
P         -3.29803       -0.10123       -1.27430
P          3.10362        0.08595       -1.74122
P         -2.41602       -1.50990        0.26997
P         -2.43077        1.51549        0.06186
P          2.42392       -1.50715       -0.25627
P          2.42586        1.52075       -0.10258
P         -3.09405        0.10770        1.72926
P          3.29267       -0.06763        1.26678
Cl         1.43857        0.17007       -3.03742
Cl        -5.28678       -0.05852       -0.61897
Cl         5.28426       -0.02876        0.61970
Cl        -1.42298        0.21836        3.01598
Ag         0.00364       -1.52546        0.00282
Ag        -0.00269        1.52179       -0.02564
```

6.2.2 NBO analysis

```
Summary of Natural Population Analysis:

                                     Natural Population
             Natural    -----------------------------------------------
  Atom No    Charge        Core      Valence    Rydberg      Total
 ------------------------------------------------------------------------
                                      [...]
    P189    0.32150      9.99875     4.60281    0.07694    14.67850
    P190    0.33228      9.99870     4.60040    0.06862    14.66772
    P191    0.17285      9.99841     4.75203    0.07671    14.82715
```

```
    P192    0.17217      9.99841     4.75220    0.07722    14.82783
    P193    0.17270      9.99841     4.75221    0.07668    14.82730
    P194    0.17228      9.99840     4.75200    0.07732    14.82772
    P195    0.33200      9.99870     4.60069    0.06861    14.66800
    P196    0.32144      9.99875     4.60278    0.07703    14.67856
   Cl197   -0.24955      9.99972     7.22630    0.02353    17.24955
   Cl198   -0.22114      9.99971     7.19271    0.02872    17.22114
   Cl199   -0.22117      9.99971     7.19277    0.02869    17.22117
   Cl200   -0.24984      9.99972     7.22658    0.02354    17.24984
   Ag201    0.59061     35.99245    10.38835    0.02858    46.40939
   Ag202    0.59161     35.99241    10.38575    0.03022    46.40839
 ===============================================================
 * Total *  2.00000    335.90442   489.76757    2.32801   828.00000

                                    [...]

Wiberg bond index matrix in the NAO basis:

                                    [...]

     Atom  189     190     191     192     193     194     195     196     197
     ---- ------  ------  ------  ------  ------  ------  ------  ------  ------
 189.  P  0.0000  0.0010  0.9096  0.9070  0.0012  0.0012  0.0459  0.0001  0.0005
 190.  P  0.0010  0.0000  0.0024  0.0024  0.9171  0.9185  0.0007  0.0458  0.8949
 191.  P  0.9096  0.0024  0.0000  0.0374  0.0358  0.0041  0.9170  0.0011  0.0025
 192.  P  0.9070  0.0024  0.0374  0.0000  0.0041  0.0349  0.9190  0.0012  0.0031
 193.  P  0.0012  0.9171  0.0358  0.0041  0.0000  0.0374  0.0024  0.9098  0.0382
 194.  P  0.0012  0.9185  0.0041  0.0349  0.0374  0.0000  0.0024  0.9070  0.0387
 195.  P  0.0459  0.0007  0.9170  0.9190  0.0024  0.0024  0.0000  0.0010  0.0005
 196.  P  0.0001  0.0458  0.0011  0.0012  0.9098  0.9070  0.0010  0.0000  0.0267
 197. Cl  0.0005  0.8949  0.0025  0.0031  0.0382  0.0387  0.0005  0.0267  0.0000
 198. Cl  0.9361  0.0006  0.0486  0.0483  0.0018  0.0019  0.0344  0.0001  0.0002
 199. Cl  0.0001  0.0346  0.0018  0.0019  0.0486  0.0483  0.0006  0.9360  0.0117
 200. Cl  0.0267  0.0005  0.0381  0.0387  0.0025  0.0031  0.8945  0.0006  0.0003
 201. Ag  0.0128  0.0192  0.3137  0.0104  0.3139  0.0105  0.0192  0.0128  0.0114
 202. Ag  0.0124  0.0188  0.0107  0.3119  0.0106  0.3119  0.0188  0.0123  0.0154

     Atom  198     199     200     201     202
     ---- ------  ------  ------  ------  ------
 189.  P  0.9361  0.0001  0.0267  0.0128  0.0124
 190.  P  0.0006  0.0346  0.0005  0.0192  0.0188
 191.  P  0.0486  0.0018  0.0381  0.3137  0.0107
 192.  P  0.0483  0.0019  0.0387  0.0104  0.3119
 193.  P  0.0018  0.0486  0.0025  0.3139  0.0106
 194.  P  0.0019  0.0483  0.0031  0.0105  0.3119
 195.  P  0.0344  0.0006  0.8945  0.0192  0.0188
 196.  P  0.0001  0.9360  0.0006  0.0128  0.0123
 197. Cl  0.0002  0.0117  0.0003  0.0114  0.0154
 198. Cl  0.0000  0.0003  0.0117  0.0105  0.0101
 199. Cl  0.0003  0.0000  0.0002  0.0106  0.0101
 200. Cl  0.0117  0.0002  0.0000  0.0114  0.0153
 201. Ag  0.0105  0.0106  0.0114  0.0000  0.0426
 202. Ag  0.0101  0.0101  0.0153  0.0426  0.0000
```

Wiberg bond index, Totals by atom:

Atom		1
	[...]	
189.	P	3.0409
190.	P	3.0233
191.	P	3.4597
192.	P	3.4568
193.	P	3.4599
194.	P	3.4567
195.	P	3.0233
196.	P	3.0409
197.	Cl	1.1094
198.	Cl	1.1361
199.	Cl	1.1361
200.	Cl	1.1092
201.	Ag	0.8981
202.	Ag	0.8992

[...]

NBI: Natural Binding Index (NCU strength parameters)

[...]

Atom		189	190	191	192	193	194	195	196	197
189.	P	0.0000	0.0312	0.9537	0.9524	0.0340	0.0348	0.2141	0.0111	0.0232
190.	P	0.0312	0.0000	0.0488	0.0487	0.9577	0.9584	0.0259	0.2140	0.9460
191.	P	0.9537	0.0488	0.0000	0.1934	0.1892	0.0639	0.9576	0.0338	0.0500
192.	P	0.9524	0.0487	0.1934	0.0000	0.0637	0.1869	0.9587	0.0346	0.0561
193.	P	0.0340	0.9577	0.1892	0.0637	0.0000	0.1935	0.0487	0.9539	0.1954
194.	P	0.0348	0.9584	0.0639	0.1869	0.1935	0.0000	0.0486	0.9524	0.1968
195.	P	0.2141	0.0259	0.9576	0.9587	0.0487	0.0486	0.0000	0.0310	0.0213
196.	P	0.0111	0.2140	0.0338	0.0346	0.9539	0.9524	0.0310	0.0000	0.1634
197.	Cl	0.0232	0.9460	0.0500	0.0561	0.1954	0.1968	0.0213	0.1634	0.0000
198.	Cl	0.9675	0.0249	0.2205	0.2198	0.0426	0.0438	0.1856	0.0114	0.0155
199.	Cl	0.0114	0.1860	0.0425	0.0437	0.2204	0.2197	0.0247	0.9675	0.1083
200.	Cl	0.1635	0.0213	0.1953	0.1968	0.0501	0.0560	0.9458	0.0237	0.0178
201.	Ag	0.1131	0.1386	0.5601	0.1021	0.5603	0.1024	0.1386	0.1131	0.1068
202.	Ag	0.1112	0.1370	0.1035	0.5585	0.1032	0.5585	0.1370	0.1111	0.1243

Atom		198	199	200	201	202
189.	P	0.9675	0.0114	0.1635	0.1131	0.1112
190.	P	0.0249	0.1860	0.0213	0.1386	0.1370
191.	P	0.2205	0.0425	0.1953	0.5601	0.1035
192.	P	0.2198	0.0437	0.1968	0.1021	0.5585
193.	P	0.0426	0.2204	0.0501	0.5603	0.1032
194.	P	0.0438	0.2197	0.0560	0.1024	0.5585
195.	P	0.1856	0.0247	0.9458	0.1386	0.1370
196.	P	0.0114	0.9675	0.0237	0.1131	0.1111
197.	Cl	0.0155	0.1083	0.0178	0.1068	0.1243
198.	Cl	0.0000	0.0162	0.1080	0.1025	0.1004
199.	Cl	0.0162	0.0000	0.0154	0.1027	0.1003
200.	Cl	0.1080	0.0154	0.0000	0.1068	0.1237
201.	Ag	0.1025	0.1027	0.1068	0.0000	0.2063
202.	Ag	0.1004	0.1003	0.1237	0.2063	0.0000

```
NATURAL BOND ORBITAL ANALYSIS:

    (Occupancy)   Bond orbital / Coefficients / Hybrids
 ------------------ Lewis ---------------------------------------------------------
                                      [...]
 141. (1.96502) LP ( 1) P189           s( 71.05%)p 0.41( 28.83%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.8429  0.0010 -0.0027
                                        0.0000  0.0582  0.0113  0.0009  0.0000
                                        0.0368  0.0013  0.0013  0.0000  0.5321
                                        0.0159  0.0089 -0.0002  0.0003 -0.0044
                                        0.0032 -0.0040  0.0019 -0.0050  0.0054
                                       -0.0297  0.0127
 142. (1.96799) LP ( 1) P190           s( 72.07%)p 0.39( 27.81%)d 0.00(  0.12%)
                                        0.0000  0.0000  0.8490  0.0014 -0.0002
                                        0.0000  0.4665  0.0094  0.0098  0.0000
                                       -0.0081 -0.0001  0.0002  0.0000  0.2454
                                       -0.0017  0.0023  0.0005  0.0001 -0.0178
                                        0.0032  0.0005 -0.0006 -0.0242  0.0135
                                        0.0069 -0.0032
 143. (1.77449) LP ( 1) P191           s( 55.50%)p 0.80( 44.39%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.7448  0.0139 -0.0038
                                        0.0000  0.6646  0.0327  0.0011  0.0000
                                       -0.0019 -0.0109 -0.0025  0.0000  0.0308
                                        0.0057 -0.0003 -0.0028  0.0079  0.0105
                                       -0.0081  0.0001  0.0003  0.0233 -0.0158
                                       -0.0042  0.0065
 144. (1.77714) LP ( 1) P192           s( 55.30%)p 0.81( 44.60%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.7435  0.0143 -0.0039
                                        0.0000  0.6667  0.0334  0.0012  0.0000
                                        0.0003  0.0109  0.0021  0.0000  0.0146
                                        0.0003  0.0002  0.0035 -0.0083  0.0050
                                       -0.0034  0.0013  0.0003  0.0241 -0.0168
                                       -0.0053  0.0071
 145. (1.77428) LP ( 1) P193           s( 55.48%)p 0.80( 44.41%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.7447  0.0139 -0.0038
                                        0.0000 -0.6649 -0.0328 -0.0011  0.0000
                                       -0.0003 -0.0109 -0.0025  0.0000 -0.0281
                                       -0.0055  0.0003  0.0029 -0.0080  0.0103
                                       -0.0079  0.0001 -0.0004  0.0234 -0.0159
                                       -0.0043  0.0066
 146. (1.77730) LP ( 1) P194           s( 55.32%)p 0.81( 44.58%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.7436  0.0142 -0.0039
                                        0.0000 -0.6667 -0.0333 -0.0012  0.0000
                                        0.0022  0.0110  0.0021  0.0000 -0.0093
                                       -0.0004 -0.0003 -0.0035  0.0084  0.0052
                                       -0.0035 -0.0011 -0.0006  0.0241 -0.0167
                                       -0.0053  0.0071
 147. (1.96799) LP ( 1) P195           s( 72.07%)p 0.39( 27.82%)d 0.00(  0.12%)
                                        0.0000  0.0000  0.8489  0.0014 -0.0002
                                        0.0000 -0.4654 -0.0093 -0.0098  0.0000
                                       -0.0109 -0.0001  0.0000  0.0000 -0.2476
                                        0.0017 -0.0023 -0.0007 -0.0001 -0.0180
                                        0.0033 -0.0007  0.0008 -0.0242  0.0135
                                        0.0068 -0.0032
```

