Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

How Lewis acidic is your cation? Putting phosphenium ions on the fluoride-ion affinity scale.

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This document contains the SCF energies, ZPEs, XYZ coordinates and vibrational frequencies for the stationary points reported in the main section of the publication.

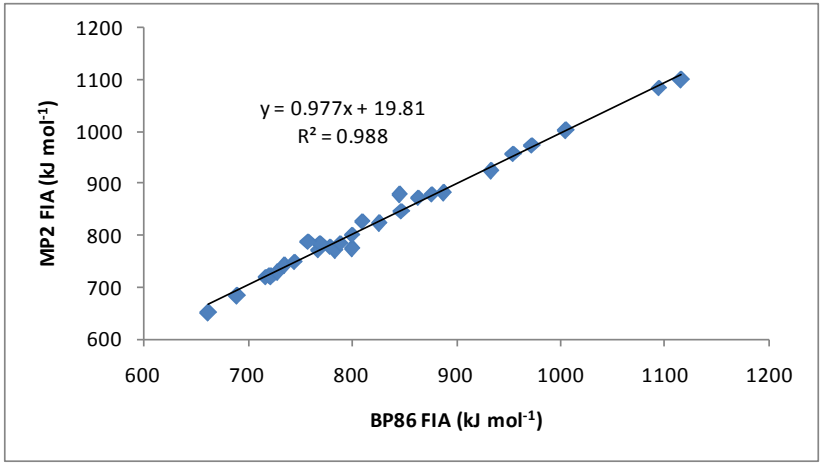
Table S1 – Summary of energetic data. SCF energies and ZPEs are in Hartrees. The chemical potential and thermal energy corrections are in kJ mol^{-1} and are calculated at 298.15K. Thermal-energy-corrected energies (at both levels of theory) were used to calculate FIAs.

Structure	Compound number	(RI-)BP86/SVP Energy (a.u.)	(RI-)MP2/def2-TZVPP Energy (a.u.)	ZPE (a.u.)	Chem. Pot. (kJ mol-1)	Energy Corr. (kJ mol-1)	S (kJ mol-1 K-1)	Thermal Corrected BP86 Energy (kJ mol-1)	Thermal Corrected MP2 Energy (kJ mol-1)
OCF3-		-412.637275	-412.4365159	0.015425	-28.68	51.60	0.2776	-1083119	-1082592
OCF2		-312.803019	-312.6254593	0.013794	-30.03	44.95	0.2598	-821060	-820594
Grutzmacher's	**1**	-1813.608916		0.649337	1532.42	1802.14	0.9130	-4758919	
Grutzmacher's-F	**1-F**	-1913.608919		0.650613	1526.17	1809.95	0.9601	-5021411	
(H2C2N2Me2)P+	**2**	-607.620027	-606.8815256	0.120357	233.38	336.01	0.3526	-1594664	-1592725
(H2C2N2Me2)PF	**2-F**	-707.626633	-706.8604535	0.120631	225.83	341.33	0.3957	-1857176	-1855165
aminocatP+	**3**	-761.169081	-760.2098187	0.166792	347.85	464.10	0.3982	-1997602	-1995084
aminocatPF	**3-F**	-861.186540	-860.2014455	0.167633	342.2	470.58	0.4389	-2260142	-2257556
(H4C2N2Me2)P+	**4**	-608.806954	-608.0629476	0.142915	289.00	396.92	0.3703	-1597719	-1595766
(H4C2N2Me2)PF	**4-F**	-708.834677	-708.0688883	0.144127	288.05	403.22	0.3946	-1860285	-1858275
(Me2N)2P+	**5**	-609.992165	-609.2468990	0.162602	336.78	452.79	0.3974	-1600774	-1598818
(Me2N)2PF	**5-F**	-710.021676	-709.2528336	0.163379	333.2	458.54	0.4287	-1863346	-1861328
(iPr2N)(mes)P+	**6**	-981.975266	-980.6740565	0.358138	805.13	996.85	0.6513	-2576686	-2573270
(iPr2N)(mes)PF	**6-F**	-1082.006027	-1080.682378	0.361182	812.84	1007.00	0.6595	-2839256	-2835782
iPr2NPdiCF3PhP+	**7**	-1537.734316		0.288207	616.32	817.50	0.6831	-4035733	
iPr2NPdiCF3PhPF	**7-F**	-1637.764048		0.290545	620.58	826.44	0.6988	-4298302	
iPr2NP(CF3)(CF2)PhPF	**7_carb**	-1537.690886		0.287173	612.31	815.86	0.6910	-4035620	
(iPr2N)(diMePh)P+	**8**	-942.687766	-941.4442422	0.331520	740.95	922.30	0.6166	-2473631	-2470366
(iPr2N)(diMePh)PF	**8-F**	-1042.721201	-1041.454752	0.334809	752.72	932.42	0.6110	-2736208	-2732884
(Me2N)(mes)P+	**9**	-824.846557	-823.7642342	0.249549	543.5	696.08	0.5201	-2164524	-2161683
(Me2N)(mes)PF	**9-F**	-924.882004	-923.7790937	0.251804	543.92	705.36	0.5498	-2427107	-2424212
(Me2N)(diMePh)P+	**10**	-785.557709	-784.533502	0.222906	479.52	621.57	0.4848	-2061465	-2058776
(Me2N)(diMePh)PF	**10-F**	-885.597155	-884.5514074	0.225490	483.00	631.09	0.5050	-2324059	-2321314
thiocatP+	**11**	-1368.179912	-1366.644444	0.082408	131.28	236.43	0.3610	-3591233	-3587203
thiocatPF	**11-F**	-1468.233717	-1466.670472	0.084284	129.04	245.26	0.3981	-3853866	-3849762
(Me2N)(Ph)P+	**12**	-706.989634	-706.0770291	0.170358	352.25	474.37	0.4179	-1855371	-1852975
(Me2N)(Ph)PF	**12-F**	-807.036930	-806.1029572	0.171987	351.38	482.25	0.4473	-2117987	-2115536

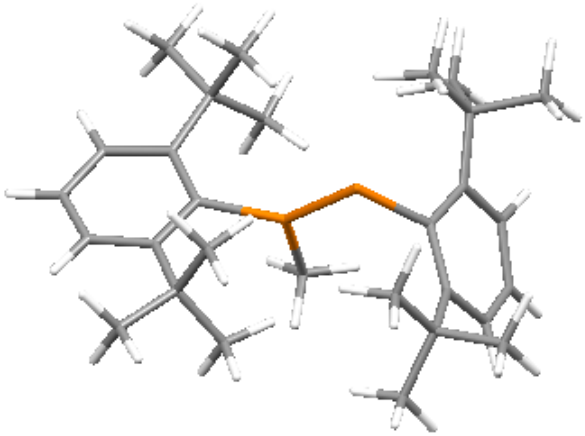
H2C2S2P+	**13**	-1214.623898	-1213.310973	0.036043	19.53	107.57	0.3036	-3188278	-3184831
H2C2S2PF	**13-F**	-1314.684061	-1313.338179	0.037644	16.39	116.02	0.3425	-3450927	-3447394
(Me2N)(tBu)P+	**14**	-633.214100	-632.4106484	0.198822	425.2	552.99	0.4369	-1661632	-1659522
(Me2N)(tBu)PF	**14-F**	-733.266229	-732.4396032	0.201078	427.65	561.76	0.4581	-1924260	-1922090
(H2N)2P+	**15**	-452.870681	-452.3751115	0.052340	71.04	148.36	0.2677	-1188635	-1187334
(H2N)2PF	**15-F**	-552.919171	-552.4068364	0.054214	68.25	156.91	0.3057	-1451253	-1449909
(H4C2ONMe)P+	**16**	-589.364942	-588.6938530	0.103576	191.44	288.84	0.3350	-1546792	-1545030
(H4C2ONMe)PF	**16-F**	-689.420472	-688.7251329	0.105307	191.19	296.69	0.3621	-1809430	-1807604
(Mes)2P+	**17**	-1039.687732	-1038.268744	0.336134	736.31	939.92	0.6913	-2728238	-2724513
(Mes)2PF	**17-F**	-1139.733142	-1138.302686	0.339784	753.25	951.32	0.6727	-2990846	-2987091
(MeS)2P+	**18**	-1217.030286	-1215.697169	0.076779	112.96	223.07	0.3777	-3194479	-3190979
(MeS)2PF	**18-F**	-1317.090983	-1315.735225	0.078969	111.37	232.87	0.4159	-3457128	-3453570
H4C2S2P+	**19**	-1215.831966	-1214.506295	0.058749	77.36	168.82	0.3151	-3191388	-3187908
H4C2S2PF	**19-F**	-1315.902208	-1314.552524	0.061004	76.24	178.37	0.3508	-3454062	-3450520
Me2NPCl+	**20**	-935.617263	-934.6419671	0.082488	134.66	234.44	0.3430	-2455758	-2453198
Me2NPClF	**20-F**	-1035.688072	-1034.688660	0.084741	134.56	244.06	0.3756	-2718435	-2715811
Ph2P+	**21**	-803.977452	-802.8968050	0.177932	366.90	496.05	0.4415	-2109942	-2107106
Ph2PF	**21-F**	-904.041252	-902.9442805	0.179968	364.01	504.79	0.4805	-2372601	-2369721
(MeO)2P+	**22**	-571.119593	-570.5163111	0.083044	134.61	237.16	0.3523	-1498949	-1497366
(MeO)2PF	**22-F**	-671.198158	-670.5717205	0.085472	135.65	246.39	0.3797	-1761646	-1760002
catP+	**23**	-722.263745	-721.4349051	0.087210	149.08	245.82	0.3328	-1895694	-1893518
catPF	**23-F**	-822.348013	-821.500263	0.089378	148.22	254.99	0.3664	-2158406	-2156181
(C6F5)PhP+	**24**	-1299.777755	-1298.506483	0.137930	245.99	403.27	0.5359	-3411511	-3408174
(C6F5)PhPF	**24-F**	-1399.855178	-1398.573222	0.140110	245.99	412.44	0.5693	-3674205	-3670840
(H2C2O2)P+	**25**	-568.700412	-568.0973053	0.041161	38.26	118.39	0.2771	-1492718	-1491135
(H2C2O2)PF	**25-F**	-668.789540	-668.164794	0.043063	36.53	127.00	0.3117	-1755443	-1753803
(H4C2O2)P+	**26**	-569.915097	-569.3175754	0.064061	91.22	181.05	0.3096	-1495844	-1494275
(H4C2O2)PF	**26-F**	-670.008692	-669.3857650	0.066750	96.73	190.35	0.3223	-1758580	-1756945
P(PH2)2+	**27**	-1025.948418	-1024.72069	0.035239	17.13	107.85	0.3126	-2693004	-2689781
P(F)(PH2)2+	**27-F**	-1126.040539	-1124.789984	0.037947	16.67	118.18	0.3488	-2955736	-2952453
I2P+	**28**	-363.923506	-934.9207191	0.001886	-76.82	16.15	0.3201	-955281	-2454148
I2PF	**28-F**	-464.034830	-1035.005265	0.004313	-77.57	26.18	0.3563	-1218063	-2716860
Me2P+	**29**	-420.711374	-420.1864158	0.069211	111.16	195.76	0.2921	-1104169	-1102791
Me2PF	**29-F**	-520.833671	-520.2870024	0.074980	120.99	212.71	0.3159	-1366973	-1365538
Br2P+	**30**	-5489.266795	-5485.751712	0.002355	-71.14	16.76	0.3032	-14409306	-14400079

