

Prototypical phosphine complexes of antimony(III)

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Supporting Information

SECTION 1: I.R. / Raman characterization of selected compounds:

Cl₃(PMe₃)Sb.

Raman (int): 66.46(25), 77.0(36), 85.7(43), 91.5(32), 119.5(36), 127.2(68), 139.7(45), 144.6(57), 158.1(23), 159.0(23), 161.9(23), 193.7(25), 211.1(68), 229.4(18), 243.9(54), 255.5(30), 266.1(52), 277.6(63), 310.4(102), 346.1(27), 1406.8(9), 1415.4(11), 2911.0(100), 2977.5(20), 2983.3(27), 2986.2(18), 3003.6(18), 3007.4(7).

Cl₃(PPh₃)Sb.

I.R. (Nujol mull, KBr plates, cm⁻¹): 499, 516, 615, 664, 668, 691, 712, 743, 845, 853, 925, 967, 994, 1022, 1036, 1070, 1093, 1167, 1180, 1306, 1377, 1395, 1405, 1436, 1457, 1718, 2321, 2854, 2926.

Cl₃(PMe₃)₂Sb.

Raman (int): 116(17), 130(11), 149(16), 173(6), 187(2), 206(3), 223(12), 257(38), 265(23), 328(2), 352(6), 668(35)747(6), 754(8), 757(7), 758(6), 947(2), 1303(3), 1307(3), 1402(6), 1411(7), 1420(7), 2794(2), 2899(100), 2904(69), 2909(42), 2972(33), 2982(20), 3000(11), 3015(3).

Cl₃(PPh₃)₂Sb.

I.R. (Nujol mull, KBr plates, cm⁻¹): 441, 489, 498, 516, 545, 616, 668, 691, 713, 723, 742, 774, 845, 853, 893, 926, 966, 994, 1022, 1026, 1070, 1092, 1157, 1169, 1305, 1377, 1399, 1437, 1457, 1463, 1718, 2345, 2363, 2669, 2724, 2924, 3421.

[Ph₂(PMe₃)Sb][OTf].

I.R. (Nujol mull, KBr plates): 448 (m), 515 (m), 571 (m), 637 (m), 664 (w), 695 (m), 728 (s), 756 (m), 853 (m), 959 (s), 996 (w), 1028 (m), 1064 (w), 1154 (s), 1223 (m), 1268 (s), 1294 (w), 1377 (s), 1460 (s), 1718 (m), 2725 (w), 2918 (s).

[Cl₂(PPh₃)₂Sb][OTf].

IR (Nujol mull, cm⁻¹, [relative intensities]): 1450, 1436, 1419, 1395, 1298, 1226, 1212, 1165, 1095, 1028, 1017, 998, 747, 725, 711, 691, 634, 619, 570, 516, 498, 493, 419, 398, 375, 354, 335, 328, 324, 304.

[Ph₂(PMe₃)₂Sb][OTf].

Raman (int): 65.5(28), 92.5(100), 133.9(50), 144.6(18), 159.9(28), 170.6(23), 226.5(31), 248.7(15), 263.2(21), 267.9(20), 312.3(19), 321.0(20), 341.2(8), 347.1(17), 571.1(7), 652.7(21), 669.1(31), 744.3(19), 748.2(11), 755.9(17), 996.96(46), 998.89(35), 1022.0(18), 1028.78(41), 1225.5(8), 1305.5(9), 1414.5(12), 1576.5(21), 2911.9(62), 2980.4(36), 2989.1(18), 3041.2(20), 3051.8(34).

[Cl(PMe₃)₂Sb][OTf]₂.

I.R. (Nujol mull, KBr plates, cm⁻¹): 514, 573, 638, 667, 722, 754, 759, 786, 848, 857, 866, 961, 1019, 1027, 1077, 1157, 1169, 1207, 1268, 1287, 1339, 1366, 1376, 1456, 1464, 1717, 2040, 2340, 2360, 2670, 2726, 2852, 2923, 2952.