```
148. (1.96505) LP ( 1) P196            s( 71.05%)p 0.41( 28.83%)d 0.00(  0.11%)
                                        0.0000  0.0000  0.8429  0.0010 -0.0027
                                        0.0000 -0.0604 -0.0114 -0.0009  0.0000
                                        0.0274  0.0012  0.0011  0.0000 -0.5324
                                       -0.0159 -0.0088  0.0002 -0.0003 -0.0046
                                        0.0033  0.0028 -0.0012 -0.0051  0.0054
                                       -0.0299  0.0127
                                      [...]
161. (1.99853) LP ( 1)Ag201            s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.0002  0.0000  0.0000  0.0000
                                        0.0000  0.0009  0.0005 -0.0003 -0.0001
                                        0.0000  0.0000 -0.0001  0.0000  0.0000
                                        0.0000  0.0009 -0.0022 -0.0001 -0.0003
                                       -0.0890  0.0016 -0.0011  0.0000  0.0033
                                        0.0000  0.0000  0.0000  0.9957  0.0080
                                        0.0098  0.0011 -0.0107 -0.0001 -0.0001
                                        0.0000 -0.0204 -0.0002 -0.0002  0.0000
                                       -0.0004  0.0004 -0.0002  0.0000  0.0000
                                        0.0000 -0.0003  0.0004  0.0000  0.0000
                                        0.0001  0.0000  0.0000  0.0000
162. (1.99782) LP ( 2)Ag201            s(  0.05%)p 0.15(  0.01%)d99.99( 99.94%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.0222 -0.0009 -0.0005 -0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0071 -0.0048 -0.0011  0.0000
                                        0.0000 -0.0001  0.0001  0.0000  0.0000
                                        0.0029  0.0000  0.0000  0.0000  0.1685
                                       -0.0009  0.0006  0.0000 -0.0229 -0.0002
                                       -0.0002  0.0000 -0.3469 -0.0045 -0.0061
                                       -0.0011 -0.9220 -0.0081 -0.0066 -0.0012
                                        0.0000  0.0000  0.0000  0.0000 -0.0005
                                        0.0006  0.0000  0.0000  0.0001 -0.0001
                                        0.0000  0.0000 -0.0008  0.0006
163. (1.98330) LP ( 3)Ag201            s(  2.68%)p 0.01(  0.02%)d36.30( 97.30%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.1637  0.0015  0.0015 -0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0115  0.0053  0.0025  0.0006
                                        0.0000  0.0000 -0.0001  0.0000  0.0000
                                        0.0010  0.0000  0.0000  0.0000  0.3611
                                       -0.0015 -0.0031 -0.0003  0.0029 -0.0001
                                        0.0000  0.0000  0.8799 -0.0025 -0.0100
                                        0.0001 -0.2612 -0.0052  0.0047  0.0006
                                        0.0000  0.0000  0.0000  0.0000  0.0006
                                       -0.0004  0.0000  0.0000  0.0001 -0.0001
                                        0.0000  0.0000  0.0004 -0.0006
```

```
164. (1.97847) LP ( 4)Ag201            s(  0.14%)p 0.01(  0.00%)d99.99( 99.86%)
                                                f 0.00(  0.00%)
                                        0.0000  0.0376 -0.0003  0.0003 -0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0026  0.0006  0.0002 -0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                       -0.0211  0.0002  0.0001  0.0000 -0.9164
                                        0.0092  0.0015  0.0012 -0.0014  0.0000
                                        0.0000  0.0000  0.2875 -0.0017 -0.0027
                                       -0.0001 -0.2748 -0.0010  0.0016  0.0002
                                        0.0000  0.0000  0.0000  0.0000  0.0003
                                       -0.0001  0.0000  0.0000  0.0003  0.0001
                                        0.0000  0.0000  0.0002 -0.0002
165. (1.97718) LP ( 5)Ag201            s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                f 0.00(  0.00%)
                                        0.0000  0.0004  0.0000  0.0000  0.0000
                                        0.0000  0.0012 -0.0005 -0.0005 -0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0006  0.0005  0.0002  0.0000
                                        0.9958 -0.0074 -0.0045 -0.0010 -0.0200
                                        0.0002  0.0001  0.0000  0.0891  0.0010
                                       -0.0006 -0.0001  0.0053  0.0000  0.0000
                                        0.0000 -0.0047  0.0000  0.0000  0.0000
                                        0.0000  0.0001 -0.0002  0.0002  0.0000
                                        0.0000 -0.0001  0.0000  0.0000  0.0000
                                       -0.0007  0.0006  0.0000  0.0000
166. (1.99849) LP ( 1)Ag202            s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                f 0.00(  0.00%)
                                        0.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000 -0.0003 -0.0001  0.0002  0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0009  0.0017  0.0001  0.0002
                                       -0.0215  0.0020 -0.0003  0.0003  0.0017
                                        0.0000  0.0000  0.0000  0.9994  0.0076
                                        0.0102  0.0012 -0.0119 -0.0001 -0.0002
                                        0.0000 -0.0224 -0.0002 -0.0002  0.0000
                                        0.0005 -0.0004  0.0002 -0.0001  0.0000
                                        0.0000  0.0004 -0.0004  0.0000  0.0000
                                       -0.0001  0.0000  0.0000  0.0000
167. (1.99798) LP ( 2)Ag202            s(  0.06%)p 0.15(  0.01%)d99.99( 99.93%)
                                                f 0.00(  0.00%)
                                        0.0000  0.0239 -0.0004 -0.0002 -0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0074  0.0052  0.0014  0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0020  0.0000  0.0000  0.0000  0.0665
                                       -0.0009  0.0002  0.0001 -0.0250 -0.0002
                                       -0.0002  0.0000 -0.3187 -0.0050 -0.0064
                                       -0.0011 -0.9447 -0.0081 -0.0067 -0.0013
                                        0.0000  0.0000  0.0000  0.0000  0.0005
                                       -0.0006  0.0000  0.0000 -0.0001  0.0000
                                        0.0000  0.0000  0.0008 -0.0006
```

```
168. (1.98368) LP ( 3)Ag202            s(  2.70%)p 0.01(  0.02%)d36.06( 97.28%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.1642  0.0015  0.0013 -0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0124 -0.0056 -0.0025 -0.0006
                                        0.0000 -0.0003  0.0000  0.0000  0.0000
                                       -0.0011  0.0000  0.0000  0.0000  0.1870
                                       -0.0017 -0.0018  0.0000  0.0040  0.0000
                                        0.0000  0.0000  0.9226 -0.0016 -0.0106
                                        0.0000 -0.2941 -0.0045  0.0052  0.0007
                                        0.0000  0.0000  0.0000  0.0000 -0.0008
                                        0.0005  0.0000  0.0000 -0.0002  0.0001
                                        0.0000  0.0000 -0.0005  0.0006
169. (1.97847) LP ( 4)Ag202            s(  0.07%)p 0.01(  0.00%)d99.99( 99.93%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.0272 -0.0003  0.0004  0.0000
                                        0.0000  0.0000  0.0001  0.0000  0.0000
                                        0.0000  0.0020 -0.0004  0.0000  0.0002
                                        0.0000 -0.0001  0.0000  0.0000  0.0000
                                       -0.0068  0.0001  0.0000  0.0000 -0.9800
                                        0.0102  0.0021  0.0013  0.0007  0.0000
                                        0.0000  0.0000  0.1552 -0.0010 -0.0017
                                       -0.0002 -0.1207 -0.0012  0.0009  0.0001
                                        0.0000  0.0000  0.0000  0.0000 -0.0002
                                        0.0001  0.0000  0.0000 -0.0004  0.0000
                                        0.0000  0.0000 -0.0002  0.0001
170. (1.97645) LP ( 5)Ag202            s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0015  0.0004  0.0005  0.0005
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0002 -0.0003 -0.0004  0.0000
                                        0.9997 -0.0070 -0.0049 -0.0011 -0.0066
                                        0.0001  0.0000  0.0000  0.0216  0.0003
                                       -0.0006  0.0000  0.0025  0.0000  0.0000
                                        0.0000  0.0002  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0002 -0.0002  0.0000
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0007 -0.0006  0.0000  0.0000
                                    [...]
375. (1.95132) BD ( 1) P189- P191
             ( 48.15%)   0.6939* P189 s( 10.89%)p 8.07( 87.84%)d 0.12(  1.28%)
                                        0.0000  0.0000  0.3299 -0.0016  0.0041
                                        0.0000  0.2894 -0.0113 -0.0015  0.0000
                                        0.6618 -0.0137 -0.0058  0.0000 -0.5966
                                       -0.0189  0.0039  0.0307  0.0033 -0.0510
                                        0.0096 -0.0720 -0.0109 -0.0143 -0.0074
                                        0.0544 -0.0243
             ( 51.85%)   0.7201* P191 s( 11.21%)p 7.84( 87.83%)d 0.09(  0.96%)
                                        0.0000  0.0000  0.3345 -0.0004  0.0138
                                        0.0000 -0.4051 -0.0140  0.0061  0.0000
                                       -0.4746  0.0072  0.0034  0.0000  0.6989
                                       -0.0145  0.0010  0.0480 -0.0096 -0.0484
                                        0.0049 -0.0526 -0.0176 -0.0276  0.0237
                                       -0.0004  0.0213
```