Br2PF	**30-F**	-5589.393238	-5585.855322	0.004869	-71.29	26.80	0.3373	-14672128	-14662841
Cl2P+	**31**	-1261.198397	-1259.993526	0.003139	-62.99	17.98	0.2799	-3310625	-3307463
Cl2PF	**31-F**	-1361.337156	-1360.107691	0.005704	-62.84	27.86	0.3125	-3573480	-3570252
F2P+	**32**	-540.503818	-540.0607352	0.005269	-51.51	22.39	0.2562	-1418798	-1417635
F3P	**32-F**	-640.676473	-640.2067236	0.008203	-47.50	32.34	0.2761	-1681741	-1680508
H2P+	**33**	-342.064199	-341.6615818	0.013119	-17.46	41.94	0.2075	-897874	-896817
H2PF	**33-F**	-442.247039	-441.8152223	0.018752	-13.2	57.21	0.2445	-1160839	-1159705
SbF5	**34**	-504.340725	-738.3567709	0.010352	-56.28	47.06	0.3549	-1323845	-1938137
SbF5-	**34-F**	-604.281477	-838.279014	0.012463	-49.13	55.55	0.3594	-1586181	-2200424
Me3C+	**35**	-157.412627	-157.1658146	0.112579	217.57	312.56	0.3269	-412893	-412245
Me3CF	**35-F**	-257.490166	-257.2214768	0.119576	240.79	330.83	0.3103	-675578	-674873
Me3Si+	**36**	-408.807432	-408.2381403	0.105301	188.89	297.87	0.3738	-1072819	-1071325
Me3SiF	**36-F**	-508.927550	-508.3395593	0.109944	207.67	310.89	0.3545	-1335621	-1334078
(CF3)P(F)CF2+	**37**	-1015.717580	-1014.983297	0.028282	-21.42	98.96	0.4121	-2666157	-2664230
(CF3)2PF	**37-F**	-1115.851512	-1115.095582	0.031248	-17.20	108.78	0.4308	-2928999	-2927015
AsF5		-2734.777396	-2733.217082	0.012600	-45.32	50.42	0.3294	-7178738	-7174642
AsF6-		-2834.694320	-2833.117132	0.014952	-36.81	58.86	0.3292	-7441011	-7436871

Chart S1 – The correlation between FIAs calculated at the BP86/SV(P) level and MP2/def2-TZVPP level.



1: [{$(CH_3)_3C$}$_2C_6H_3$ CH_3PP{$(CH_3)_3C$}$_2C_6H_3$]$^+$



(RI-)BP86/SV(P) level:

SCF Energy = -1813.6089164600 E_h
Zero Point Energy = 0.0360429 E_h
Symmetry = C_s

XYZ Coordinates:
76

P	-0.32724	0.01416	-0.64743
P	1.18396	0.08142	0.76376
C	-2.10435	0.06987	-0.16698
H	-2.47354	1.11655	-0.21370
H	-2.21349	-0.31641	0.86857
C	-0.12943	-0.04337	-2.48320
C	-0.04667	1.18600	-3.23970
C	-0.28284	1.09824	-4.62741
H	-0.25533	2.00609	-5.24131
C	-0.55533	-0.11499	-5.25983
C	0.36733	2.57507	-2.67086
C	0.38479	3.68174	-3.75522
H	1.10450	3.46515	-4.57292
H	0.70855	4.63513	-3.28523
H	-0.61872	3.85991	-4.19929
C	-0.61493	3.06690	-1.58389
H	-1.65431	3.12201	-1.97633
H	-0.32499	4.08200	-1.23585
H	-0.61572	2.41779	-0.68155
C	1.81827	2.46810	-2.12717
H	2.52176	2.20558	-2.94696
H	1.93031	1.69356	-1.33910
H	2.14326	3.44151	-1.69838
H	-0.76364	-0.13916	-6.34169
C	0.15486	0.05390	2.32491
C	-0.42953	1.26677	2.83587
C	-1.55307	1.13632	3.67994
H	-2.05094	2.04062	4.06261
C	-2.04000	-0.11367	4.07413
C	0.15554	2.70239	2.70042
C	1.40712	2.80971	1.81004
H	2.22056	2.12679	2.14362
H	1.82306	3.84071	1.86896
H	1.19386	2.63067	0.73305
C	0.60361	3.12816	4.13171
H	-0.24294	3.14313	4.84987
H	1.03833	4.15184	4.10205
H	1.37703	2.43684	4.53206
C	-0.91120	3.70361	2.18969
H	-1.77995	3.77974	2.87705
H	-1.29795	3.41765	1.18823
H	-0.47115	4.72155	2.10627
H	-2.94184	-0.18543	4.70368
C	-1.31527	-1.26425	3.74811
C	-0.17689	-1.22057	2.91316
C	0.68616	-2.51626	2.87890
C	1.95365	-2.43400	2.00917
H	2.61477	-1.58679	2.29933
H	2.55634	-3.36043	2.13936
H	1.72922	-2.37255	0.92010
C	1.17713	-2.74933	4.34071
H	0.33553	-2.89708	5.04935
H	1.81545	-3.65951	4.38232
H	1.78037	-1.88836	4.70297
C	-0.14231	-3.74259	2.42192
H	-1.02488	-3.92453	3.07101
H	-0.50602	-3.62062	1.37941
H	0.48496	-4.66044	2.45805
H	-1.62770	-2.22535	4.18557
H	-2.68554	-0.55393	-0.87665
C	-0.51262	-1.30375	-4.53036
C	-0.27821	-1.32475	-3.13997
C	-0.09041	-2.71971	-2.46784
C	-0.27232	-3.88867	-3.46969
H	0.45386	-3.84849	-4.30933
H	-0.09324	-4.84601	-2.93466
H	-1.30079	-3.93462	-3.88926
C	-1.11094	-2.97808	-1.33451
H	-2.15664	-2.85452	-1.69396
H	-1.00398	-4.01979	-0.96072
H	-0.95926	-2.31872	-0.45099
C	1.36777	-2.80940	-1.94341
H	2.09043	-2.73122	-2.78474
H	1.61057	-2.00062	-1.22356
H	1.53726	-3.78502	-1.43661
H	-0.66084	-2.24614	-5.07080

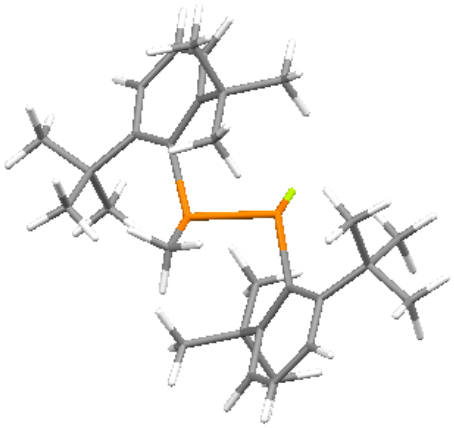
$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	13.76	0.01645	YES	YES
8		a	30.95	0.00265	YES	YES
9		a	34.41	0.06186	YES	YES
10		a	52.26	0.12618	YES	YES
11		a	59.59	0.19627	YES	YES
12		a	67.28	0.02437	YES	YES
13		a	72.21	0.04681	YES	YES
14		a	78.88	0.08447	YES	YES
15		a	87.85	0.09640	YES	YES
16		a	93.02	0.28804	YES	YES
17		a	98.81	0.00715	YES	YES
18		a	107.31	0.00655	YES	YES
19		a	112.61	0.10670	YES	YES
20		a	127.15	0.11049	YES	YES
21		a	145.88	0.39575	YES	YES