Raman (int): 79.9(17), 86.4(18), 109.9(15), 129.1(22), 143.6(29), 148.4(24), 166.7(12), 177.3(25), 196.6(41), 218.8(36), 226.7(38), 262.2(14), 265.1(17), 275.7(9), 317.2(31), 342.2(50), 347.1(73), 355.7(45), 514.8(5), 575.6(15), 636.3(5), 671.0(34), 756.9(8), 763.6(47), 1022.0(27), 1028.8(100), 2915.5(39), 2923.5(41), 2327.4(41), 2932.2(31), 2987.2(13), 2990.1(13), 2996.8(20), 3006.5(24), 3010.3(15), 3020.9(6).

[(CH₃CN)₆Mg][Cl₄(PMe₃)Sb]₂.

Raman (int): 65.5(28), 92.5(100), 133.9(50), 144.6(18), 159.9(28), 170.6(23), 226.5(31), 248.7(15), 263.2(21), 267.9(20), 312.3(19), 321.0(20), 341.2(8), 347.1(17), 571.1(7), 652.7(21), 669.1(31), 744.3(19), 748.2(11), 755.9(17), 996.96(46), 998.89(35), 1022.0(18), 1028.78(41), 1225.5(8), 1305.5(9), 1414.5(12), 1576.5(21), 2911.9(62), 2980.4(36), 2989.1(18), 3041.2(20), 3051.8(34).

Cl₂(Ph)(PPh₃)Sb.

Raman (int): 91(100), 128(3), 150(16), 181(4), 198(12), 217(3), 249(9), 267(7), 311(12), 343(33), 410(13), 444(7), 518(22), 617(3), 685(2), 714(4), 749(3), 998(50), 1025(18), 1096(30), 1161(6), 1184(4), 1434(4), 1480(3), 1573(4), 1584(54), 3043(4), 3057(35), 3071(2),

SECTION 2: Cartesian Coordinates for calculated structures

Full reference for Gaussian 09: Gaussian 09, Revision **D.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[*pyr*-Cl₃(PMe₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -461.154219733

Sb	1.03451	0.00045	-0.00032
Cl	0.61183	2.28800	-1.01500
Cl	0.61421	-0.26460	2.48835
Cl	0.61391	-2.02284	-1.47351
P	-1.55197	-0.00060	0.00035
C	-2.20840	-1.54413	0.68534
H	-1.84681	-1.65769	1.70908
H	-3.30266	-1.52659	0.67757
H	-1.84683	-2.37944	0.08265
C	-2.20954	0.17768	-1.67846
H	-1.84798	-0.65201	-2.28886
H	-3.30377	0.17520	-1.65873
H	-1.84859	1.11741	-2.10075
C	-2.20932	1.36387	0.99465
H	-3.30355	1.34753	0.98345
H	-1.84755	1.25985	2.01936
H	-1.84846	2.30749	0.58107

[*mer*-Cl₃(PMe₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -461.144923169

Sb	-0.86401	-0.00001	-0.45593
Cl	-0.71901	2.56152	-0.48635
Cl	-0.71893	-2.56154	-0.48635
Cl	-1.20573	-0.00002	1.92152
P	1.68165	0.00002	0.07632
C	2.15014	-1.45657	1.04247
H	1.91220	-2.36012	0.47959
H	3.21698	-1.42184	1.28485
H	1.55998	-1.46550	1.96169
C	2.15011	1.45663	1.04246
H	1.55995	1.46555	1.96168
H	3.21694	1.42193	1.28484
H	1.91214	2.36017	0.47957
C	2.66801	0.00003	-1.44879
H	3.73762	0.00004	-1.21825
H	2.42836	-0.88998	-2.03644

H	2.42834	0.89002	-2.03645
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[*fac*-Cl₃(PMe₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -461.155031395