```
 376. (1.95156) BD ( 1) P189- P192
              ( 48.16%)   0.6940* P189 s( 10.85%)p 8.10( 87.88%)d 0.12(  1.27%)
                                     0.0000  0.0000  0.3294 -0.0018  0.0047
                                     0.0000  0.2891 -0.0102 -0.0021  0.0000
                                    -0.7386  0.0103  0.0059  0.0000 -0.4990
                                    -0.0206  0.0018 -0.0374 -0.0023 -0.0459
                                     0.0099  0.0809  0.0035 -0.0246 -0.0080
                                     0.0355 -0.0248
              ( 51.84%)   0.7200* P192 s( 11.37%)p 7.71( 87.67%)d 0.08(  0.96%)
                                     0.0000  0.0000  0.3369 -0.0012  0.0142
                                     0.0000 -0.3864 -0.0152  0.0059  0.0000
                                     0.5741 -0.0098 -0.0031  0.0000  0.6303
                                    -0.0121  0.0012 -0.0526  0.0095 -0.0398
                                     0.0033  0.0466  0.0261 -0.0373  0.0224
                                    -0.0121  0.0164
 377. (1.98529) BD ( 1) P189-Cl198
              ( 33.74%)   0.5808* P189 s(  7.14%)p12.77( 91.19%)d 0.23(  1.67%)
                                     0.0000  0.0000  0.2667 -0.0159  0.0032
                                     0.0000 -0.8969  0.0541 -0.0098  0.0000
                                    -0.0222 -0.0011 -0.0003  0.0000 -0.3220
                                    -0.0174 -0.0031  0.0061  0.0000  0.0917
                                    -0.0003  0.0047 -0.0027  0.0711  0.0406
                                    -0.0073 -0.0385
              ( 66.26%)   0.8140*Cl198 s( 14.30%)p 5.94( 84.92%)d 0.06(  0.79%)
                                     0.0000  0.0000  0.3779 -0.0134  0.0006
                                     0.0000  0.8796 -0.0200  0.0028  0.0000
                                     0.0173 -0.0004  0.0001  0.0000  0.2734
                                    -0.0084  0.0022  0.0022  0.0004  0.0359
                                     0.0051  0.0009 -0.0001  0.0728  0.0046
                                    -0.0349 -0.0023
 378. (1.95694) BD ( 1) P190- P193
              ( 48.16%)   0.6940* P190 s( 10.58%)p 8.35( 88.34%)d 0.10(  1.08%)
                                     0.0000  0.0000  0.3252 -0.0048  0.0013
                                     0.0000 -0.3104 -0.0136 -0.0045  0.0000
                                     0.7273 -0.0127 -0.0080  0.0000 -0.5074
                                     0.0131  0.0022 -0.0495  0.0091  0.0537
                                    -0.0135 -0.0638 -0.0092 -0.0149 -0.0134
                                     0.0181 -0.0186
              ( 51.84%)   0.7200* P193 s( 10.81%)p 8.17( 88.26%)d 0.09(  0.94%)
                                     0.0000  0.0000  0.3284 -0.0035  0.0130
                                     0.0000  0.3348  0.0156 -0.0039  0.0000
                                    -0.5112  0.0088  0.0058  0.0000  0.7132
                                    -0.0127 -0.0003 -0.0422  0.0114  0.0296
                                     0.0054 -0.0553 -0.0197 -0.0461  0.0274
                                     0.0062  0.0140
```

```
 379. (1.95803) BD ( 1) P190- P194
              ( 48.34%)   0.6953* P190 s( 10.65%)p 8.29( 88.28%)d 0.10(  1.07%)
                                        0.0000  0.0000  0.3263 -0.0047  0.0015
                                        0.0000 -0.2985 -0.0131 -0.0043  0.0000
                                       -0.6757  0.0137  0.0072  0.0000 -0.5801
                                        0.0113  0.0033  0.0441 -0.0090  0.0575
                                       -0.0145  0.0603  0.0153 -0.0099 -0.0123
                                        0.0287 -0.0162
              ( 51.66%)   0.7187* P194 s( 10.70%)p 8.26( 88.36%)d 0.09(  0.94%)
                                        0.0000  0.0000  0.3268 -0.0033  0.0129
                                        0.0000  0.3522  0.0143 -0.0041  0.0000
                                        0.4298 -0.0069 -0.0063  0.0000  0.7578
                                       -0.0151 -0.0009  0.0396 -0.0123  0.0358
                                        0.0036  0.0579  0.0140 -0.0389  0.0284
                                        0.0164  0.0163
 380. (1.98730) BD ( 1) P190-Cl197
              ( 32.56%)   0.5706* P190 s(  6.61%)p13.87( 91.70%)d 0.25(  1.68%)
                                        0.0000  0.0000  0.2569 -0.0094 -0.0059
                                        0.0000 -0.7666  0.0209 -0.0025  0.0000
                                       -0.0358  0.0024 -0.0001  0.0000  0.5711
                                        0.0392  0.0008  0.0060  0.0018 -0.0778
                                       -0.0487 -0.0018 -0.0050  0.0823  0.0029
                                       -0.0249  0.0307
              ( 67.44%)   0.8212*Cl197 s( 14.22%)p 5.99( 85.09%)d 0.05(  0.70%)
                                        0.0000  0.0000  0.3768 -0.0121 -0.0004
                                        0.0000  0.7326 -0.0162  0.0040  0.0000
                                        0.0376 -0.0006  0.0000  0.0000 -0.5589
                                        0.0125  0.0003  0.0042  0.0004 -0.0735
                                       -0.0021 -0.0035 -0.0004  0.0370  0.0047
                                        0.0109 -0.0001
 381. (1.95704) BD ( 1) P191- P195
              ( 51.82%)   0.7199* P191 s( 10.80%)p 8.17( 88.26%)d 0.09(  0.94%)
                                        0.0000  0.0000  0.3284 -0.0034  0.0130
                                        0.0000 -0.3337 -0.0157  0.0040  0.0000
                                       -0.5225  0.0091  0.0058  0.0000 -0.7055
                                        0.0125  0.0003  0.0427 -0.0116  0.0287
                                        0.0057  0.0547  0.0207 -0.0471  0.0269
                                        0.0047  0.0133
              ( 48.18%)   0.6941* P195 s( 10.58%)p 8.35( 88.34%)d 0.10(  1.08%)
                                        0.0000  0.0000  0.3252 -0.0049  0.0015
                                        0.0000  0.3103  0.0134  0.0044  0.0000
                                        0.7352 -0.0125 -0.0080  0.0000  0.4960
                                       -0.0135 -0.0019  0.0504 -0.0094  0.0527
                                       -0.0133  0.0641  0.0084 -0.0159 -0.0136
                                        0.0165 -0.0188
```

```
382. (1.95803) BD ( 1) P192- P195
              ( 51.65%)   0.7187* P192 s( 10.69%)p 8.26( 88.37%)d 0.09(  0.94%)
                                        0.0000  0.0000  0.3267 -0.0032  0.0129
                                        0.0000 -0.3444 -0.0142  0.0041  0.0000
                                        0.4189 -0.0066 -0.0061  0.0000 -0.7675
                                        0.0151  0.0012 -0.0382  0.0121  0.0360
                                        0.0031 -0.0585 -0.0128 -0.0382  0.0285
                                        0.0186  0.0167
              ( 48.35%)   0.6953* P195 s( 10.66%)p 8.28( 88.27%)d 0.10(  1.07%)
                                        0.0000  0.0000  0.3264 -0.0047  0.0015
                                        0.0000  0.2935  0.0130  0.0044  0.0000
                                       -0.6663  0.0139  0.0072  0.0000  0.5934
                                       -0.0112 -0.0034 -0.0427  0.0088  0.0576
                                       -0.0145 -0.0599 -0.0160 -0.0094 -0.0119
                                        0.0311 -0.0159
383. (1.95152) BD ( 1) P193- P196
              ( 51.85%)   0.7201* P193 s( 11.22%)p 7.83( 87.82%)d 0.09(  0.96%)
                                        0.0000  0.0000  0.3347 -0.0003  0.0137
                                        0.0000  0.4008  0.0140 -0.0060  0.0000
                                       -0.4879  0.0073  0.0035  0.0000 -0.6921
                                        0.0144 -0.0010 -0.0484  0.0096 -0.0471
                                        0.0048  0.0524  0.0187 -0.0292  0.0235
                                       -0.0016  0.0206
              ( 48.15%)   0.6939* P196 s( 10.89%)p 8.07( 87.83%)d 0.12(  1.28%)
                                        0.0000  0.0000  0.3299 -0.0015  0.0041
                                        0.0000 -0.2838  0.0114  0.0015  0.0000
                                        0.6737 -0.0136 -0.0058  0.0000  0.5858
                                        0.0189 -0.0038 -0.0313 -0.0029 -0.0497
                                        0.0096  0.0739  0.0099 -0.0160 -0.0077
                                        0.0526 -0.0246
384. (1.95144) BD ( 1) P194- P196
              ( 51.83%)   0.7199* P194 s( 11.36%)p 7.72( 87.68%)d 0.08(  0.96%)
                                        0.0000  0.0000  0.3367 -0.0011  0.0142
                                        0.0000  0.3831  0.0152 -0.0059  0.0000
                                        0.5627 -0.0096 -0.0030  0.0000 -0.6425
                                        0.0121 -0.0011  0.0518 -0.0096 -0.0411
                                        0.0037 -0.0479 -0.0251 -0.0362  0.0227
                                       -0.0101  0.0171
              ( 48.17%)   0.6941* P196 s( 10.85%)p 8.10( 87.88%)d 0.12(  1.27%)
                                        0.0000  0.0000  0.3294 -0.0018  0.0047
                                        0.0000 -0.2901  0.0104  0.0021  0.0000
                                       -0.7281  0.0104  0.0058  0.0000  0.5136
                                        0.0205 -0.0020  0.0363  0.0028 -0.0465
                                        0.0096 -0.0802 -0.0047 -0.0230 -0.0078
                                        0.0384 -0.0247
```

```
385. (1.98730) BD ( 1) P195-Cl200
              ( 32.55%)   0.5706* P195 s(  6.61%)p13.88( 91.71%)d 0.25(  1.68%)
                                        0.0000  0.0000  0.2568 -0.0093 -0.0060
                                        0.0000  0.7692 -0.0211  0.0023  0.0000
                                       -0.0483  0.0029 -0.0003  0.0000 -0.5667
                                       -0.0389 -0.0008 -0.0078 -0.0027 -0.0771
                                       -0.0488  0.0026  0.0060  0.0826  0.0031
                                       -0.0256  0.0301
              ( 67.45%)   0.8212*Cl200 s( 14.22%)p 5.98( 85.09%)d 0.05(  0.69%)
                                        0.0000  0.0000  0.3769 -0.0121 -0.0003
                                        0.0000 -0.7351  0.0163 -0.0038  0.0000
                                        0.0488 -0.0009  0.0001  0.0000  0.5547
                                       -0.0125 -0.0004 -0.0056 -0.0005 -0.0733
                                       -0.0021  0.0046  0.0004  0.0372  0.0047
                                        0.0101 -0.0002
386. (1.98528) BD ( 1) P196-Cl199
              ( 33.73%)   0.5808* P196 s(  7.14%)p12.77( 91.19%)d 0.23(  1.67%)
                                        0.0000  0.0000  0.2667 -0.0160  0.0033
                                        0.0000  0.8982 -0.0540  0.0099  0.0000
                                       -0.0203 -0.0005 -0.0004  0.0000  0.3182
                                        0.0178  0.0031 -0.0050 -0.0003  0.0914
                                       -0.0008 -0.0041  0.0023  0.0715  0.0406
                                       -0.0079 -0.0386
              ( 66.27%)   0.8140*Cl199 s( 14.30%)p 5.94( 84.92%)d 0.06(  0.79%)
                                        0.0000  0.0000  0.3779 -0.0133  0.0006
                                        0.0000 -0.8807  0.0200 -0.0027  0.0000
                                        0.0159 -0.0004  0.0000  0.0000 -0.2698
                                        0.0084 -0.0022 -0.0023 -0.0003  0.0353
                                        0.0051 -0.0008  0.0000  0.0730  0.0046
                                       -0.0352 -0.0023
---------------- non-Lewis ----------------------------------------------------
387. (0.45619) LV ( 1)Ag201           s( 96.84%)p 0.00(  0.22%)d 0.03(  2.94%)
                                                  f 0.00(  0.00%)
                                        0.0000  0.9841 -0.0010 -0.0011  0.0004
                                        0.0000 -0.0001  0.0001  0.0000  0.0000
                                        0.0000 -0.0435  0.0116  0.0128 -0.0032
                                        0.0000  0.0003 -0.0002 -0.0001  0.0000
                                        0.0002  0.0000  0.0000  0.0000 -0.0289
                                       -0.0069 -0.0028  0.0014 -0.0002 -0.0002
                                       -0.0001  0.0000 -0.1499 -0.0177 -0.0016
                                        0.0044  0.0746 -0.0090 -0.0040 -0.0032
                                        0.0000  0.0000  0.0000  0.0000  0.0013
                                       -0.0009 -0.0001  0.0000  0.0005 -0.0002
                                        0.0000  0.0000  0.0026 -0.0015
388. (0.45392) LV ( 1)Ag202           s( 96.88%)p 0.00(  0.23%)d 0.03(  2.89%)
                                                  f 0.00(  0.00%)
                                        0.0000  0.9843 -0.0011 -0.0009  0.0004
                                        0.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0446 -0.0121 -0.0122  0.0028
                                        0.0000 -0.0007  0.0001  0.0002  0.0000
                                        0.0003  0.0001  0.0000  0.0000 -0.0057
                                        0.0011 -0.0028  0.0002 -0.0002 -0.0002
                                        0.0000  0.0000 -0.1509 -0.0180 -0.0029
                                        0.0044  0.0752 -0.0057 -0.0025 -0.0034
                                        0.0001  0.0000  0.0000  0.0000 -0.0016
                                        0.0012 -0.0001  0.0000 -0.0007  0.0003
                                        0.0000  0.0000 -0.0030  0.0016
```