22	a	161.08	0.63066	YES	YES
23	a	175.25	1.87019	YES	YES
24	a	181.30	4.98267	YES	YES
25	a	187.83	2.34842	YES	YES
26	a	201.93	0.78738	YES	YES
27	a	208.12	0.51370	YES	YES
28	a	213.32	3.62949	YES	YES
29	a	220.56	4.85373	YES	YES
30	a	228.64	3.32256	YES	YES
31	a	237.18	2.09788	YES	YES
32	a	244.12	4.13545	YES	YES
33	a	253.32	0.29069	YES	YES
34	a	256.74	0.29566	YES	YES
35	a	261.73	0.98699	YES	YES
36	a	266.48	0.33733	YES	YES
37	a	269.91	2.77505	YES	YES
38	a	271.49	0.67664	YES	YES
39	a	279.53	0.76038	YES	YES
40	a	294.16	0.77264	YES	YES
41	a	306.23	1.26201	YES	YES
42	a	310.26	1.66681	YES	YES
43	a	318.40	0.37643	YES	YES
44	a	326.44	0.79368	YES	YES
45	a	328.52	0.73014	YES	YES
46	a	338.67	0.99943	YES	YES
47	a	341.30	2.97567	YES	YES
48	a	345.00	0.85511	YES	YES
49	a	345.95	4.07475	YES	YES
50	a	364.71	1.67496	YES	YES
51	a	373.83	2.34202	YES	YES
52	a	375.98	7.57256	YES	YES
53	a	378.30	4.48544	YES	YES
54	a	384.61	1.66089	YES	YES
55	a	386.22	2.78345	YES	YES
56	a	395.56	0.35331	YES	YES
57	a	400.15	0.56685	YES	YES
58	a	413.63	1.39971	YES	YES
59	a	420.81	1.05919	YES	YES
60	a	425.46	7.20391	YES	YES
61	a	456.90	3.31955	YES	YES
62	a	466.49	32.10801	YES	YES
63	a	496.63	1.93363	YES	YES
64	a	498.63	0.13483	YES	YES
65	a	502.79	1.65785	YES	YES
66	a	506.17	0.44923	YES	YES
67	a	530.34	6.17461	YES	YES
68	a	534.34	2.10891	YES	YES
69	a	537.76	4.88885	YES	YES
70	a	553.98	1.94185	YES	YES
71	a	578.60	1.81850	YES	YES
72	a	624.31	5.50602	YES	YES
73	a	634.21	0.95103	YES	YES
74	a	705.85	3.83251	YES	YES
75	a	708.82	0.23296	YES	YES
76	a	714.92	23.09694	YES	YES
77	a	728.99	17.63818	YES	YES
78	a	733.45	0.09725	YES	YES
79	a	735.43	0.20835	YES	YES
80	a	742.75	4.89227	YES	YES
81	a	794.63	15.98227	YES	YES
82	a	801.10	13.84142	YES	YES
83	a	810.92	0.78302	YES	YES
84	a	815.99	0.72364	YES	YES
85	a	846.54	1.73688	YES	YES
86	a	850.08	5.14753	YES	YES
87	a	854.93	10.61936	YES	YES
88	a	884.74	67.61561	YES	YES
89	a	892.43	0.87936	YES	YES
90	a	895.13	0.68853	YES	YES
91	a	897.38	1.05996	YES	YES
92	a	902.60	2.51507	YES	YES
93	a	904.52	1.28801	YES	YES
94	a	907.29	3.80981	YES	YES
95	a	910.57	1.07721	YES	YES
96	a	915.21	1.19085	YES	YES
97	a	915.98	1.26015	YES	YES
98	a	921.81	0.52804	YES	YES
99	a	923.19	1.50216	YES	YES
100	a	925.70	0.47820	YES	YES
101	a	929.03	0.27068	YES	YES
102	a	930.74	0.26763	YES	YES
103	a	971.10	2.39835	YES	YES
104	a	985.18	1.15559	YES	YES
105	a	990.04	0.71587	YES	YES
106	a	993.30	2.09678	YES	YES
107	a	994.52	2.21692	YES	YES
108	a	1000.82	2.26102	YES	YES
109	a	1002.24	0.08142	YES	YES
110	a	1003.00	0.36398	YES	YES
111	a	1007.05	0.07728	YES	YES
112	a	1008.35	0.92134	YES	YES
113	a	1011.05	0.83627	YES	YES
114	a	1013.36	0.84775	YES	YES
115	a	1090.80	14.37523	YES	YES
116	a	1094.98	4.93343	YES	YES
117	a	1112.01	11.84256	YES	YES
118	a	1131.39	9.71716	YES	YES
119	a	1134.86	3.84713	YES	YES
120	a	1141.69	4.80339	YES	YES
121	a	1168.27	0.25370	YES	YES
122	a	1172.57	3.70034	YES	YES
123	a	1173.16	5.87550	YES	YES
124	a	1191.16	11.33301	YES	YES
125	a	1192.02	0.98887	YES	YES
126	a	1193.25	1.50687	YES	YES
127	a	1194.56	3.16615	YES	YES
128	a	1195.43	16.18572	YES	YES
129	a	1197.72	1.57804	YES	YES
130	a	1198.14	1.78950	YES	YES
131	a	1228.65	16.61874	YES	YES
132	a	1234.64	9.74051	YES	YES
133	a	1237.75	13.35978	YES	YES
134	a	1241.46	13.14631	YES	YES
135	a	1256.63	7.37263	YES	YES
136	a	1280.81	4.29667	YES	YES
137	a	1296.57	4.41919	YES	YES
138	a	1335.27	17.98145	YES	YES
139	a	1337.85	2.45607	YES	YES
140	a	1339.28	3.30993	YES	YES
141	a	1341.79	4.84075	YES	YES
142	a	1342.72	10.91103	YES	YES
143	a	1345.81	6.41612	YES	YES
144	a	1346.30	1.11210	YES	YES
145	a	1355.11	4.40078	YES	YES
146	a	1361.76	1.29718	YES	YES
147	a	1364.11	18.04497	YES	YES
148	a	1375.29	13.54349	YES	YES
149	a	1377.77	13.39061	YES	YES
150	a	1378.74	6.75518	YES	YES
151	a	1380.38	8.61880	YES	YES
152	a	1384.16	9.96138	YES	YES
153	a	1387.08	2.56178	YES	YES

154	a	1408.31	11.47982	YES	YES
155	a	1409.83	17.92455	YES	YES
156	a	1414.34	0.86930	YES	YES
157	a	1415.22	0.57160	YES	YES
158	a	1415.46	0.45835	YES	YES
159	a	1417.24	9.88984	YES	YES
160	a	1418.83	8.86736	YES	YES
161	a	1420.04	1.09698	YES	YES
162	a	1420.79	7.02067	YES	YES
163	a	1422.83	1.96769	YES	YES
164	a	1423.65	10.96650	YES	YES
165	a	1424.83	4.45342	YES	YES
166	a	1429.80	2.64523	YES	YES
167	a	1435.01	22.63761	YES	YES
168	a	1436.29	12.54157	YES	YES
169	a	1440.57	4.52910	YES	YES
170	a	1441.84	11.79913	YES	YES
171	a	1443.21	7.30921	YES	YES
172	a	1443.61	15.77388	YES	YES
173	a	1447.11	11.66052	YES	YES
174	a	1450.99	6.84145	YES	YES
175	a	1451.46	14.52009	YES	YES
176	a	1454.24	21.78289	YES	YES
177	a	1457.05	12.80977	YES	YES
178	a	1462.18	23.90325	YES	YES
179	a	1464.92	10.87205	YES	YES
180	a	1567.14	9.80528	YES	YES
181	a	1573.67	12.15785	YES	YES
182	a	1581.97	10.53398	YES	YES
183	a	1583.49	7.51940	YES	YES
184	a	2929.29	59.28511	YES	YES
185	a	2932.77	81.13117	YES	YES
186	a	2935.17	17.49423	YES	YES
187	a	2942.74	36.40565	YES	YES
188	a	2948.33	10.78027	YES	YES
189	a	2948.74	26.62236	YES	YES
190	a	2949.02	5.07729	YES	YES
191	a	2949.33	12.68517	YES	YES
192	a	2952.48	7.94430	YES	YES
193	a	2952.62	3.09114	YES	YES
194	a	2956.22	12.47923	YES	YES
195	a	2957.39	10.61281	YES	YES
196	a	2964.37	0.48277	YES	YES
197	a	3006.28	48.44533	YES	YES
198	a	3007.48	28.21543	YES	YES

1-F: {$(CH_3)_3C$}$_2C_6H_3$ CH_3PP{$(CH_3)_3C$}$_2C_6H_3F$



(RI-)BP86/SV(P) level:

SCF Energy = -1913.6089192870 E_h
Zero Point Energy 0.0360429 E_h
Symmetry = C_1

XYZ Coordinates:
77

P	0.71342	-0.55771	-0.62095
P	-0.77936	0.64830	0.61213
C	0.03348	-0.25233	-2.35255
H	-0.57288	-1.14685	-2.61064
H	0.88047	-0.18233	-3.06678
H	-0.60587	0.64524	-2.47178
F	-0.22131	0.22758	2.12451
C	-2.31587	-0.33527	0.18244
C	2.34408	0.34065	-0.23370
C	-2.41881	-1.74534	-0.10536
C	2.50671	1.72430	0.14576
C	-3.30115	-2.13599	-1.13817
H	-3.35714	-3.19687	-1.42864
C	3.46540	2.02884	1.14196
H	3.55017	3.06416	1.50712
C	-4.12678	-1.22104	-1.79620
C	4.32866	1.06847	1.66542
C	-4.19881	0.09535	-1.32991
H	-4.95209	0.76605	-1.76662
C	4.33800	-0.20794	1.09686
H	5.10192	-0.92408	1.43053
C	-3.34376	0.56303	-0.30931
C	3.38769	-0.59852	0.13102
C	-1.80394	-2.92480	0.70957
C	1.87184	2.99364	-0.50841
C	-3.01219	-3.70442	1.31428
H	-3.68942	-4.12003	0.53784
H	-3.61662	-3.04630	1.97682
H	-2.63704	-4.55526	1.92682
C	0.93312	2.72214	-1.69329
H	1.41636	2.08039	-2.45955
H	0.66511	3.68669	-2.17961
H	-0.01094	2.24723	-1.36742
C	-0.92118	-2.51581	1.90156
H	-1.44546	-1.81459	2.58317
H	0.02453	-2.03783	1.58334
H	-0.65900	-3.42667	2.48510
C	1.11485	3.85587	0.53455
H	1.77627	4.19718	1.36019
H	0.27412	3.28505	0.98472
H	0.69550	4.76467	0.04684
C	-0.99428	-3.88100	-0.20212
H	-1.60856	-4.31311	-1.02206
H	-0.59685	-4.73063	0.39711
H	-0.13232	-3.34578	-0.65587
C	3.05239	3.82929	-1.09240
H	3.77089	4.16321	-0.31480
H	2.65383	4.73901	-1.59619
H	3.61967	3.23953	-1.84605
H	-4.77341	-1.55209	-2.62620
H	5.03861	1.32954	2.46774
C	3.59550	-2.02244	-0.48855
C	-3.65930	1.97327	0.29997
C	-2.89730	3.12211	-0.40970
H	-3.06591	3.08859	-1.50942
H	-1.80618	3.06500	-0.22346
H	-3.26168	4.10747	-0.03956
C	3.05860	-2.13418	-1.93681
H	3.44563	-1.31101	-2.57757
H	1.94974	-2.12260	-1.97845
H	3.38459	-3.09978	-2.38432
C	-3.38282	1.99606	1.82638
H	-3.98919	1.22347	2.34908
H	-3.65894	2.99117	2.24160
H	-2.31777	1.81863	2.08562
C	2.95202	-3.11139	0.40645