Sb	-0.85718	0.00000	-0.51289
Cl	-3.26379	0.00000	-0.23014
Cl	-0.51389	-1.82542	0.98980
Cl	-0.51389	1.82542	0.98980
P	2.24345	0.00000	-0.21847
C	2.62811	0.00000	1.57358
H	3.70940	0.00000	1.74943
H	2.18388	0.88338	2.03807
H	2.18388	-0.88338	2.03808
C	3.22284	1.43405	-0.82300
H	2.79082	2.35852	-0.42997
H	4.26869	1.36791	-0.50329
H	3.19093	1.48023	-1.91546
C	3.22284	-1.43405	-0.82300
H	4.26869	-1.36791	-0.50329
H	2.79082	-2.35852	-0.42997
H	3.19092	-1.48024	-1.91546

[*pyr*-Cl₃(PPh₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -1036.50602861

Sb	-0.02905	0.01046	-2.19677
Cl	-2.32524	1.02153	-1.85015
Cl	2.00224	1.49499	-1.90595
Cl	0.24946	-2.48957	-1.90153
P	0.00614	-0.00225	0.46642
C	-1.59405	-0.50531	1.13929
C	-2.25380	0.28292	2.08892
C	-2.17779	-1.70152	0.69720
C	-3.48774	-0.12345	2.59246
H	-1.81159	1.21057	2.43033
C	-3.40848	-2.10028	1.20734
H	-1.67504	-2.31351	-0.04198
C	-4.06600	-1.31255	2.15329
H	-3.99635	0.49322	3.32605
H	-3.85773	-3.02394	0.85834
H	-5.02940	-1.62417	2.54368

C	0.38652	1.63763	1.12423
C	1.41733	1.81681	2.05362
C	-0.36359	2.74091	0.69158
C	1.69428	3.09015	2.54676
H	2.00449	0.97030	2.38731
C	-0.08140	4.00770	1.19109
H	-1.15908	2.61001	-0.03210
C	0.94756	4.18512	2.11705
H	2.49674	3.22378	3.26461
H	-0.66144	4.85831	0.84933
H	1.16870	5.17646	2.49914
C	1.25151	-1.14865	1.09998
C	0.91435	-2.12597	2.04317
C	2.57114	-1.05256	0.63476
C	1.89064	-2.99966	2.51734
H	-0.10379	-2.20953	2.40244
C	3.53932	-1.92732	1.11564
H	2.83765	-0.30195	-0.09955
C	3.20142	-2.90238	2.05518
H	1.62299	-3.75759	3.24605
H	4.55738	-1.85176	0.74875
H	3.95870	-3.58733	2.42265

[*mer*-Cl₃(PPh₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -1036.46184064

Sb	-1.57970	1.11893	-0.98714
Cl	0.16814	3.01023	-1.03739
Cl	-2.69027	-1.15518	-1.33483
Cl	-2.49157	1.54673	1.19554
P	0.38635	-0.29112	0.13155
C	-0.19043	-1.56979	1.26867
C	-0.10502	-1.35695	2.65238
C	-0.77911	-2.74868	0.78504
C	-0.59715	-2.31206	3.53682
H	0.34951	-0.45420	3.04028
C	-1.26073	-3.70111	1.67725
H	-0.87279	-2.91425	-0.27852
C	-1.17385	-3.48485	3.05201
H	-0.52784	-2.13752	4.60526
H	-1.71576	-4.60802	1.29385
H	-1.55703	-4.22794	3.74384
C	1.58443	0.71428	1.04103
C	2.95312	0.44689	0.92025
C	1.14413	1.73584	1.89254
C	3.87311	1.18921	1.65671

H	3.30112	-0.33048	0.25006
C	2.06933	2.46872	2.62886
H	0.08987	1.96932	1.96680
C	3.43259	2.19728	2.51268
H	4.93329	0.98115	1.55707
H	1.72401	3.26429	3.28022
H	4.15149	2.77809	3.08147
C	1.29098	-1.06423	-1.22997
C	1.76334	-2.38023	-1.16721
C	1.56739	-0.27653	-2.35746
C	2.48951	-2.90874	-2.23251
H	1.56772	-2.98783	-0.29255
C	2.29463	-0.81168	-3.41645
H	1.24196	0.75867	-2.39674
C	2.75165	-2.12848	-3.35778
H	2.85052	-3.93055	-2.18089
H	2.50442	-0.19823	-4.28602
H	3.31401	-2.54479	-4.18713