```
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.50 kcal/mol
    (Intermolecular threshold: 0.05 kcal/mol)
                                                          E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO      kcal/mol   a.u.    a.u.
 ===========================================================================
from unit  1 to unit  3
  143. LP ( 1) P191           387. LV ( 1)Ag201           82.87    0.53   0.187
                                     [...]
from unit  1 to unit  4
  144. LP ( 1) P192           388. LV ( 1)Ag202           82.62    0.52   0.186
                                     [...]
from unit  2 to unit  3
  145. LP ( 1) P193           387. LV ( 1)Ag201           82.92    0.53   0.188
                                     [...]
from unit  2 to unit  4
  146. LP ( 1) P194           388. LV ( 1)Ag202           82.60    0.52   0.186
                                     [...]


NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

 1 pass over DM reduced the maximum off-diagonal element to 0.20E-09

 Hybridization/Polarization Analysis of NLMOs in NAO Basis:
 NLMO / Occupancy / Percent from Parent NBO / Atomic Hybrid Contributions
 ---------------------------------------------------------------------------
                                     [...]
141. (2.00000)  98.2403% LP ( 1) P189
                          0.055%  C  1 s( 38.16%)p 1.61( 61.47%)d 0.01(  0.38%)
                          0.056%  C  2 s( 37.46%)p 1.66( 62.19%)d 0.01(  0.35%)
                          0.071%  C 12 s( 35.58%)p 1.80( 64.13%)d 0.01(  0.30%)
                          0.070%  C 13 s( 36.34%)p 1.74( 63.35%)d 0.01(  0.31%)
                          0.026%  C 21 s( 12.57%)p 6.88( 86.45%)d 0.08(  0.98%)
                          0.023%  C 23 s( 13.99%)p 6.08( 85.03%)d 0.07(  0.97%)
                          0.032%  C 37 s(  6.33%)p14.65( 92.78%)d 0.14(  0.88%)
                          0.030%  C 38 s(  5.39%)p17.37( 93.63%)d 0.18(  0.98%)
                          0.076%  H 82 s( 99.06%)p 0.01(  0.94%)
                          0.077%  H 86 s( 99.08%)p 0.01(  0.92%)
                          0.099%  H105 s( 99.40%)p 0.01(  0.60%)
                          0.097%  H106 s( 99.40%)p 0.01(  0.60%)
                         98.241%  P189 s( 70.78%)p 0.41( 29.10%)d 0.00(  0.12%)
                          0.126%  P191 s(  1.50%)p22.82( 34.21%)d42.88( 64.29%)
                          0.122%  P192 s(  1.21%)p27.85( 33.74%)d53.69( 65.05%)
                          0.365%  P195 s(  8.86%)p 8.43( 74.65%)d 1.86( 16.50%)
                          0.077% Cl198 s(  1.68%)p19.88( 33.33%)d38.75( 64.99%)
                          0.143% Cl200 s( 17.17%)p 4.72( 81.06%)d 0.10(  1.77%)
                          0.040% Ag201 s( 84.60%)p 0.09(  7.41%)d 0.09(  7.70%)
                                                 f 0.00(  0.29%)
                          0.036% Ag202 s( 84.07%)p 0.09(  7.95%)d 0.09(  7.68%)
                                                 f 0.00(  0.30%)
```