H	3.38779	-3.08680	1.42969
H	3.13461	-4.12434	-0.02029
H	1.85699	-2.96129	0.49720
C	-5.17674	2.28332	0.15033
H	-5.81058	1.44897	0.52314
H	-5.47241	2.50543	-0.89751
H	-5.42025	3.18981	0.74762
C	5.11678	-2.33624	-0.59453
H	5.60069	-2.49748	0.39181
H	5.66804	-1.52695	-1.12238
H	5.25429	-3.27719	-1.17162

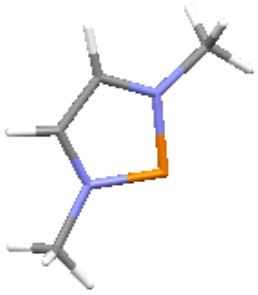
$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.00	0.09613	YES	YES
8	a	13.87	0.06239	YES	YES
9	a	33.27	0.09819	YES	YES
10	a	40.34	0.06670	YES	YES
11	a	43.21	0.08967	YES	YES
12	a	49.45	0.18879	YES	YES
13	a	63.19	0.25801	YES	YES
14	a	68.22	0.14680	YES	YES
15	a	82.31	0.08856	YES	YES
16	a	92.07	0.02681	YES	YES
17	a	96.50	0.03486	YES	YES
18	a	113.12	0.10520	YES	YES
19	a	117.23	0.05779	YES	YES
20	a	122.76	0.44742	YES	YES
21	a	132.29	0.40818	YES	YES
22	a	146.96	0.38403	YES	YES
23	a	167.17	0.70911	YES	YES
24	a	179.29	0.18311	YES	YES
25	a	182.56	0.65139	YES	YES
26	a	193.16	0.37672	YES	YES
27	a	200.56	0.33955	YES	YES
28	a	203.98	0.41383	YES	YES
29	a	213.70	0.35392	YES	YES
30	a	216.20	0.40598	YES	YES
31	a	219.17	0.48269	YES	YES
32	a	222.91	1.20021	YES	YES
33	a	235.92	1.45381	YES	YES
34	a	242.58	2.38628	YES	YES
35	a	246.49	0.25393	YES	YES
36	a	253.46	0.07923	YES	YES
37	a	258.88	0.37369	YES	YES
38	a	260.33	0.51150	YES	YES
39	a	265.78	0.02790	YES	YES
40	a	270.62	0.78956	YES	YES
41	a	276.22	0.64584	YES	YES
42	a	288.57	2.88577	YES	YES
43	a	290.22	0.08844	YES	YES
44	a	292.82	0.63358	YES	YES
45	a	302.76	0.21637	YES	YES
46	a	312.12	3.86001	YES	YES
47	a	313.42	0.41449	YES	YES
48	a	323.71	0.52791	YES	YES
49	a	347.21	0.49808	YES	YES
50	a	350.63	2.19429	YES	YES
51	a	354.41	0.31519	YES	YES
52	a	360.29	0.57708	YES	YES
53	a	364.61	3.10765	YES	YES
54	a	374.29	0.16293	YES	YES
55	a	378.68	3.10401	YES	YES
56	a	381.67	2.46825	YES	YES
57	a	387.01	3.28112	YES	YES
58	a	400.12	0.64146	YES	YES
59	a	405.45	1.42124	YES	YES
60	a	415.73	1.33788	YES	YES
61	a	426.70	1.88222	YES	YES
62	a	427.63	1.77588	YES	YES
63	a	435.83	3.71993	YES	YES
64	a	472.54	25.84962	YES	YES
65	a	477.55	0.25784	YES	YES
66	a	501.18	0.99704	YES	YES
67	a	514.02	0.80351	YES	YES
68	a	516.98	11.75908	YES	YES
69	a	524.70	17.17015	YES	YES
70	a	532.60	4.29596	YES	YES
71	a	537.14	0.74521	YES	YES
72	a	550.22	0.69804	YES	YES
73	a	554.22	7.96801	YES	YES
74	a	633.21	3.86008	YES	YES
75	a	634.96	4.55217	YES	YES
76	a	650.85	4.83113	YES	YES
77	a	698.52	4.74042	YES	YES
78	a	701.17	1.85174	YES	YES
79	a	730.12	29.56746	YES	YES
80	a	730.66	2.52379	YES	YES
81	a	733.43	2.32063	YES	YES
82	a	741.10	13.73744	YES	YES
83	a	747.36	59.05336	YES	YES
84	a	788.71	10.19452	YES	YES
85	a	792.66	17.45848	YES	YES
86	a	816.21	1.16799	YES	YES
87	a	816.98	0.47802	YES	YES
88	a	844.67	19.86352	YES	YES
89	a	854.97	0.12582	YES	YES
90	a	856.17	26.54913	YES	YES
91	a	880.41	0.76740	YES	YES
92	a	882.72	18.67082	YES	YES
93	a	885.67	0.43002	YES	YES
94	a	899.70	4.50140	YES	YES
95	a	900.99	2.36628	YES	YES
96	a	901.81	1.41679	YES	YES
97	a	904.57	1.26112	YES	YES
98	a	913.42	1.27010	YES	YES
99	a	919.35	0.56351	YES	YES
100	a	919.65	0.21535	YES	YES
101	a	920.89	0.07352	YES	YES
102	a	923.95	0.87299	YES	YES
103	a	927.37	1.40416	YES	YES
104	a	932.43	0.71247	YES	YES
105	a	936.72	0.47640	YES	YES
106	a	955.45	2.28177	YES	YES
107	a	961.03	3.21690	YES	YES
108	a	991.43	1.50948	YES	YES
109	a	999.21	5.05125	YES	YES
110	a	1007.57	1.41735	YES	YES
111	a	1007.73	0.24834	YES	YES
112	a	1007.99	0.53977	YES	YES
113	a	1008.81	0.53527	YES	YES
114	a	1009.61	2.15713	YES	YES
115	a	1010.91	0.95281	YES	YES
116	a	1012.77	1.08156	YES	YES
117	a	1013.73	1.07198	YES	YES

118	a	1089.86	14.15525	YES	YES
119	a	1092.90	1.18310	YES	YES
120	a	1115.63	11.35866	YES	YES
121	a	1118.97	7.90828	YES	YES
122	a	1130.79	3.45050	YES	YES
123	a	1132.87	5.84330	YES	YES
124	a	1172.40	1.55692	YES	YES
125	a	1172.89	6.17035	YES	YES
126	a	1175.91	15.41788	YES	YES
127	a	1176.66	4.56439	YES	YES
128	a	1180.31	13.64812	YES	YES
129	a	1183.70	15.29475	YES	YES
130	a	1192.47	2.41464	YES	YES
131	a	1193.73	4.39881	YES	YES
132	a	1197.64	7.23320	YES	YES
133	a	1200.51	5.77644	YES	YES
134	a	1222.15	9.84112	YES	YES
135	a	1228.27	10.26373	YES	YES
136	a	1242.41	8.68095	YES	YES
137	a	1244.18	8.72707	YES	YES
138	a	1264.37	3.03886	YES	YES
139	a	1285.40	1.57127	YES	YES
140	a	1291.94	0.97698	YES	YES
141	a	1333.23	9.13382	YES	YES
142	a	1334.90	6.55446	YES	YES
143	a	1336.23	6.14797	YES	YES
144	a	1337.41	3.42457	YES	YES
145	a	1337.98	8.21872	YES	YES
146	a	1340.23	3.36596	YES	YES
147	a	1343.09	1.59368	YES	YES
148	a	1344.34	3.20960	YES	YES
149	a	1362.66	9.17416	YES	YES
150	a	1364.33	4.98246	YES	YES
151	a	1370.48	6.23180	YES	YES
152	a	1371.90	13.72911	YES	YES
153	a	1372.49	11.94003	YES	YES
154	a	1373.89	2.52959	YES	YES
155	a	1397.41	13.32499	YES	YES
156	a	1408.49	0.26500	YES	YES
157	a	1408.74	2.98760	YES	YES
158	a	1412.66	5.32667	YES	YES
159	a	1413.68	0.14903	YES	YES
160	a	1416.40	3.13895	YES	YES
161	a	1418.76	12.13474	YES	YES
162	a	1419.49	17.65432	YES	YES
163	a	1421.20	0.20354	YES	YES
164	a	1421.79	1.84339	YES	YES
165	a	1421.98	0.68507	YES	YES
166	a	1423.72	3.89564	YES	YES
167	a	1425.34	4.12476	YES	YES
168	a	1427.87	14.25618	YES	YES
169	a	1430.47	2.00161	YES	YES
170	a	1433.68	7.57303	YES	YES
171	a	1434.31	1.89497	YES	YES
172	a	1437.03	0.41485	YES	YES
173	a	1440.91	3.41492	YES	YES
174	a	1442.74	7.21624	YES	YES
175	a	1443.78	21.62460	YES	YES
176	a	1445.59	0.26566	YES	YES
177	a	1450.70	1.34748	YES	YES
178	a	1453.90	2.10020	YES	YES
179	a	1459.48	20.80285	YES	YES
180	a	1463.03	25.19358	YES	YES
181	a	1463.65	6.70010	YES	YES
182	a	1466.55	7.31936	YES	YES
183	a	1568.28	13.91284	YES	YES
184	a	1572.34	9.35395	YES	YES
185	a	1578.30	14.91028	YES	YES
186	a	1581.55	7.99481	YES	YES
187	a	2936.02	28.98809	YES	YES
188	a	2936.56	22.40043	YES	YES
189	a	2937.04	21.58784	YES	YES
190	a	2938.02	16.59005	YES	YES
191	a	2938.31	10.12807	YES	YES
192	a	2938.93	13.77668	YES	YES
193	a	2940.77	36.95154	YES	YES
194	a	2941.21	28.47115	YES	YES
195	a	2944.41	35.58329	YES	YES
196	a	2945.38	36.62288	YES	YES
197	a	2954.13	25.49515	YES	YES
198	a	2955.97	29.03238	YES	YES