[*fac*-Cl₃(PPh₃)Sb]

Theory/Basis: B3LYP-D/Def2-TZVPP/6-311

E(RB3LYP) = -1036.46918978

Sb	-2.26752	-0.02326	-0.46238
Cl	-4.69126	-0.00322	-0.55053
Cl	-2.16446	-1.83563	1.08194
Cl	-2.13244	1.79024	1.07964
P	0.80097	-0.00534	-0.04311
C	1.54516	1.25192	-1.13736
C	0.98957	2.54064	-1.10744
C	2.61961	0.99042	-1.99628
C	1.50880	3.54919	-1.91470
H	0.15580	2.75512	-0.44573
C	3.13145	2.00139	-2.80895
H	3.05380	-0.00218	-2.03025
C	2.57936	3.28096	-2.76881
H	1.07399	4.54289	-1.88047
H	3.96479	1.78836	-3.47104
H	2.97954	4.06616	-3.40217
C	1.57087	-1.57261	-0.56230
C	1.21163	-2.09859	-1.81296
C	2.45164	-2.29338	0.25146
C	1.73510	-3.31249	-2.24637
H	0.52694	-1.55176	-2.45549
C	2.96717	-3.51512	-0.18100

H	2.73313	-1.90063	1.22165
C	2.61352	-4.02546	-1.42838
H	1.45274	-3.70604	-3.21752
H	3.64798	-4.06664	0.45951
H	3.01609	-4.97633	-1.76211
C	1.51225	0.34907	1.59519
C	0.81617	-0.08509	2.73094
C	2.72962	1.02525	1.74786
C	1.34091	0.14213	4.00162
H	-0.13490	-0.59400	2.62101
C	3.24707	1.25596	3.02027
H	3.26593	1.37474	0.87241
C	2.55500	0.81243	4.14784
H	0.79503	-0.19538	4.87657
H	4.18936	1.78307	3.13150
H	2.95825	0.99556	5.13877

[Cl₃(PMe₃)Sb] - pyr
 Theory/Basis: MP2/Def2-TZVPP
 EMP2: -2079.1908276

Sb	-1.03678	-0.00624	-0.08823
Cl	-0.41542	-1.74728	-1.75854
Cl	-0.76863	-0.61843	2.31188
Cl	-0.53025	2.35541	-0.69924
P	1.49617	0.00900	0.12733
C	2.05739	1.20548	1.35343
H	3.14487	1.17902	1.41339
H	1.72314	2.19592	1.05409
H	1.62319	0.94891	2.31673
C	2.29891	0.43356	-1.42997
H	1.96536	1.42178	-1.73732
H	3.37972	0.42845	-1.29303
H	2.01351	-0.29859	-2.18151
C	2.13591	-1.59999	0.62906
H	3.22122	-1.54885	0.70906
H	1.70193	-1.86462	1.59028
H	1.85004	-2.33798	-0.11656

[Cl₂(PMe₃)Sb]¹⁺
 Theory/Basis: MP2/Def2-TZVPP
 EMP2: -1619.2243502

Sb	-0.85471	0.00000	-0.66254
Cl	-1.19851	-1.76726	0.79297

Cl	-1.19851	1.76726	0.79297
P	1.60668	0.00000	0.04449
C	2.42575	-1.47005	-0.59382
H	3.46371	-1.47739	-0.26199
H	1.92057	-2.35690	-0.21450
H	2.39772	-1.47322	-1.68198
C	1.72108	0.00000	1.83683
H	1.23294	-0.88828	2.23199
H	2.77400	0.00000	2.11923
H	1.23294	0.88829	2.23199
C	2.42575	1.47004	-0.59382
H	1.92058	2.35690	-0.21450
H	3.46371	1.47739	-0.26199
H	2.39772	1.47322	-1.68199