```
142. (2.00000)  98.3739% LP ( 1) P190
                          0.088%  C  3 s( 37.71%)p 1.65( 62.19%)d 0.00(  0.10%)
                          0.082%  C  4 s( 37.80%)p 1.64( 62.08%)d 0.00(  0.12%)
                          0.012%  C 27 s( 17.35%)p 4.71( 81.66%)d 0.06(  0.99%)
                          0.013%  C 30 s( 14.96%)p 5.60( 83.75%)d 0.09(  1.29%)
                          0.046%  C 41 s( 21.74%)p 3.52( 76.55%)d 0.08(  1.71%)
                          0.049%  C 43 s( 21.33%)p 3.61( 77.05%)d 0.08(  1.62%)
                          0.126%  H 93 s( 99.19%)p 0.01(  0.81%)
                          0.117%  H 95 s( 99.16%)p 0.01(  0.84%)
                         98.376%  P190 s( 71.74%)p 0.39( 28.15%)d 0.00(  0.12%)
                          0.039%  P191 s( 65.78%)p 0.48( 31.27%)d 0.04(  2.95%)
                          0.038%  P192 s( 63.89%)p 0.52( 33.11%)d 0.05(  3.00%)
                          0.169%  P193 s(  1.73%)p32.01( 55.32%)d24.86( 42.96%)
                          0.162%  P194 s(  1.88%)p28.98( 54.33%)d23.35( 43.79%)
                          0.066%  P196 s( 13.18%)p 5.57( 73.37%)d 1.02( 13.46%)
                          0.066% Cl197 s(  0.15%)p99.99( 20.96%)d99.99( 78.89%)
                          0.031% Cl199 s( 11.37%)p 6.78( 77.07%)d 1.02( 11.56%)
                          0.215% Ag201 s( 93.67%)p 0.03(  2.39%)d 0.04(  3.86%)
                                                   f 0.00(  0.08%)
                          0.204% Ag202 s( 93.32%)p 0.03(  2.55%)d 0.04(  4.04%)
                                                   f 0.00(  0.09%)
143. (2.00000)  87.7442% LP ( 1) P191
                          0.029%  C 12 s( 66.60%)p 0.44( 29.01%)d 0.07(  4.39%)
                          0.060%  C 23 s( 19.49%)p 4.11( 80.12%)d 0.02(  0.38%)
                          0.027%  C 34 s(  2.73%)p35.60( 97.25%)d 0.01(  0.01%)
                          0.078%  C 37 s( 27.75%)p 2.58( 71.68%)d 0.02(  0.57%)
                          0.198%  C 38 s(  7.74%)p11.72( 90.72%)d 0.20(  1.54%)
                          0.014%  C 43 s( 37.56%)p 1.65( 62.09%)d 0.01(  0.35%)
                          0.076%  C 51 s( 14.15%)p 6.03( 85.30%)d 0.04(  0.55%)
                          0.050%  C 61 s( 34.65%)p 1.84( 63.70%)d 0.05(  1.64%)
                          0.020%  H 89 s( 99.78%)p 0.00(  0.22%)
                          0.011%  H105 s( 95.75%)p 0.04(  4.25%)
                          0.062%  H159 s( 99.12%)p 0.01(  0.88%)
                          0.011%  H172 s( 99.42%)p 0.01(  0.58%)
                          0.537%  P189 s(  5.05%)p16.80( 84.78%)d 2.02( 10.17%)
                          0.012%  P190 s(  8.79%)p 9.71( 85.43%)d 0.66(  5.78%)
                         87.803%  P191 s( 53.01%)p 0.88( 46.85%)d 0.00(  0.14%)
                          0.199%  P192 s( 46.71%)p 0.80( 37.50%)d 0.34( 15.78%)
                          0.288%  P193 s( 70.22%)p 0.39( 27.69%)d 0.03(  2.09%)
                          0.047%  P194 s( 52.55%)p 0.73( 38.31%)d 0.17(  9.14%)
                          0.218%  P195 s(  8.78%)p 8.07( 70.85%)d 2.32( 20.37%)
                          0.013%  P196 s(  7.18%)p11.91( 85.57%)d 1.01(  7.25%)
                          0.216% Cl198 s( 13.13%)p 6.48( 85.11%)d 0.13(  1.76%)
                          0.066% Cl200 s( 13.14%)p 6.38( 83.91%)d 0.22(  2.95%)
                          9.562% Ag201 s( 95.98%)p 0.01(  0.85%)d 0.03(  3.07%)
                                                   f 0.00(  0.11%)
                          0.300% Ag202 s( 92.57%)p 0.03(  2.91%)d 0.05(  4.39%)
                                                   f 0.00(  0.13%)
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 144. (2.00000)  87.9489% LP ( 1) P192
                          0.030%  C 13 s( 64.06%)p 0.49( 31.45%)d 0.07(  4.49%)
                          0.063%  C 21 s( 16.12%)p 5.18( 83.49%)d 0.02(  0.40%)
                          0.027%  C 29 s(  2.71%)p35.90( 97.28%)d 0.00(  0.01%)
                          0.196%  C 37 s(  8.16%)p11.06( 90.27%)d 0.19(  1.57%)
                          0.078%  C 38 s( 27.97%)p 2.55( 71.45%)d 0.02(  0.58%)
                          0.013%  C 41 s( 37.37%)p 1.67( 62.24%)d 0.01(  0.39%)
                          0.076%  C 49 s( 16.55%)p 5.01( 82.89%)d 0.03(  0.56%)
                          0.050%  C 59 s( 35.01%)p 1.81( 63.43%)d 0.04(  1.56%)
                          0.022%  H 91 s( 99.80%)p 0.00(  0.20%)
                          0.011%  H106 s( 95.23%)p 0.05(  4.77%)
                          0.066%  H162 s( 99.30%)p 0.01(  0.70%)
                          0.496%  P189 s(  4.91%)p17.15( 84.15%)d 2.23( 10.95%)
                          0.014%  P190 s( 10.76%)p 7.64( 82.15%)d 0.66(  7.09%)
                          0.217%  P191 s( 51.23%)p 0.68( 34.72%)d 0.27( 14.05%)
                         88.001%  P192 s( 52.95%)p 0.89( 46.91%)d 0.00(  0.13%)
                          0.043%  P193 s( 52.13%)p 0.74( 38.39%)d 0.18(  9.48%)
                          0.317%  P194 s( 69.16%)p 0.42( 28.76%)d 0.03(  2.09%)
                          0.215%  P195 s(  8.86%)p 7.98( 70.71%)d 2.30( 20.43%)
                          0.016%  P196 s(  8.26%)p10.24( 84.59%)d 0.86(  7.15%)
                          0.199% Cl198 s( 13.04%)p 6.52( 85.02%)d 0.15(  1.95%)
                          0.069% Cl200 s( 12.18%)p 6.92( 84.32%)d 0.29(  3.50%)
                          0.273% Ag201 s( 92.17%)p 0.03(  2.85%)d 0.05(  4.83%)
                                                   f 0.00(  0.15%)
                          9.397% Ag202 s( 95.99%)p 0.01(  0.87%)d 0.03(  3.02%)
                                                   f 0.00(  0.11%)
 145. (2.00000)  87.7796% LP ( 1) P193
                          0.050%  C 16 s( 35.13%)p 1.80( 63.22%)d 0.05(  1.65%)
                          0.073%  C 30 s( 14.80%)p 5.72( 84.63%)d 0.04(  0.57%)
                          0.014%  C 38 s( 38.26%)p 1.60( 61.36%)d 0.01(  0.37%)
                          0.079%  C 41 s( 27.84%)p 2.57( 71.60%)d 0.02(  0.57%)
                          0.198%  C 43 s(  7.74%)p11.72( 90.72%)d 0.20(  1.54%)
                          0.027%  C 46 s(  2.67%)p36.44( 97.32%)d 0.00(  0.01%)
                          0.064%  C 54 s( 18.34%)p 4.43( 81.29%)d 0.02(  0.37%)
                          0.029%  C 63 s( 66.13%)p 0.45( 29.48%)d 0.07(  4.40%)
                          0.010%  H 96 s( 99.42%)p 0.01(  0.58%)
                          0.062%  H110 s( 99.12%)p 0.01(  0.88%)
                          0.011%  H165 s( 95.77%)p 0.04(  4.23%)
                          0.020%  H177 s( 99.78%)p 0.00(  0.22%)
                          0.014%  P189 s(  7.14%)p11.98( 85.55%)d 1.02(  7.31%)
                          0.220%  P190 s(  8.88%)p 7.98( 70.86%)d 2.28( 20.26%)
                          0.329%  P191 s( 69.69%)p 0.41( 28.50%)d 0.03(  1.81%)
                          0.046%  P192 s( 52.40%)p 0.73( 38.45%)d 0.17(  9.15%)
                         87.838%  P193 s( 53.00%)p 0.88( 46.86%)d 0.00(  0.14%)
                          0.200%  P194 s( 46.56%)p 0.81( 37.68%)d 0.34( 15.76%)
                          0.012%  P195 s(  9.11%)p 9.33( 85.01%)d 0.65(  5.88%)
                          0.537%  P196 s(  5.10%)p16.61( 84.66%)d 2.01( 10.24%)
                          0.067% Cl197 s( 13.14%)p 6.39( 83.96%)d 0.22(  2.90%)
                          0.217% Cl199 s( 13.24%)p 6.42( 84.96%)d 0.14(  1.80%)
                          9.485% Ag201 s( 95.96%)p 0.01(  0.86%)d 0.03(  3.06%)
                                                   f 0.00(  0.11%)
                          0.297% Ag202 s( 92.55%)p 0.03(  2.91%)d 0.05(  4.40%)
                                                   f 0.00(  0.13%)
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 146. (2.00000)  87.9268% LP ( 1) P194
                          0.049%  C 17 s( 34.74%)p 1.83( 63.68%)d 0.05(  1.58%)
                          0.079%  C 27 s( 15.71%)p 5.33( 83.75%)d 0.03(  0.54%)
                          0.013%  C 37 s( 36.92%)p 1.70( 62.71%)d 0.01(  0.37%)
                          0.027%  C 40 s(  2.75%)p35.41( 97.24%)d 0.01(  0.01%)
                          0.196%  C 41 s(  8.13%)p11.11( 90.30%)d 0.19(  1.58%)
                          0.078%  C 43 s( 28.02%)p 2.55( 71.39%)d 0.02(  0.59%)
                          0.059%  C 53 s( 17.37%)p 4.73( 82.22%)d 0.02(  0.41%)
                          0.030%  C 64 s( 64.89%)p 0.47( 30.63%)d 0.07(  4.48%)
                          0.065%  H112 s( 99.29%)p 0.01(  0.71%)
                          0.011%  H166 s( 95.32%)p 0.05(  4.68%)
                          0.022%  H178 s( 99.80%)p 0.00(  0.20%)
                          0.016%  P189 s(  8.37%)p10.10( 84.55%)d 0.85(  7.08%)
                          0.213%  P190 s(  8.78%)p 8.03( 70.51%)d 2.36( 20.71%)
                          0.044%  P191 s( 52.22%)p 0.73( 38.28%)d 0.18(  9.51%)
                          0.285%  P192 s( 69.43%)p 0.41( 28.22%)d 0.03(  2.35%)
                          0.217%  P193 s( 51.15%)p 0.68( 34.84%)d 0.27( 14.00%)
                         87.979%  P194 s( 52.97%)p 0.89( 46.90%)d 0.00(  0.13%)
                          0.014%  P195 s( 11.06%)p 7.40( 81.85%)d 0.64(  7.09%)
                          0.494%  P196 s(  4.93%)p17.07( 84.15%)d 2.21( 10.92%)
                          0.071% Cl197 s( 12.30%)p 6.85( 84.26%)d 0.28(  3.44%)
                          0.197% Cl199 s( 13.26%)p 6.40( 84.80%)d 0.15(  1.95%)
                          0.275% Ag201 s( 92.16%)p 0.03(  2.87%)d 0.05(  4.82%)
                                                   f 0.00(  0.15%)
                          9.454% Ag202 s( 96.00%)p 0.01(  0.87%)d 0.03(  3.02%)
                                                   f 0.00(  0.11%)
 147. (2.00000)  98.3728% LP ( 1) P195
                          0.047%  C 37 s( 22.11%)p 3.45( 76.19%)d 0.08(  1.70%)
                          0.050%  C 38 s( 21.06%)p 3.67( 77.33%)d 0.08(  1.60%)
                          0.012%  C 49 s( 17.29%)p 4.72( 81.69%)d 0.06(  1.02%)
                          0.013%  C 51 s( 15.62%)p 5.32( 83.13%)d 0.08(  1.25%)
                          0.087%  C 69 s( 37.63%)p 1.65( 62.27%)d 0.00(  0.10%)
                          0.082%  C 70 s( 38.00%)p 1.63( 61.88%)d 0.00(  0.12%)
                          0.126%  H169 s( 99.19%)p 0.01(  0.81%)
                          0.117%  H174 s( 99.16%)p 0.01(  0.84%)
                          0.065%  P189 s( 13.19%)p 5.56( 73.32%)d 1.02( 13.49%)
                          0.169%  P191 s(  1.75%)p31.72( 55.38%)d24.55( 42.87%)
                          0.162%  P192 s(  1.85%)p29.44( 54.57%)d23.51( 43.58%)
                          0.039%  P193 s( 65.59%)p 0.48( 31.58%)d 0.04(  2.83%)
                          0.038%  P194 s( 63.62%)p 0.53( 33.46%)d 0.05(  2.92%)
                         98.374%  P195 s( 71.73%)p 0.39( 28.15%)d 0.00(  0.12%)
                          0.031% Cl198 s( 11.30%)p 6.82( 77.12%)d 1.02( 11.58%)
                          0.066% Cl200 s(  0.15%)p99.99( 21.06%)d99.99( 78.79%)
                          0.215% Ag201 s( 93.68%)p 0.03(  2.38%)d 0.04(  3.86%)
                                                   f 0.00(  0.08%)
                          0.205% Ag202 s( 93.38%)p 0.03(  2.53%)d 0.04(  4.00%)
                                                   f 0.00(  0.09%)
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 148. (2.00000)  98.2421% LP ( 1) P196
                          0.032%  C 41 s(  6.96%)p13.24( 92.17%)d 0.12(  0.87%)
                          0.030%  C 43 s(  5.17%)p18.17( 93.85%)d 0.19(  0.99%)
                          0.027%  C 53 s( 12.10%)p 7.18( 86.92%)d 0.08(  0.98%)
                          0.023%  C 54 s( 14.04%)p 6.06( 85.00%)d 0.07(  0.97%)
                          0.072%  C 63 s( 35.57%)p 1.80( 64.13%)d 0.01(  0.30%)
                          0.069%  C 64 s( 36.36%)p 1.74( 63.32%)d 0.01(  0.31%)
                          0.055%  C 71 s( 38.37%)p 1.60( 61.24%)d 0.01(  0.38%)
                          0.056%  C 72 s( 37.55%)p 1.65( 62.10%)d 0.01(  0.35%)
                          0.100%  H165 s( 99.40%)p 0.01(  0.60%)
                          0.095%  H166 s( 99.39%)p 0.01(  0.61%)
                          0.076%  H179 s( 99.06%)p 0.01(  0.94%)
                          0.077%  H180 s( 99.08%)p 0.01(  0.92%)
                          0.363%  P190 s(  8.88%)p 8.40( 74.63%)d 1.86( 16.49%)
                          0.126%  P193 s(  1.54%)p22.23( 34.16%)d41.85( 64.30%)
                          0.123%  P194 s(  1.12%)p30.09( 33.83%)d57.86( 65.05%)
                         98.243%  P196 s( 70.78%)p 0.41( 29.10%)d 0.00(  0.12%)
                          0.142% Cl197 s( 17.16%)p 4.72( 81.05%)d 0.10(  1.79%)
                          0.077% Cl199 s(  1.70%)p19.78( 33.60%)d38.09( 64.70%)
                          0.041% Ag201 s( 84.81%)p 0.09(  7.24%)d 0.09(  7.65%)
                                                 f 0.00(  0.29%)
                          0.036% Ag202 s( 84.24%)p 0.09(  7.79%)d 0.09(  7.67%)
                                                 f 0.00(  0.30%)
                                      [...]
 161. (2.00000)  99.9266% LP ( 1)Ag201
                         99.927% Ag201 s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
 162. (2.00000)  99.8908% LP ( 2)Ag201
                         99.891% Ag201 s(  0.05%)p 0.15(  0.01%)d99.99( 99.94%)
                                                 f 0.00(  0.00%)
 163. (2.00000)  99.1565% LP ( 3)Ag201
                          0.029%  C 37 s( 35.31%)p 1.81( 64.06%)d 0.02(  0.63%)
                          0.029%  C 41 s( 35.38%)p 1.81( 63.99%)d 0.02(  0.63%)
                          0.026%  P189 s( 16.94%)p 3.80( 64.46%)d 1.10( 18.60%)
                          0.126%  P191 s(  8.37%)p 6.70( 56.05%)d 4.25( 35.59%)
                          0.085%  P192 s( 40.08%)p 1.15( 45.91%)d 0.35( 14.01%)
                          0.127%  P193 s(  8.39%)p 6.68( 56.06%)d 4.24( 35.55%)
                          0.085%  P194 s( 40.09%)p 1.15( 45.94%)d 0.35( 13.97%)
                          0.026%  P196 s( 17.29%)p 3.72( 64.33%)d 1.06( 18.38%)
                          0.011% Cl198 s( 12.70%)p 6.55( 83.24%)d 0.32(  4.06%)
                          0.011% Cl199 s( 12.61%)p 6.61( 83.38%)d 0.32(  4.00%)
                         99.157% Ag201 s(  2.72%)p 0.01(  0.02%)d35.80( 97.27%)
                                                 f 0.00(  0.00%)
                          0.163% Ag202 s( 83.85%)p 0.12(  9.80%)d 0.07(  5.98%)
                                                 f 0.00(  0.37%)
 164. (2.00000)  98.9101% LP ( 4)Ag201
                          0.010%  C 16 s( 42.09%)p 1.34( 56.45%)d 0.03(  1.46%)
                          0.115%  P189 s( 14.40%)p 5.64( 81.24%)d 0.30(  4.37%)
                          0.114%  P190 s( 11.27%)p 7.76( 87.45%)d 0.11(  1.29%)
                          0.263%  P191 s(  0.10%)p99.99( 83.08%)d99.99( 16.83%)
                          0.262%  P193 s(  0.10%)p99.99( 82.98%)d99.99( 16.91%)
                          0.118%  P195 s( 11.24%)p 7.78( 87.49%)d 0.11(  1.27%)
                          0.118%  P196 s( 14.52%)p 5.58( 81.08%)d 0.30(  4.40%)
                         98.910% Ag201 s(  0.14%)p 0.01(  0.00%)d99.99( 99.86%)
                                                 f 0.00(  0.00%)
                          0.013% Ag202 s( 83.91%)p 0.07(  5.50%)d 0.12( 10.19%)
                                                 f 0.00(  0.41%)
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165. (2.00000)  98.8503% LP ( 5)Ag201
                          0.117%  C 38 s( 36.01%)p 1.75( 63.06%)d 0.03(  0.93%)
                          0.122%  C 43 s( 34.55%)p 1.87( 64.54%)d 0.03(  0.91%)
                          0.053%  P189 s( 18.86%)p 3.88( 73.08%)d 0.43(  8.06%)
                          0.055%  P190 s(  7.53%)p11.66( 87.81%)d 0.62(  4.66%)
                          0.311%  P191 s(  1.85%)p45.13( 83.58%)d 7.87( 14.57%)
                          0.304%  P193 s(  1.85%)p45.09( 83.21%)d 8.10( 14.95%)
                          0.049%  P195 s(  7.26%)p12.06( 87.62%)d 0.70(  5.12%)
                          0.049%  P196 s( 18.99%)p 3.83( 72.64%)d 0.44(  8.37%)
                          0.011% Cl198 s( 11.29%)p 7.73( 87.30%)d 0.13(  1.42%)
                          0.010% Cl199 s( 11.55%)p 7.54( 87.04%)d 0.12(  1.41%)
                         98.850% Ag201 s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
166. (2.00000)  99.9244% LP ( 1)Ag202
                         99.924% Ag202 s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
167. (2.00000)  99.8991% LP ( 2)Ag202
                          0.011%  P192 s( 18.54%)p 2.09( 38.77%)d 2.30( 42.69%)
                          0.011%  P194 s( 18.63%)p 2.08( 38.72%)d 2.29( 42.65%)
                         99.899% Ag202 s(  0.06%)p 0.15(  0.01%)d99.99( 99.93%)
                                                 f 0.00(  0.00%)
168. (2.00000)  99.1762% LP ( 3)Ag202
                          0.029%  C 38 s( 35.51%)p 1.80( 63.84%)d 0.02(  0.64%)
                          0.029%  C 43 s( 35.51%)p 1.80( 63.85%)d 0.02(  0.64%)
                          0.019%  P189 s( 16.78%)p 3.65( 61.34%)d 1.30( 21.88%)
                          0.088%  P191 s( 38.59%)p 1.25( 48.18%)d 0.34( 13.23%)
                          0.127%  P192 s(  8.27%)p 6.73( 55.70%)d 4.35( 36.03%)
                          0.087%  P193 s( 38.60%)p 1.25( 48.16%)d 0.34( 13.24%)
                          0.127%  P194 s(  8.23%)p 6.77( 55.73%)d 4.38( 36.04%)
                          0.019%  P196 s( 16.69%)p 3.68( 61.48%)d 1.31( 21.83%)
                          0.162% Ag201 s( 83.63%)p 0.11(  9.44%)d 0.08(  6.53%)
                                                 f 0.00(  0.40%)
                         99.176% Ag202 s(  2.73%)p 0.01(  0.02%)d35.63( 97.25%)
                                                 f 0.00(  0.00%)
169. (2.00000)  98.9089% LP ( 4)Ag202
                          0.102%  P189 s( 13.45%)p 6.13( 82.51%)d 0.30(  4.04%)
                          0.132%  P190 s( 10.73%)p 8.20( 88.00%)d 0.12(  1.26%)
                          0.268%  P192 s(  0.06%)p99.99( 83.46%)d99.99( 16.49%)
                          0.269%  P194 s(  0.06%)p99.99( 83.48%)d99.99( 16.46%)
                          0.132%  P195 s( 10.72%)p 8.21( 88.00%)d 0.12(  1.29%)
                          0.102%  P196 s( 13.45%)p 6.13( 82.52%)d 0.30(  4.03%)
                         98.909% Ag202 s(  0.07%)p 0.01(  0.00%)d99.99( 99.93%)
                                                 f 0.00(  0.00%)
170. (2.00000)  98.8123% LP ( 5)Ag202
                          0.124%  C 37 s( 35.44%)p 1.80( 63.67%)d 0.03(  0.89%)
                          0.124%  C 41 s( 35.50%)p 1.79( 63.61%)d 0.03(  0.89%)
                          0.079%  P189 s( 18.64%)p 4.01( 74.73%)d 0.36(  6.63%)
                          0.033%  P190 s(  5.06%)p17.39( 87.97%)d 1.38(  6.97%)
                          0.312%  P192 s(  1.72%)p48.31( 83.31%)d 8.68( 14.97%)
                          0.312%  P194 s(  1.71%)p48.60( 83.32%)d 8.73( 14.97%)
                          0.033%  P195 s(  4.91%)p17.95( 88.06%)d 1.43(  7.03%)
                          0.079%  P196 s( 18.64%)p 4.01( 74.74%)d 0.35(  6.62%)
                          0.010% Cl198 s(  9.38%)p 9.47( 88.83%)d 0.19(  1.79%)
                          0.010% Cl199 s(  9.24%)p 9.63( 88.97%)d 0.19(  1.79%)
                         98.812% Ag202 s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                                 f 0.00(  0.00%)
                                      [...]
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 375. (2.00000)  97.5371% BD ( 1) P189- P191
                          0.014%  C 11 s(  3.89%)p24.39( 94.78%)d 0.34(  1.34%)
                          0.019%  C 12 s(  3.86%)p24.51( 94.68%)d 0.38(  1.46%)
                          0.015%  C 20 s(  1.73%)p56.22( 97.13%)d 0.66(  1.15%)
                          0.078%  C 23 s( 37.18%)p 1.65( 61.38%)d 0.04(  1.44%)
                          0.032%  C 34 s(  0.42%)p99.99( 99.33%)d 0.62(  0.26%)
                          0.107%  C 37 s( 32.53%)p 2.06( 66.86%)d 0.02(  0.61%)
                          0.340%  C 38 s( 15.81%)p 5.22( 82.58%)d 0.10(  1.61%)
                          0.017%  C 48 s( 12.24%)p 6.91( 84.55%)d 0.26(  3.22%)
                          0.021%  C 49 s(  1.64%)p59.82( 98.18%)d 0.11(  0.18%)
                          0.180%  C 51 s( 10.22%)p 8.75( 89.44%)d 0.03(  0.35%)
                          0.053%  C 61 s(  4.63%)p20.46( 94.73%)d 0.14(  0.64%)
                          0.027%  H 82 s( 99.75%)p 0.00(  0.25%)
                          0.016%  H105 s( 99.60%)p 0.00(  0.40%)
                          0.052%  H159 s( 99.94%)p 0.00(  0.06%)
                         47.113%  P189 s( 12.27%)p 7.05( 86.49%)d 0.10(  1.23%)
                         50.594%  P191 s( 13.36%)p 6.41( 85.70%)d 0.07(  0.94%)
                          0.237%  P192 s( 28.66%)p 1.79( 51.22%)d 0.70( 20.12%)
                          0.522%  P195 s( 11.17%)p 6.99( 78.06%)d 0.96( 10.77%)
                          0.098% Cl198 s(  5.84%)p10.80( 63.10%)d 5.32( 31.06%)
                          0.199% Cl200 s( 16.16%)p 5.09( 82.31%)d 0.10(  1.54%)
                          0.101% Ag201 s( 38.44%)p 0.19(  7.35%)d 1.38( 53.04%)
                                                 f 0.03(  1.17%)
                          0.025% Ag202 s( 20.49%)p 2.01( 41.15%)d 1.86( 38.16%)
                                                 f 0.01(  0.20%)
 376. (2.00000)  97.5483% BD ( 1) P189- P192
                          0.015%  C  9 s(  3.79%)p25.06( 94.93%)d 0.34(  1.28%)
                          0.020%  C 13 s(  4.03%)p23.46( 94.61%)d 0.34(  1.36%)
                          0.014%  C 19 s(  2.10%)p45.90( 96.54%)d 0.65(  1.36%)
                          0.083%  C 21 s( 35.38%)p 1.79( 63.27%)d 0.04(  1.35%)
                          0.034%  C 29 s(  0.49%)p99.99( 99.27%)d 0.50(  0.24%)
                          0.348%  C 37 s( 16.58%)p 4.94( 81.88%)d 0.09(  1.54%)
                          0.116%  C 38 s( 32.29%)p 2.08( 67.12%)d 0.02(  0.59%)
                          0.016%  C 45 s( 12.93%)p 6.48( 83.77%)d 0.26(  3.30%)
                          0.176%  C 49 s( 10.39%)p 8.59( 89.25%)d 0.03(  0.36%)
                          0.023%  C 51 s(  1.64%)p59.87( 98.18%)d 0.11(  0.18%)
                          0.050%  C 59 s(  4.75%)p19.93( 94.61%)d 0.13(  0.64%)
                          0.026%  H 86 s( 99.75%)p 0.00(  0.25%)
                          0.017%  H106 s( 99.56%)p 0.00(  0.44%)
                          0.051%  H162 s( 99.95%)p 0.00(  0.05%)
                         47.033%  P189 s( 12.06%)p 7.19( 86.71%)d 0.10(  1.24%)
                          0.264%  P191 s( 28.88%)p 1.82( 52.52%)d 0.64( 18.60%)
                         50.670%  P192 s( 13.54%)p 6.32( 85.52%)d 0.07(  0.94%)
                          0.504%  P195 s( 11.36%)p 6.84( 77.73%)d 0.96( 10.91%)
                          0.090% Cl198 s(  6.09%)p 9.97( 60.71%)d 5.45( 33.20%)
                          0.191% Cl200 s( 16.51%)p 4.95( 81.82%)d 0.10(  1.66%)
                          0.025% Ag201 s( 24.53%)p 1.64( 40.33%)d 1.42( 34.94%)
                                                 f 0.01(  0.20%)
                          0.098% Ag202 s( 40.22%)p 0.19(  7.58%)d 1.27( 50.98%)
                                                 f 0.03(  1.22%)
```