2: $[(CH)_2\{N(CH_3)\}_2P]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -607.6200269769 E_h
Zero Point Energy = 0.1203573 E_h
Symmetry = C_{2V}

XYZ Coordinates:
15

N	0.00000	-1.19856	-0.10501
P	0.00000	0.00000	1.11975
N	0.00000	1.19856	-0.10501
C	0.00000	-0.69216	-1.37817
C	0.00000	0.69216	-1.37817
H	0.00000	1.35812	-2.25286
H	0.00000	-1.35812	-2.25286
C	0.00000	-2.64671	0.18123
C	0.00000	2.64671	0.18123
H	0.00000	2.80730	1.27771
H	-0.90830	3.11284	-0.25349
H	0.90830	3.11284	-0.25349
H	-0.90830	-3.11284	-0.25349
H	0.00000	-2.80730	1.27771
H	0.90830	-3.11284	-0.25349

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	22.03	0.03297	YES YES
8		a	54.03	0.12061	YES YES
9		a	108.47	0.65451	YES YES
10		a	143.10	1.87741	YES YES
11		a	161.89	3.23946	YES YES
12		a	220.77	0.84890	YES YES

13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

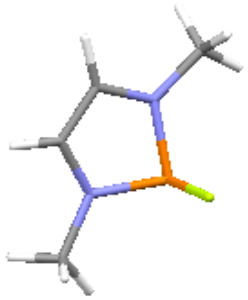
(RI-)MP2/def2-TZVPP level

SCF Energy = -606.8815255634 E_h
Symmetry = C_{2V}

XYZ Coordinates:
15

N	0.00000	-1.18003	-0.10091
P	0.00000	0.00000	1.10355
N	0.00000	1.18003	-0.10091
C	0.00000	-0.68696	-1.36666
C	0.00000	0.68696	-1.36666
H	0.00000	1.34585	-2.22023
H	0.00000	-1.34585	-2.22023
C	0.00000	-2.62589	0.18335
C	0.00000	2.62589	0.18335
H	0.00000	2.77469	1.25879
H	-0.89205	3.07157	-0.24557
H	0.89205	3.07157	-0.24557
H	-0.89205	-3.07157	-0.24557
H	0.00000	-2.77469	1.25879
H	0.89205	-3.07157	-0.24557

2-F: (CH)$_2${N(CH$_3$)}$_2$PF



(RI-)BP86/SV(P) level:

SCF Energy = -707.6266329546 E_h
Zero Point Energy = 0.1206311 E_h
Symmetry = C_s

XYZ Coordinates:
16

N	-0.16566	0.39817	-1.20117
P	-0.50577	-0.79894	0.00000
N	-0.16566	0.39817	1.20117
C	0.44178	1.55455	-0.68071
C	0.44178	1.55455	0.68071
H	0.83415	2.32909	1.35351
H	0.83415	2.32909	-1.35351
C	-0.29751	0.15648	-2.62729
C	-0.29751	0.15648	2.62729
H	-0.93739	-0.73675	2.79128
H	-0.78385	1.02234	3.13203
H	0.68694	-0.03175	3.11826
H	-0.78385	1.02234	-3.13203
H	-0.93739	-0.73675	-2.79128
H	0.68694	-0.03175	-3.11826
F	0.90767	-1.72213	0.00000

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES
15	a	331.59	0.65752	YES YES
16	a	431.69	25.51929	YES YES
17	a	435.65	24.98526	YES YES
18	a	505.39	1.25012	YES YES
19	a	523.48	2.22561	YES YES
20	a	528.83	0.84803	YES YES
21	a	549.42	11.99635	YES YES
22	a	726.13	1.43402	YES YES
23	a	729.50	5.41704	YES YES
24	a	820.34	66.34508	YES YES
25	a	1102.54	231.73283	YES YES
26	a	1125.45	315.13040	YES YES
27	a	1148.81	88.79335	YES YES
28	a	1154.27	19.36874	YES YES
29	a	1170.73	346.92142	YES YES

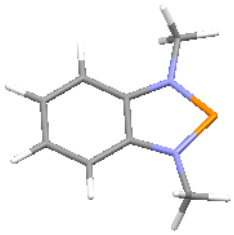
(RI-)MP2/def2-TZVPP level

SCF Energy = -706.8604534901 E_h
Symmetry = C_s

XYZ Coordinates:
16

N	-0.19832	0.38595	-1.17742
P	-0.49343	-0.78945	0.00000
N	-0.19832	0.38595	1.17742
C	0.43205	1.52624	-0.67466
C	0.43205	1.52624	0.67466
H	0.81490	2.28294	1.33819
H	0.81490	2.28294	-1.33819
C	-0.27745	0.13123	-2.60283
C	-0.27745	0.13123	2.60283
H	-0.93761	-0.71547	2.77693
H	-0.69193	0.99878	3.11395
H	0.69999	-0.09942	3.02803
H	-0.69193	0.99878	-3.11395
H	-0.93761	-0.71547	-2.77693
H	0.69999	-0.09942	-3.02803
F	0.91357	-1.63954	0.00000

3: [C_6H_4{NCH_3}$_2$P]+



(RI-)BP86/SV(P) level:

SCF Energy = -761.1690806451 E_h
Zero Point Energy = 0.1667923E_h
Symmetry = C_{2V}

XYZ Coordinates:
21

N	0.00000	-1.20895	0.89417
P	0.00000	0.00000	2.09427
N	0.00000	1.20895	0.89417
C	0.00000	-0.71427	-0.40244
C	0.00000	0.71427	-0.40244
C	0.00000	1.44008	-1.61389
C	0.00000	-1.44008	-1.61389
H	0.00000	-2.53977	-1.62299
C	0.00000	-0.71064	-2.80406
C	0.00000	0.71064	-2.80406
H	0.00000	2.53977	-1.62299
H	0.00000	-1.24872	-3.76511
H	0.00000	1.24872	-3.76511
C	0.00000	-2.64616	1.20507
C	0.00000	2.64616	1.20507
H	-0.90779	-3.12437	0.78078
H	0.00000	-2.78724	2.30463
H	0.90779	-3.12437	0.78078
H	0.00000	2.78724	2.30463
H	-0.90779	3.12437	0.78078
H	0.90779	3.12437	0.78078

vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1	138.41	2.99649	YES	YES
8	a2	144.16	0.00000	NO	YES
9	b1	173.03	3.85994	YES	YES
10	a2	174.52	0.00000	NO	YES
11	b1	191.92	1.14261	YES	YES
12	b2	239.88	0.01904	YES	YES
13	a1	256.78	1.18714	YES	YES
14	a2	318.61	0.00000	NO	YES
15	b1	397.02	6.84629	YES	YES
16	b2	432.83	3.25320	YES	YES
17	a1	471.30	0.02468	YES	YES
18	a1	498.48	2.06616	YES	YES
19	b1	515.87	0.03519	YES	YES
20	b2	531.89	6.39905	YES	YES
21	a2	550.58	0.00000	NO	YES
22	a1	673.75	1.69598	YES	YES
23	b2	715.34	0.67223	YES	YES
24	b1	748.28	62.55957	YES	YES
25	a2	759.72	0.00000	NO	YES
26	a2	850.61	0.00000	NO	YES
27	a1	866.62	3.49652	YES	YES
28	b2	868.86	15.65714	YES	YES
29	b1	941.57	0.20448	YES	YES
30	a2	991.31	0.00000	NO	YES
31	a1	1016.03	0.79658	YES	YES
32	b2	1035.30	42.84118	YES	YES
33	a2	1096.32	0.00000	NO	YES
34	a1	1100.93	17.34663	YES	YES
35	b1	1105.57	0.00257	YES	YES
36	b2	1127.39	15.10554	YES	YES
37	a1	1152.77	0.63401	YES	YES
38	b2	1178.08	22.95363	YES	YES
39	a1	1191.79	0.60423	YES	YES
40	b2	1267.29	9.17887	YES	YES
41	a1	1315.66	2.63622	YES	YES
42	b2	1318.29	1.21720	YES	YES
43	a1	1405.30	3.96278	YES	YES
44	b2	1406.97	0.70323	YES	YES
45	a1	1408.53	1.49813	YES	YES
46	a2	1420.15	0.00000	NO	YES
47	b1	1421.02	39.46891	YES	YES
48	b2	1441.11	0.11052	YES	YES
49	a1	1442.19	32.19954	YES	YES
50	a1	1460.08	0.48879	YES	YES
51	b2	1487.82	10.12876	YES	YES
52	a1	1584.68	29.53799	YES	YES
53	b2	1606.23	0.62757	YES	YES
54	a1	2970.56	0.59095	YES	YES
55	b2	2970.63	5.84924	YES	YES
56	b1	3066.16	0.00075	YES	YES
57	a2	3066.26	0.00000	NO	YES
58	a1	3081.08	0.22439	YES	YES
59	b2	3081.33	0.25985	YES	YES
60	b2	3122.43	0.03837	YES	YES
61	a1	3131.14	0.05991	YES	YES
62	b2	3139.72	0.16857	YES	YES
63	a1	3143.22	0.38366	YES	YES