[Cl₄(PMe₃)Sb]¹⁻

Theory/Basis: MP2/Def2-TZVPP

EMP2: -2539.0275944

Sb	0.70380	-0.00000	-0.65911
Cl	1.78284	-1.73597	0.84101
Cl	-0.88036	-1.91700	-1.52573
Cl	1.78285	1.73596	0.84101
Cl	-0.88035	1.91700	-1.52573
P	-1.21811	0.00000	1.02862
C	-1.20098	-1.44527	2.11320
H	-0.27487	-1.45798	2.68114
H	-2.06749	-1.41605	2.77446
H	-1.22726	-2.33128	1.48178
C	-1.20097	1.44527	2.11321
H	-2.06747	1.41605	2.77447
H	-0.27486	1.45797	2.68114
H	-1.22725	2.33128	1.48179
C	-2.86990	0.00001	0.29679
H	-2.96493	-0.88631	-0.32460
H	-3.60648	0.00001	1.10114
H	-2.96492	0.88633	-0.32460

[Cl₂(PMe₃)₂Sb]¹⁺

Theory/Basis: MP2/Def2-TZVPP

EMP2: -2079.619648

Sb	0.00000	-0.00000	1.00076
Cl	0.28758	2.41723	0.40163

Cl	-0.28759	-2.41723	0.40162
P	-2.03932	0.11448	-0.53413
P	2.03932	-0.11447	-0.53413
C	3.31493	0.87084	0.27332
H	3.51238	0.47001	1.26637
H	4.22655	0.81644	-0.32147
H	2.98081	1.90141	0.35658
C	1.78637	0.56660	-2.18339
H	1.32401	1.54745	-2.09935
H	2.75601	0.65867	-2.67329
H	1.16000	-0.10701	-2.76362
C	2.70641	-1.77429	-0.72600
H	3.64208	-1.70635	-1.28145
H	2.89071	-2.21245	0.25269
H	1.99601	-2.40314	-1.25497
C	-2.70640	1.77430	-0.72600
H	-3.64207	1.70635	-1.28145
H	-2.89071	2.21245	0.25269
H	-1.99601	2.40314	-1.25496
C	-3.31493	-0.87083	0.27332
H	-4.22655	-0.81644	-0.32147
H	-2.98082	-1.90141	0.35657
H	-3.51238	-0.47000	1.26637
C	-1.78637	-0.56659	-2.18339
H	-1.32402	-1.54745	-2.09935
H	-2.75601	-0.65866	-2.67329
H	-1.16000	0.10701	-2.76362

[Cl(PMe₃)₂Sb]²⁺

Theory/Basis: MP2/Def2-TZVPP

EMP2: -1619.5154434

Sb	0.00000	-0.63065	-0.82080
P	1.99673	0.63850	0.16007
P	-1.99673	0.63850	0.16007
C	3.32478	-0.55690	-0.04928
H	3.44912	-0.80838	-1.10183
H	4.24882	-0.10992	0.32158
H	3.10907	-1.45791	0.52368
C	1.86240	1.04507	1.90515
H	2.85408	1.33940	2.25460
H	1.17717	1.87590	2.05373
H	1.53182	0.17358	2.46768
C	2.37002	2.11423	-0.79780
H	1.58751	2.86104	-0.67809

H	3.31214	2.52877	-0.43481
H	2.48006	1.86092	-1.85140
C	-2.37002	2.11424	-0.79779
H	-3.31214	2.52877	-0.43481
H	-1.58750	2.86104	-0.67809
H	-2.48005	1.86092	-1.85140
C	-1.86240	1.04506	1.90515
H	-1.17717	1.87590	2.05374
H	-2.85409	1.33940	2.25460
H	-1.53182	0.17357	2.46768
C	-3.32478	-0.55689	-0.04928
H	-4.24882	-0.10991	0.32157
H	-3.44912	-0.80838	-1.10184
H	-3.10907	-1.45791	0.52367
Cl	0.00000	-2.04397	1.01480