```
 377. (2.00000)  99.2598% BD ( 1) P189-Cl198
                           0.018%  C 21 s( 14.29%)p 5.95( 85.02%)d 0.05(  0.69%)
                           0.018%  C 23 s( 14.87%)p 5.68( 84.44%)d 0.05(  0.69%)
                          33.601%  P189 s(  8.92%)p10.04( 89.51%)d 0.18(  1.57%)
                           0.146%  P191 s( 13.49%)p 4.08( 55.05%)d 2.33( 31.46%)
                           0.145%  P192 s( 13.44%)p 4.08( 54.79%)d 2.36( 31.76%)
                           0.067%  P195 s( 20.05%)p 3.59( 71.93%)d 0.40(  8.02%)
                          65.782% Cl198 s( 14.39%)p 5.89( 84.81%)d 0.06(  0.79%)
                           0.030% Cl200 s(  8.19%)p11.14( 91.25%)d 0.07(  0.56%)
                           0.050% Ag201 s( 64.63%)p 0.12(  8.08%)d 0.42( 27.18%)
                                                f 0.00(  0.11%)
                           0.047% Ag202 s( 68.25%)p 0.10(  7.05%)d 0.36( 24.60%)
                                                f 0.00(  0.11%)
 378. (2.00000)  97.8196% BD ( 1) P190- P193
                           0.013%  C  3 s( 19.72%)p 3.96( 78.12%)d 0.11(  2.16%)
                           0.016%  C 15 s(  3.96%)p23.93( 94.86%)d 0.30(  1.17%)
                           0.058%  C 30 s( 31.66%)p 2.09( 66.20%)d 0.07(  2.14%)
                           0.130%  C 41 s( 28.35%)p 2.51( 71.07%)d 0.02(  0.58%)
                           0.314%  C 43 s( 13.34%)p 6.37( 84.96%)d 0.13(  1.70%)
                           0.025%  C 46 s(  0.43%)p99.99( 99.28%)d 0.69(  0.29%)
                           0.019%  C 53 s(  0.94%)p99.99( 98.85%)d 0.23(  0.21%)
                           0.128%  C 54 s( 10.69%)p 8.32( 88.88%)d 0.04(  0.43%)
                           0.013%  C 55 s( 19.96%)p 3.82( 76.23%)d 0.19(  3.81%)
                           0.060%  C 63 s(  9.87%)p 9.06( 89.37%)d 0.08(  0.76%)
                           0.039%  H 93 s( 99.70%)p 0.00(  0.30%)
                           0.022%  H110 s( 99.88%)p 0.00(  0.12%)
                           0.015%  H153 s( 99.31%)p 0.01(  0.69%)
                           0.016%  H165 s( 99.70%)p 0.00(  0.30%)
                          47.130%  P190 s( 12.09%)p 7.19( 86.87%)d 0.09(  1.05%)
                           0.029%  P191 s( 66.98%)p 0.41( 27.24%)d 0.09(  5.77%)
                          50.932%  P193 s( 14.09%)p 6.03( 85.00%)d 0.06(  0.91%)
                           0.269%  P194 s( 20.73%)p 3.06( 63.35%)d 0.77( 15.92%)
                           0.231%  P196 s(  2.37%)p34.72( 82.16%)d 6.54( 15.47%)
                           0.071% Cl197 s(  4.97%)p11.11( 55.26%)d 8.00( 39.77%)
                           0.077% Cl199 s( 13.15%)p 6.10( 80.19%)d 0.51(  6.66%)
                           0.229% Ag201 s( 71.68%)p 0.07(  4.90%)d 0.32( 22.82%)
                                                f 0.01(  0.60%)
                           0.030% Ag202 s( 17.25%)p 2.64( 45.59%)d 2.14( 36.88%)
                                                f 0.02(  0.27%)
```