(RI-)MP2/def2-TZVPP level

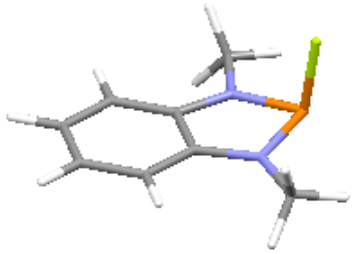
SCF Energy = -760.2098187358 E_h
Symmetry = C_{2V}

XYZ Coordinates:
21

N	0.00000	-1.19073	0.88782
P	0.00000	0.00000	2.06869
N	0.00000	1.19073	0.88782
C	0.00000	-0.70667	-0.39643
C	0.00000	0.70667	-0.39643
C	0.00000	1.43270	-1.59483
C	0.00000	-1.43270	-1.59483
H	0.00000	-2.51301	-1.60146
C	0.00000	-0.70612	-2.77087
C	0.00000	0.70612	-2.77087
H	0.00000	2.51301	-1.60146
H	0.00000	-1.23135	-3.71537
H	0.00000	1.23135	-3.71537
C	0.00000	-2.62818	1.18742
C	0.00000	2.62818	1.18742
H	-0.89169	-3.08216	0.76379
H	0.00000	-2.76544	2.26477
H	0.89169	-3.08216	0.76379

H	0.00000	2.76544	2.26477
H	-0.89169	3.08216	0.76379
H	0.89169	3.08216	0.76379

3-F: $C_6H_4\{NCH_3\}_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -861.1865403285 E_h
Zero Point Energy = 0.1676333 E_h
Symmetry = C_{2V}

XYZ Coordinates:
22

N	-0.32978	-0.61973	-1.21121
P	-0.29989	-1.85773	0.00000
N	-0.32978	-0.61973	1.21121
C	-0.10637	0.67012	-0.71171
C	-0.10637	0.67012	0.71171
C	0.07242	1.86443	1.42440
C	0.07242	1.86443	-1.42440
H	0.07854	1.86769	-2.52540
C	0.24602	3.06462	-0.70227
C	0.24602	3.06462	0.70227
H	0.07854	1.86769	2.52540
H	0.38681	4.00907	-1.25267
H	0.38681	4.00907	1.25267
C	-0.40878	-0.90397	-2.63293
C	-0.40878	-0.90397	2.63293
H	-1.18166	-0.26658	-3.12049
H	-0.69561	-1.96693	-2.77965
H	0.56572	-0.73306	-3.14792
H	-0.69561	-1.96693	2.77965
H	-1.18166	-0.26658	3.12049
H	0.56572	-0.73306	3.14792
F	1.31371	-2.30304	0.00000

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	89.28	1.73663	YES	YES
8	a"	104.20	0.74538	YES	YES
9	a'	105.45	3.94699	YES	YES
10	a"	144.13	0.73819	YES	YES
11	a'	177.40	0.37013	YES	YES
12	a"	186.43	0.36153	YES	YES
13	a"	237.03	0.02400	YES	YES
14	a'	257.27	1.07696	YES	YES
15	a'	259.49	2.51777	YES	YES
16	a"	300.78	0.59215	YES	YES
17	a'	381.39	5.94568	YES	YES
18	a"	426.72	6.11870	YES	YES
19	a'	456.35	1.08828	YES	YES
20	a'	493.57	8.35646	YES	YES
21	a'	502.36	10.43889	YES	YES
22	a"	534.54	13.97349	YES	YES
23	a"	562.98	0.00001	YES	YES
24	a'	679.39	10.47117	YES	YES
25	a"	705.85	2.23080	YES	YES
26	a'	712.09	112.38149	YES	YES
27	a'	725.16	112.62282	YES	YES
28	a"	740.63	0.00016	YES	YES
29	a"	827.23	1.52809	YES	YES
30	a"	834.08	6.97956	YES	YES
31	a'	869.06	93.11380	YES	YES
32	a'	884.46	4.13318	YES	YES
33	a"	940.23	0.00449	YES	YES
34	a'	1024.46	11.62029	YES	YES
35	a"	1043.54	31.64423	YES	YES
36	a"	1107.58	20.85797	YES	YES
37	a"	1111.92	2.32450	YES	YES
38	a'	1112.23	0.96392	YES	YES
39	a'	1119.16	3.79180	YES	YES
40	a'	1139.57	0.03808	YES	YES
41	a"	1183.77	23.34545	YES	YES
42	a'	1210.00	70.92107	YES	YES
43	a"	1276.08	11.82202	YES	YES
44	a"	1304.81	82.72320	YES	YES
45	a'	1323.76	120.02985	YES	YES
46	a'	1404.93	2.82812	YES	YES
47	a"	1406.76	0.23732	YES	YES
48	a'	1412.20	1.94305	YES	YES
49	a"	1418.45	1.94308	YES	YES
50	a'	1419.22	17.32080	YES	YES
51	a"	1451.14	1.91032	YES	YES
52	a'	1460.16	62.90341	YES	YES
53	a"	1467.15	19.78374	YES	YES
54	a'	1498.33	167.24789	YES	YES
55	a'	1605.10	0.12877	YES	YES
56	a"	1608.59	19.46922	YES	YES
57	a"	2920.30	134.65594	YES	YES
58	a'	2921.13	5.96847	YES	YES
59	a"	2989.89	0.37550	YES	YES
60	a'	2989.92	44.53456	YES	YES
61	a'	3038.30	10.21773	YES	YES
62	a"	3038.63	0.06295	YES	YES
63	a"	3094.66	0.01360	YES	YES
64	a'	3106.16	12.47090	YES	YES
65	a"	3115.29	22.47787	YES	YES
66	a'	3121.82	8.68987	YES	YES

(RI-)MP2/def2-TZVPP level

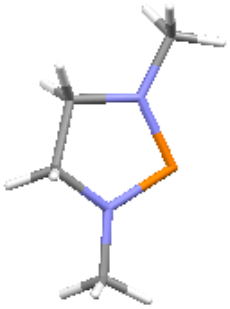
SCF Energy = -860.201445535 E_h
Symmetry = C_s

XYZ Coordinates:
22

N	-0.36090	-0.62979	-1.18816
P	-0.27598	-1.83326	0.00000
N	-0.36090	-0.62979	1.18816
C	-0.12491	0.65168	-0.70244
C	-0.12491	0.65168	0.70244
C	0.06291	1.82966	1.41560
C	0.06291	1.82966	-1.41560
H	0.06938	1.83013	-2.49681
C	0.24700	3.01512	-0.69740
C	0.24700	3.01512	0.69740
H	0.06938	1.83013	2.49681
H	0.39618	3.94209	-1.23323
H	0.39618	3.94209	1.23323
C	-0.38673	-0.90064	-2.61079

C	-0.38673	-0.90064	2.61079
H	-1.12823	-0.26860	-3.09891
H	-0.66071	-1.94106	-2.76950
H	0.58720	-0.72183	-3.06922
H	-0.66071	-1.94106	2.76950
H	-1.12823	-0.26860	3.09891
H	0.58720	-0.72183	3.06922
F	1.31529	-2.19510	0.00000

4: $[(CH_2)_2\{N(CH_3)\}_2P]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -608.8069544766 E_h
Zero Point Energy = 0.1429152 E_h
Symmetry = C_1

XYZ Coordinates:
17

N	1.21528	-0.02545	-0.02102
P	0.00002	1.10353	0.00010
N	-1.21530	-0.02547	0.02117
C	0.76859	-1.43546	0.09170
C	-0.76855	-1.43546	-0.09163
H	-1.07824	-1.82314	-1.08861
H	-1.28010	-2.04604	0.68277
H	1.07822	-1.82323	1.08865
H	1.28012	-2.04592	-0.68278
C	2.64841	0.27765	-0.01945
H	2.80774	1.37473	-0.05506
H	3.13460	-0.18454	-0.90634
H	3.12273	-0.12573	0.90258
C	-2.64847	0.27766	0.01910
H	-2.80784	1.37488	0.04995
H	-3.13448	-0.18080	0.90807
H	-3.12298	-0.12966	-0.90110

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES
15	a	331.59	0.65752	YES YES
16	a	431.69	25.51929	YES YES
17	a	435.65	24.98526	YES YES
18	a	505.39	1.25012	YES YES
19	a	523.48	2.22561	YES YES
20	a	528.83	0.84803	YES YES
21	a	549.42	11.99635	YES YES
22	a	726.13	1.43402	YES YES
23	a	729.50	5.41704	YES YES
24	a	820.34	66.34508	YES YES
25	a	1102.54	231.73283	YES YES
26	a	1125.45	315.13040	YES YES
27	a	1148.81	88.79335	YES YES
28	a	1154.27	19.36874	YES YES
29	a	1170.73	346.92142	YES YES

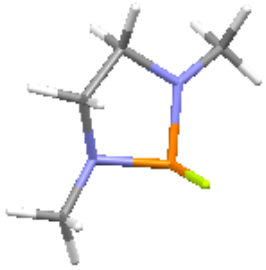
(RI-)MP2/def2-TZVPP level

SCF Energy = -608.0629475704 E_h
Symmetry = C_1

XYZ Coordinates:
17

N	1.19656	-0.02000	-0.04184
P	-0.00000	1.07845	-0.00001
N	-1.19656	-0.02000	0.04189
C	0.75404	-1.41776	0.13166
C	-0.75404	-1.41774	-0.13167
H	-0.99308	-1.72581	-1.14992
H	-1.28996	-2.05716	0.56584
H	0.99304	-1.72586	1.14990
H	1.28993	-2.05715	-0.56589
C	2.62902	0.27928	-0.02281
H	2.78070	1.35328	-0.08242
H	3.10677	-0.19927	-0.87396
H	3.06570	-0.09671	0.90018
C	-2.62902	0.27928	0.02279
H	-2.78069	1.35326	0.08275
H	-3.10682	-0.19951	0.87378
H	-3.06564	-0.09642	-0.90034

4-F: $(CH_2)_2\{N(CH_3)\}_2PF$



(RI-)BP86/SV(P) level:
SCF Energy = -708.8346774044 E_h
Zero Point Energy = 0.1441270 E_h
Symmetry = C_1