```
 379. (2.00000)  97.8758% BD ( 1) P190- P194
                          0.012%  C  4 s( 19.24%)p 4.09( 78.73%)d 0.11(  2.03%)
                          0.016%  C 14 s(  4.49%)p20.99( 94.31%)d 0.27(  1.19%)
                          0.057%  C 27 s( 30.84%)p 2.17( 67.00%)d 0.07(  2.17%)
                          0.023%  C 40 s(  0.51%)p99.99( 99.19%)d 0.60(  0.30%)
                          0.300%  C 41 s( 12.73%)p 6.72( 85.49%)d 0.14(  1.78%)
                          0.122%  C 43 s( 28.15%)p 2.53( 71.22%)d 0.02(  0.63%)
                          0.013%  C 52 s( 19.74%)p 3.88( 76.53%)d 0.19(  3.73%)
                          0.120%  C 53 s( 11.40%)p 7.73( 88.14%)d 0.04(  0.46%)
                          0.022%  C 54 s(  0.93%)p99.99( 98.88%)d 0.20(  0.19%)
                          0.063%  C 64 s(  9.40%)p 9.56( 89.87%)d 0.08(  0.74%)
                          0.038%  H 95 s( 99.72%)p 0.00(  0.28%)
                          0.023%  H112 s( 99.87%)p 0.00(  0.13%)
                          0.017%  H154 s( 99.45%)p 0.01(  0.55%)
                          0.018%  H166 s( 99.69%)p 0.00(  0.31%)
                         47.328%  P190 s( 12.07%)p 7.20( 86.90%)d 0.09(  1.04%)
                          0.027%  P192 s( 70.07%)p 0.34( 24.11%)d 0.08(  5.82%)
                          0.263%  P193 s( 22.23%)p 2.77( 61.66%)d 0.73( 16.11%)
                         50.777%  P194 s( 13.88%)p 6.14( 85.20%)d 0.07(  0.92%)
                          0.232%  P196 s(  2.34%)p35.02( 82.10%)d 6.63( 15.56%)
                          0.072% Cl197 s(  5.92%)p 9.18( 54.30%)d 6.72( 39.78%)
                          0.077% Cl199 s( 13.24%)p 6.06( 80.27%)d 0.49(  6.49%)
                          0.029% Ag201 s( 17.08%)p 2.38( 40.61%)d 2.46( 41.99%)
                                                   f 0.02(  0.32%)
                          0.213% Ag202 s( 67.72%)p 0.09(  5.83%)d 0.38( 25.81%)
                                                   f 0.01(  0.64%)
 380. (2.00000)  99.3608% BD ( 1) P190-Cl197
                          0.033%  C 41 s( 27.51%)p 2.60( 71.61%)d 0.03(  0.88%)
                          0.032%  C 43 s( 27.56%)p 2.60( 71.51%)d 0.03(  0.94%)
                          0.016%  H 93 s( 99.50%)p 0.01(  0.50%)
                          0.020%  H 95 s( 99.58%)p 0.00(  0.42%)
                          0.010%  H110 s( 98.85%)p 0.01(  1.15%)
                          0.013%  H112 s( 98.98%)p 0.01(  1.02%)
                         32.468%  P190 s(  7.91%)p11.44( 90.49%)d 0.20(  1.59%)
                          0.145%  P193 s( 30.39%)p 1.02( 30.89%)d 1.27( 38.73%)
                          0.144%  P194 s( 30.38%)p 1.05( 31.81%)d 1.24( 37.81%)
                          0.032%  P196 s( 15.96%)p 4.78( 76.22%)d 0.49(  7.82%)
                         66.977% Cl197 s( 14.19%)p 6.00( 85.11%)d 0.05(  0.70%)
                          0.018% Ag201 s( 14.96%)p 2.12( 31.70%)d 3.54( 52.90%)
                                                   f 0.03(  0.45%)
                          0.023% Ag202 s(  6.14%)p 5.56( 34.15%)d 9.66( 59.30%)
                                                   f 0.07(  0.41%)
```

```
 381. (2.00000)  97.8238% BD ( 1) P191- P195
                          0.060%  C 12 s(  9.84%)p 9.08( 89.40%)d 0.08(  0.76%)
                          0.013%  C 20 s( 19.56%)p 3.92( 76.68%)d 0.19(  3.76%)
                          0.021%  C 21 s(  0.89%)p99.99( 98.91%)d 0.23(  0.20%)
                          0.123%  C 23 s( 11.12%)p 7.96( 88.44%)d 0.04(  0.45%)
                          0.025%  C 34 s(  0.49%)p99.99( 99.20%)d 0.62(  0.31%)
                          0.130%  C 37 s( 28.34%)p 2.51( 71.08%)d 0.02(  0.58%)
                          0.310%  C 38 s( 13.43%)p 6.32( 84.87%)d 0.13(  1.71%)
                          0.060%  C 51 s( 30.78%)p 2.18( 67.14%)d 0.07(  2.08%)
                          0.017%  C 58 s(  4.01%)p23.68( 94.84%)d 0.29(  1.16%)
                          0.013%  C 69 s( 19.77%)p 3.95( 78.07%)d 0.11(  2.16%)
                          0.016%  H105 s( 99.71%)p 0.00(  0.29%)
                          0.015%  H117 s( 99.31%)p 0.01(  0.69%)
                          0.022%  H159 s( 99.88%)p 0.00(  0.12%)
                          0.039%  H169 s( 99.71%)p 0.00(  0.29%)
                          0.231%  P189 s(  2.37%)p34.73( 82.21%)d 6.52( 15.42%)
                         50.917%  P191 s( 14.10%)p 6.03( 84.99%)d 0.06(  0.91%)
                          0.268%  P192 s( 20.68%)p 3.06( 63.34%)d 0.77( 15.98%)
                          0.029%  P193 s( 73.50%)p 0.28( 20.73%)d 0.08(  5.77%)
                         47.151%  P195 s( 12.09%)p 7.18( 86.86%)d 0.09(  1.04%)
                          0.077% Cl198 s( 13.19%)p 6.08( 80.17%)d 0.50(  6.64%)
                          0.071% Cl200 s(  4.98%)p11.08( 55.17%)d 8.00( 39.85%)
                          0.231% Ag201 s( 72.01%)p 0.07(  4.90%)d 0.31( 22.50%)
                                                 f 0.01(  0.59%)
                          0.030% Ag202 s( 17.59%)p 2.58( 45.31%)d 2.09( 36.82%)
                                                 f 0.02(  0.27%)
 382. (2.00000)  97.8764% BD ( 1) P192- P195
                          0.064%  C 13 s(  9.35%)p 9.61( 89.91%)d 0.08(  0.74%)
                          0.013%  C 19 s( 20.13%)p 3.78( 76.07%)d 0.19(  3.80%)
                          0.125%  C 21 s( 11.07%)p 7.99( 88.48%)d 0.04(  0.45%)
                          0.020%  C 23 s(  1.00%)p98.53( 98.80%)d 0.20(  0.20%)
                          0.024%  C 29 s(  0.42%)p99.99( 99.29%)d 0.71(  0.30%)
                          0.303%  C 37 s( 12.71%)p 6.73( 85.51%)d 0.14(  1.78%)
                          0.122%  C 38 s( 28.26%)p 2.52( 71.11%)d 0.02(  0.63%)
                          0.056%  C 49 s( 31.88%)p 2.07( 65.90%)d 0.07(  2.22%)
                          0.016%  C 57 s(  4.51%)p20.88( 94.27%)d 0.27(  1.21%)
                          0.012%  C 70 s( 18.90%)p 4.18( 79.07%)d 0.11(  2.03%)
                          0.018%  H106 s( 99.68%)p 0.00(  0.32%)
                          0.017%  H118 s( 99.46%)p 0.01(  0.54%)
                          0.023%  H162 s( 99.87%)p 0.00(  0.13%)
                          0.038%  H174 s( 99.73%)p 0.00(  0.27%)
                          0.230%  P189 s(  2.34%)p35.01( 81.96%)d 6.71( 15.70%)
                          0.264%  P191 s( 22.39%)p 2.75( 61.56%)d 0.72( 16.05%)
                         50.771%  P192 s( 13.85%)p 6.15( 85.23%)d 0.07(  0.92%)
                          0.027%  P194 s( 64.43%)p 0.46( 29.91%)d 0.09(  5.66%)
                         47.333%  P195 s( 12.07%)p 7.20( 86.90%)d 0.09(  1.04%)
                          0.077% Cl198 s( 13.26%)p 6.05( 80.23%)d 0.49(  6.51%)
                          0.072% Cl200 s(  5.94%)p 9.13( 54.23%)d 6.71( 39.84%)
                          0.029% Ag201 s( 16.55%)p 2.47( 40.93%)d 2.55( 42.19%)
                                                 f 0.02(  0.32%)
                          0.210% Ag202 s( 67.16%)p 0.09(  5.97%)d 0.39( 26.22%)
                                                 f 0.01(  0.65%)
```

```
 383. (2.00000)  97.5474% BD ( 1) P193- P196
                          0.053%  C 16 s(  4.60%)p20.61( 94.77%)d 0.14(  0.64%)
                          0.022%  C 27 s(  1.58%)p62.10( 98.25%)d 0.11(  0.17%)
                          0.172%  C 30 s( 10.69%)p 8.32( 88.95%)d 0.03(  0.36%)
                          0.017%  C 32 s( 12.40%)p 6.80( 84.36%)d 0.26(  3.23%)
                          0.107%  C 41 s( 32.52%)p 2.06( 66.86%)d 0.02(  0.62%)
                          0.336%  C 43 s( 15.92%)p 5.18( 82.46%)d 0.10(  1.62%)
                          0.032%  C 46 s(  0.48%)p99.99( 99.27%)d 0.53(  0.25%)
                          0.080%  C 54 s( 35.81%)p 1.75( 62.78%)d 0.04(  1.41%)
                          0.015%  C 55 s(  2.19%)p44.12( 96.53%)d 0.59(  1.28%)
                          0.019%  C 63 s(  3.83%)p24.75( 94.71%)d 0.38(  1.47%)
                          0.015%  C 66 s(  3.87%)p24.51( 94.80%)d 0.34(  1.33%)
                          0.052%  H110 s( 99.94%)p 0.00(  0.06%)
                          0.016%  H165 s( 99.59%)p 0.00(  0.41%)
                          0.026%  H179 s( 99.73%)p 0.00(  0.27%)
                          0.523%  P190 s( 11.19%)p 6.98( 78.04%)d 0.96( 10.78%)
                         50.608%  P193 s( 13.37%)p 6.41( 85.69%)d 0.07(  0.94%)
                          0.236%  P194 s( 28.54%)p 1.79( 51.23%)d 0.71( 20.23%)
                         47.110%  P196 s( 12.28%)p 7.04( 86.48%)d 0.10(  1.24%)
                          0.199% Cl197 s( 16.14%)p 5.10( 82.32%)d 0.10(  1.54%)
                          0.098% Cl199 s(  5.77%)p10.97( 63.31%)d 5.36( 30.92%)
                          0.102% Ag201 s( 38.97%)p 0.19(  7.30%)d 1.35( 52.56%)
                                                 f 0.03(  1.16%)
                          0.025% Ag202 s( 20.36%)p 2.01( 40.97%)d 1.89( 38.47%)
                                                 f 0.01(  0.20%)
 384. (2.00000)  97.5423% BD ( 1) P194- P196
                          0.050%  C 17 s(  4.76%)p19.85( 94.58%)d 0.14(  0.65%)
                          0.017%  C 26 s( 12.49%)p 6.75( 84.25%)d 0.26(  3.26%)
                          0.185%  C 27 s( 10.01%)p 8.96( 89.65%)d 0.03(  0.34%)
                          0.021%  C 30 s(  1.76%)p55.71( 98.05%)d 0.11(  0.19%)
                          0.033%  C 40 s(  0.42%)p99.99( 99.33%)d 0.60(  0.25%)
                          0.351%  C 41 s( 16.45%)p 4.99( 82.01%)d 0.09(  1.54%)
                          0.117%  C 43 s( 32.40%)p 2.07( 67.01%)d 0.02(  0.59%)
                          0.016%  C 52 s(  1.91%)p50.79( 96.94%)d 0.60(  1.15%)
                          0.081%  C 53 s( 37.06%)p 1.66( 61.56%)d 0.04(  1.38%)
                          0.020%  C 64 s(  4.00%)p23.68( 94.65%)d 0.34(  1.35%)
                          0.014%  C 65 s(  3.87%)p24.48( 94.85%)d 0.33(  1.28%)
                          0.010%  C 72 s(  7.64%)p11.77( 89.91%)d 0.32(  2.45%)
                          0.051%  H112 s( 99.95%)p 0.00(  0.05%)
                          0.017%  H166 s( 99.57%)p 0.00(  0.43%)
                          0.027%  H180 s( 99.76%)p 0.00(  0.24%)
                          0.499%  P190 s( 11.39%)p 6.82( 77.63%)d 0.96( 10.98%)
                          0.266%  P193 s( 28.98%)p 1.81( 52.53%)d 0.64( 18.49%)
                         50.655%  P194 s( 13.51%)p 6.33( 85.55%)d 0.07(  0.94%)
                         47.040%  P196 s( 12.05%)p 7.20( 86.71%)d 0.10(  1.23%)
                          0.189% Cl197 s( 16.53%)p 4.95( 81.79%)d 0.10(  1.68%)
                          0.090% Cl199 s(  6.04%)p10.06( 60.81%)d 5.48( 33.14%)
                          0.025% Ag201 s( 24.62%)p 1.63( 40.19%)d 1.42( 34.99%)
                                                 f 0.01(  0.20%)
                          0.097% Ag202 s( 39.12%)p 0.20(  7.67%)d 1.33( 51.98%)
                                                 f 0.03(  1.23%)
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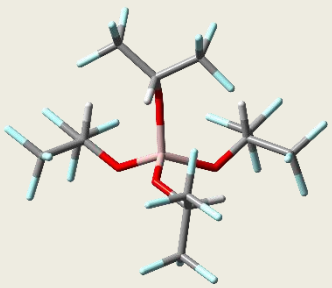
 385. (2.00000)  99.3606% BD ( 1) P195-Cl200
                          0.033%  C 37 s( 27.18%)p 2.65( 71.92%)d 0.03(  0.90%)
                          0.032%  C 38 s( 27.61%)p 2.59( 71.46%)d 0.03(  0.93%)
                          0.011%  H159 s( 98.84%)p 0.01(  1.16%)
                          0.013%  H162 s( 98.96%)p 0.01(  1.04%)
                          0.017%  H169 s( 99.51%)p 0.00(  0.49%)
                          0.020%  H174 s( 99.59%)p 0.00(  0.41%)
                          0.032%  P189 s( 16.11%)p 4.72( 76.11%)d 0.48(  7.78%)
                          0.145%  P191 s( 30.36%)p 1.02( 30.96%)d 1.27( 38.69%)
                          0.143%  P192 s( 31.43%)p 0.98( 30.72%)d 1.20( 37.85%)
                         32.455%  P195 s(  7.91%)p11.44( 90.50%)d 0.20(  1.59%)
                         66.990% Cl200 s( 14.20%)p 5.99( 85.11%)d 0.05(  0.70%)
                          0.018% Ag201 s( 14.65%)p 2.17( 31.74%)d 3.63( 53.16%)
                                                   f 0.03(  0.45%)
                          0.023% Ag202 s(  6.30%)p 5.39( 33.95%)d 9.42( 59.33%)
                                                   f 0.07(  0.42%)
 386. (2.00000)  99.2590% BD ( 1) P196-Cl199
                          0.018%  C 53 s( 14.04%)p 6.07( 85.27%)d 0.05(  0.69%)
                          0.018%  C 54 s( 15.14%)p 5.56( 84.17%)d 0.05(  0.69%)
                          0.067%  P190 s( 20.10%)p 3.58( 71.89%)d 0.40(  8.01%)
                          0.147%  P193 s( 13.50%)p 4.07( 54.97%)d 2.34( 31.53%)
                          0.145%  P194 s( 13.48%)p 4.07( 54.88%)d 2.35( 31.63%)
                         33.598%  P196 s(  8.92%)p10.04( 89.51%)d 0.18(  1.57%)
                          0.030% Cl197 s(  8.19%)p11.14( 91.25%)d 0.07(  0.56%)
                         65.784% Cl199 s( 14.39%)p 5.89( 84.82%)d 0.05(  0.79%)
                          0.051% Ag201 s( 64.71%)p 0.13(  8.19%)d 0.42( 26.99%)
                                                   f 0.00(  0.11%)
                          0.047% Ag202 s( 68.41%)p 0.10(  7.08%)d 0.36( 24.41%)
                                                   f 0.00(  0.11%)
```

6.3 $[Al(OR^F)_4]^-$

6.3.1 Optimized structure

C	-0.60906	-3.63622	-0.33289
C	-2.87917	-2.50723	-0.21228
C	-1.36934	-2.34062	-0.04774
C	3.88425	-1.18787	-1.10673
C	2.98193	-0.03405	-0.67441
C	-1.01268	0.22708	3.06679
C	1.34918	1.15162	3.11270
C	0.15081	0.77799	2.24302
C	3.58078	1.33244	-1.00865
C	-1.91525	1.64937	-1.15774
C	-2.55866	2.79963	-0.38655
C	-1.96563	1.87305	-2.67021
H	-1.20449	-2.13528	1.02813
H	2.94786	-0.07611	0.43223
H	-2.55302	0.76313	-0.96996
H	-0.21946	1.72614	1.80596
O	-0.93899	-1.34639	-0.88353
O	1.76104	-0.16874	-1.27906
O	0.53866	-0.15309	1.31629
O	-0.61789	1.50734	-0.74480
F	-0.98618	-4.63131	0.49422



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F           0.70073       -3.43670       -0.14065
F          -0.77079       -4.07567       -1.58539
F          -3.38399       -3.41354        0.64371
F           3.33906       -2.35360       -0.74039
F          -3.23316       -2.88170       -1.44666
F           4.07838       -1.23166       -2.42985
F           5.09964       -1.11918       -0.52698
F          -0.70406       -0.91063        3.70443
F          -3.49834       -1.34148        0.04150
F           1.84895        0.10999        3.78804
F          -2.04625       -0.04862        2.25291
F          -1.45238        1.09954        3.98786
F           3.78702        1.50724       -2.31937
F           2.33490        1.63564        2.34070
F           4.75852        1.53494       -0.38754
F           1.04531        2.10556        4.01117
F          -2.52592        2.53930        0.93202
F           2.74798        2.29938       -0.59989
F          -1.34076        0.86728       -3.29499
F          -3.23132        1.90473       -3.12989
F          -3.85013        2.97223       -0.72133
F          -1.93734        3.96902       -0.57144
F          -1.37474        3.01139       -3.05359
Al          0.20133       -0.04855       -0.44283
```

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