XYZ Coordinates:
18

N	1.27398	-0.18266	0.02626
P	-0.02453	0.83271	0.47836
N	-1.10728	-0.51417	0.39472
C	0.90345	-1.54330	-0.36087
C	-0.61787	-1.51107	-0.56462
H	-0.87232	-1.22674	-1.61844
H	-1.08109	-2.50326	-0.36065
H	1.18422	-2.26354	0.44977
H	1.42950	-1.86357	-1.29165
C	2.66052	0.09926	0.33592
H	2.75165	1.11844	0.76934
H	3.30568	0.05810	-0.57487

H	3.07526	-0.62790	1.07925
C	-2.54245	-0.27455	0.40823
H	-2.78504	0.50026	1.16778
H	-3.08055	-1.20780	0.69315
H	-2.94223	0.07044	-0.57942
F	-0.39036	1.61955	-0.96152

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

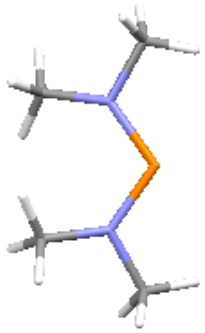
(RI-)MP2/def2-TZVPP level

SCF Energy = -708.0688882912 E_h
Symmetry = C_1

XYZ Coordinates:
18

N	1.25950	-0.13647	-0.02810
P	-0.02761	0.81898	0.45680
N	-1.06488	-0.52146	0.43132
C	0.91851	-1.51473	-0.35109
C	-0.58777	-1.50318	-0.54252
H	-0.84545	-1.20291	-1.56528
H	-1.03345	-2.47752	-0.34290
H	1.19798	-2.17321	0.47893
H	1.43872	-1.85008	-1.25024
C	2.63160	0.13522	0.34178
H	2.72253	1.16021	0.69370
H	3.29519	0.00995	-0.51498
H	2.96937	-0.53482	1.13818
C	-2.49901	-0.28109	0.40105
H	-2.75499	0.49241	1.12235
H	-3.02643	-1.19356	0.67665
H	-2.84439	0.03799	-0.58725
F	-0.45077	1.56024	-0.93868

5: $[P(NMe_2)_2]+$



(RI-)BP86/SV(P) level:

SCF Energy = -609.9921653167 E_h
Zero Point Energy = 0.1626017 E_h
Symmetry = C_1

XYZ Coordinates:
19

N	1.36596	-0.04553	-0.06710
P	-0.00060	-0.00107	0.88396
N	-1.36684	0.04712	-0.06676
C	1.56112	-0.40592	-1.47865
C	2.61433	0.26062	0.66742
C	-2.61662	-0.25946	0.66427
C	-1.55690	0.40558	-1.47925
H	-0.67425	0.93872	-1.87768
H	-2.43282	1.08668	-1.54746
H	-1.76981	-0.49455	-2.09800
H	2.42738	-1.10023	-1.54073
H	1.79231	0.49169	-2.09456
H	0.67371	-0.92481	-1.88483
H	2.39719	0.45334	1.74007
H	3.09027	1.16984	0.23901
H	3.31694	-0.59644	0.58608
H	-3.31848	0.59802	0.58256
H	-2.40226	-0.45367	1.73713
H	-3.09237	-1.16756	0.23355

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	52.25	3.37204	YES	YES
8	a	62.01	1.60483	YES	YES
9	a	180.47	17.14319	YES	YES
10	a	402.06	0.51145	YES	YES
11	a	404.01	0.50696	YES	YES
12	a	447.22	2.83071	YES	YES
13	a	739.84	3.69086	YES	YES
14	a	757.66	5.46120	YES	YES
15	a	817.70	1.30369	YES	YES
16	a	949.16	9.83394	YES	YES
17	a	960.51	14.98237	YES	YES
18	a	965.91	19.76635	YES	YES
19	a	1068.40	43.33553	YES	YES
20	a	1240.65	148.20902	YES	YES
21	a	1243.50	116.67886	YES	YES
22	a	1271.64	1.23740	YES	YES
23	a	1300.94	86.08384	YES	YES
24	a	1309.93	85.86253	YES	YES

25	a	1346.87	3.06878	YES	YES
26	a	1357.59	1.06744	YES	YES
27	a	1379.25	53.29733	YES	YES
28	a	1436.77	1.46522	YES	YES
29	a	1453.20	37.25682	YES	YES
30	a	1457.25	35.36943	YES	YES
31	a	2868.91	117.74263	YES	YES
32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

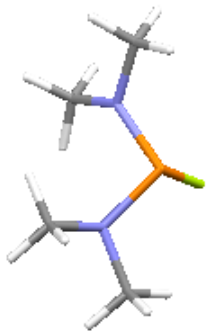
(RI-)MP2/def2-TZVPP level

SCF Energy = -609.2468989801 E_h
Symmetry = C_2

XYZ Coordinates:
19

N	1.33122	-0.04296	-0.05756
P	0.00000	0.00000	0.87609
N	-1.33122	0.04296	-0.05756
C	1.51551	-0.40757	-1.46559
C	2.59267	0.25517	0.65154
C	-2.59267	-0.25517	0.65154
C	-1.51551	0.40757	-1.46559
H	-0.64389	0.92892	-1.84191
H	-2.37324	1.07425	-1.52020
H	-1.71779	-0.47599	-2.06805
H	2.37324	-1.07425	-1.52020
H	1.71779	0.47599	-2.06805
H	0.64389	-0.92892	-1.84191
H	2.39616	0.44394	1.70472
H	3.04762	1.14063	0.21347
H	3.26388	-0.59392	0.55145
H	-3.26388	0.59392	0.55145
H	-2.39616	-0.44394	1.70472
H	-3.04762	-1.14063	0.21347

5-F: $P(NMe_2)_2F$



(RI-)BP86/SV(P) level:
SCF Energy = -710.0216762080 E_h
Zero Point Energy = 0.1633792 E_h
Symmetry = C_1

XYZ Coordinates:
20

N	1.25438	0.10017	-0.45560
P	-0.02493	-0.64153	0.50460
N	-1.36291	0.06446	-0.28399
C	1.34936	-0.38404	-1.82830
C	2.55906	0.28264	0.17192
C	-2.63128	-0.65131	-0.26280
C	-1.43495	1.46644	-0.67529
H	-0.41766	1.90650	-0.62421
H	-2.11824	2.04230	-0.00411
H	-1.81377	1.56727	-1.72063
H	1.91574	-1.34883	-1.92341
H	1.87238	0.37275	-2.45891
H	0.33376	-0.53524	-2.25137
H	2.43230	0.64525	1.21045
H	3.13639	1.05123	-0.39317
H	3.17871	-0.65403	0.18985
H	-3.37509	-0.16730	0.41772
H	-2.46537	-1.69313	0.08878
H	-3.08131	-0.69497	-1.28355
F	0.24177	0.34110	1.82725

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	52.25	3.37204	YES YES
8		a	62.01	1.60483	YES YES
9		a	180.47	17.14319	YES YES
10		a	402.06	0.51145	YES YES
11		a	404.01	0.50696	YES YES
12		a	447.22	2.83071	YES YES
13		a	739.84	3.69086	YES YES
14		a	757.66	5.46120	YES YES
15		a	817.70	1.30369	YES YES
16		a	949.16	9.83394	YES YES
17		a	960.51	14.98237	YES YES
18		a	965.91	19.76635	YES YES
19		a	1068.40	43.33553	YES YES
20		a	1240.65	148.20902	YES YES
21		a	1243.50	116.67886	YES YES
22		a	1271.64	1.23740	YES YES
23		a	1300.94	86.08384	YES YES
24		a	1309.93	85.86253	YES YES
25		a	1346.87	3.06878	YES YES
26		a	1357.59	1.06744	YES YES
27		a	1379.25	53.29733	YES YES
28		a	1436.77	1.46522	YES YES
29		a	1453.20	37.25682	YES YES
30		a	1457.25	35.36943	YES YES
31		a	2868.91	117.74263	YES YES
32		a	2877.64	84.28624	YES YES
33		a	2893.34	29.20329	YES YES
34		a	2963.18	21.64613	YES YES
35		a	2973.98	22.67130	YES YES
36		a	2979.38	17.20698	YES YES
37		a	3081.87	6.77553	YES YES
38		a	3085.00	4.78460	YES YES

(RI-)MP2/def2-TZVPP level

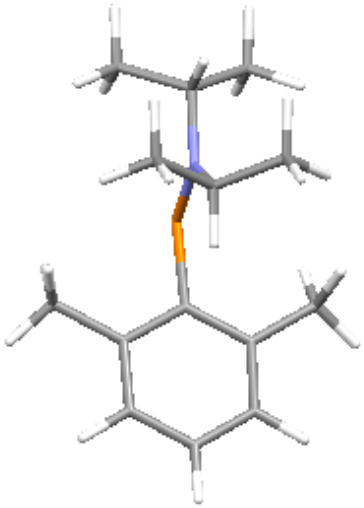
SCF Energy = -709.2528335603 E_h
Symmetry = C_1

XYZ Coordinates:
20

N	1.22993	0.17378	-0.44452
P	0.00996	-0.57986	0.50911
N	-1.32724	0.01971	-0.27571
C	1.28416	-0.33028	-1.81308
C	2.55823	0.14488	0.16376
C	-2.57395	-0.72059	-0.20320
C	-1.47319	1.39813	-0.71188
H	-0.50257	1.88525	-0.69525
H	-2.16030	1.93979	-0.05753

H	-1.87087	1.42992	-1.72842
H	1.64320	-1.36568	-1.87148
H	1.96623	0.29544	-2.38840
H	0.29884	-0.27953	-2.26925
H	2.51408	0.53662	1.17477
H	3.22408	0.77802	-0.42185
H	2.98754	-0.86489	0.19103
H	-3.28916	-0.23189	0.46368
H	-2.38228	-1.72503	0.16771
H	-3.02649	-0.79451	-1.19373
F	0.21667	0.40650	1.78002

6: [{$(CH_3)_2CH$}$_2$NP{$C_6H_3(CH_3)_2$}]$^+$



(RI-)BP86/SV(P) level:
Energy = -942.6877661176 E_h
Zero Point Energy = 0.3315202 E_h
Symmetry = C_1

XYZ Coordinates:
39

C	1.27011	0.42569	-0.03183
P	-0.38560	1.18050	-0.11480
N	-1.47521	-0.06694	0.00166
C	-2.94838	0.30003	-0.03519
C	-1.14522	-1.52522	0.12903
H	-0.03669	-1.56412	0.14581
C	-1.63803	-2.30871	-1.09987
C	-1.67046	-2.10095	1.45534
H	-3.47875	-0.66908	0.04154
C	-3.32322	0.95208	-1.37531
C	-3.33175	1.16068	1.17898
C	3.93815	-0.39860	0.05268
C	3.29757	-0.24073	-1.18634
C	1.95768	0.18334	-1.25593
C	1.91596	0.30932	1.23248
C	3.25749	-0.11652	1.24746
H	4.99047	-0.72363	0.08664
H	3.85009	-0.43565	-2.12042
C	1.27160	0.36000	-2.59277
C	1.19769	0.62968	2.52536
H	3.78129	-0.21042	2.21327
H	0.35016	1.34240	2.37704
H	1.88380	1.09601	3.26399
H	0.77720	-0.28471	3.00305
H	1.98153	0.70917	-3.37207
H	0.44436	1.11191	-2.54863
H	0.82540	-0.59298	-2.95933
H	-1.29854	-3.14307	1.55694
H	-2.77991	-2.14087	1.49674
H	-1.30103	-1.52161	2.32755
H	-1.27496	-3.35558	-1.01778
H	-1.23693	-1.88230	-2.04343
H	-2.74646	-2.34787	-1.16808
H	-4.43192	1.31459	1.18660
H	-2.84977	2.16219	1.13409
H	-3.04982	0.66880	2.13404
H	-2.84298	1.94891	-1.49149
H	-4.42340	1.10131	-1.41462
H	-3.03554	0.31150	-2.23576

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.03	0.03297	YES	YES
8		a	54.03	0.12061	YES	YES
9		a	108.47	0.65451	YES	YES
10		a	143.10	1.87741	YES	YES
11		a	161.89	3.23946	YES	YES
12		a	220.77	0.84890	YES	YES
13		a	258.07	0.23833	YES	YES
14		a	261.93	0.25719	YES	YES
15		a	331.59	0.65752	YES	YES
16		a	431.69	25.51929	YES	YES
17		a	435.65	24.98526	YES	YES
18		a	505.39	1.25012	YES	YES
19		a	523.48	2.22561	YES	YES
20		a	528.83	0.84803	YES	YES
21		a	549.42	11.99635	YES	YES
22		a	726.13	1.43402	YES	YES
23		a	729.50	5.41704	YES	YES
24		a	820.34	66.34508	YES	YES
25		a	1102.54	231.73283	YES	YES
26		a	1125.45	315.13040	YES	YES
27		a	1148.81	88.79335	YES	YES
28		a	1154.27	19.36874	YES	YES
29		a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

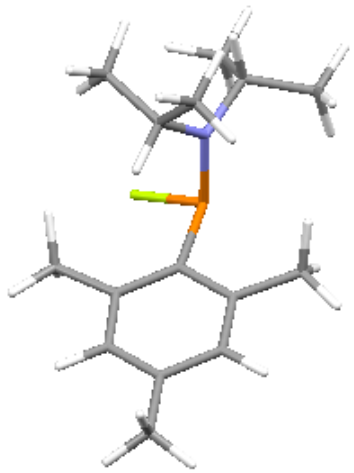
SCF Energy = -941.4442421890 E_h
Symmetry = C_1

XYZ Coordinates:
39

C	1.23202	0.47218	-0.03053
P	-0.40312	1.20374	-0.10695
N	-1.42043	-0.06346	0.00133
C	-2.89846	0.22798	-0.03966
C	-1.03576	-1.49716	0.12859
H	0.05204	-1.50145	0.16814
C	-1.49562	-2.26638	-1.10208
C	-1.58792	-2.07829	1.42293
H	-3.37305	-0.74739	0.01853
C	-3.27402	0.88588	-1.35854
C	-3.30542	1.05532	1.17006
C	3.84589	-0.42257	0.05771
C	3.21478	-0.25133	-1.17159
C	1.90053	0.20961	-1.24246
C	1.85976	0.33503	1.22300
C	3.17508	-0.12753	1.24194
H	4.86842	-0.77215	0.09247
H	3.75029	-0.46186	-2.08836
C	1.21964	0.39413	-2.57062
C	1.13682	0.65315	2.50252
H	3.68106	-0.24012	2.19214
H	0.49358	1.53171	2.40369
H	1.84400	0.86083	3.30261
H	0.51115	-0.18050	2.82434
H	1.95234	0.52638	-3.36378
H	0.57101	1.27467	-2.58108

H	0.60661	-0.47038	-2.82891
H	-1.18410	-3.08202	1.54306
H	-2.67313	-2.15953	1.40817
H	-1.28989	-1.48677	2.28570
H	-1.12136	-3.28585	-1.02724
H	-1.10258	-1.82523	-2.01542
H	-2.58072	-2.31684	-1.17213
H	-4.38884	1.15934	1.18196
H	-2.87021	2.05268	1.11968
H	-2.99524	0.57904	2.09796
H	-2.84640	1.88501	-1.43046
H	-4.35721	0.97790	-1.41321
H	-2.93586	0.29261	-2.20596

6-F: $(CH_3)_3C_6H_2N\{CH(CH_3)_2\}_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -1082.0060269960 E_h
Zero Point Energy = 0.3611824 E_h
Symmetry = C_1

XYZ Coordinates:
43

C	0.97093	0.50152	-0.02544
P	-0.77558	1.15705	-0.01164
N	-1.69979	-0.27281	0.15365
C	-3.09762	-0.11202	0.65412
C	-1.34787	-1.57313	-0.46902
H	-0.28567	-1.46773	-0.77459
C	-2.16870	-1.87394	-1.73849
C	-1.40207	-2.73277	0.54232
H	-3.56604	-1.11480	0.55303
C	-3.93239	0.86757	-0.19354
C	-3.13347	0.25725	2.14682
C	3.71707	-0.24716	0.28716
C	3.13297	-0.11009	-0.98385
C	1.78421	0.25988	-1.17523
C	1.55244	0.37931	1.27539
C	2.90317	0.00548	1.40494
C	5.15872	-0.67623	0.44600
H	3.75363	-0.29792	-1.87788
C	1.29739	0.36892	-2.60807
C	0.75076	0.62418	2.53880
H	3.33308	-0.08393	2.41829
H	-0.03342	-0.15114	2.68571
H	0.22151	1.60331	2.50951
H	1.40983	0.61546	3.43322
H	1.00166	1.40687	-2.86586
H	0.40285	-0.26039	-2.80105
H	2.09794	0.04715	-3.30768
H	-1.04082	-3.67253	0.06859
H	-2.43555	-2.92539	0.90857
H	-0.75547	-2.52031	1.42070
H	-1.79180	-2.79608	-2.23487
H	-2.09266	-1.03258	-2.46012
H	-3.24584	-2.03817	-1.50977
H	-4.18314	0.31636	2.51305
H	-2.65453	1.24633	2.31968
H	-2.59547	-0.50000	2.75699
H	-3.54372	1.90648	-0.10283
H	-4.99292	0.87167	0.14492
H	-3.90857	0.58981	-1.26838
F	-0.95415	1.55383	-1.63518
H	5.60851	-0.26446	1.37540
H	5.78145	-0.34785	-0.41425
H	5.24382	-1.78673	0.50559

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	25.86	0.31571	YES	YES
8	a	37.95	0.02088	YES	YES
9	a	40.55	0.21638	YES	YES
10	a	45.97	0.32373	YES	YES
11	a	56.35	0.10148	YES	YES
12	a	76.36	0.17162	YES	YES
13	a	96.49	0.76420	YES	YES
14	a	113.80	0.28033	YES	YES
15	a	124.00	0.70656	YES	YES
16	a	162.18	0.59674	YES	YES
17	a	180.19	4.80820	YES	YES
18	a	183.78	0.33113	YES	YES
19	a	189.51	0.50028	YES	YES
20	a	211.18	0.67917	YES	YES
21	a	225.87	0.06942	YES	YES
22	a	228.27	2.29550	YES	YES
23	a	234.60	0.17723	YES	YES
24	a	249.37	0.01762	YES	YES
25	a	265.85	0.15346	YES	YES
26	a	273.18	0.31599	YES	YES
27	a	282.83	0.48370	YES	YES
28	a	288.46	1.48839	YES	YES
29	a	312.40	0.70982	YES	YES
30	a	325.42	0.32050	YES	YES
31	a	329.60	0.10922	YES	YES
32	a	358.44	8.27189	YES	YES
33	a	370.41	3.95804	YES	YES
34	a	421.83	7.58451	YES	YES
35	a	486.59	5.87223	YES	YES
36	a	507.90	9.10264	YES	YES
37	a	513.44	10.14302	YES	YES
38	a	516.09	0.33405	YES	YES
39	a	529.09	7.42745	YES	YES
40	a	531.75	6.24104	YES	YES

41	a	552.46	2.59840	YES	YES
42	a	564.95	1.25841	YES	YES
43	a	602.10	15.94087	YES	YES
44	a	626.95	11.65430	YES	YES
45	a	713.69	99.23422	YES	YES
46	a	722.43	4.72321	YES	YES
47	a	846.36	6.92994	YES	YES
48	a	849.27	4.06759	YES	YES
49	a	863.85	17.66038	YES	YES
50	a	876.82	0.01835	YES	YES
51	a	898.68	1.30362	YES	YES
52	a	903.84	0.15768	YES	YES
53	a	919.05	0.01496	YES	YES
54	a	919.63	0.35857	YES	YES
55	a	921.54	0.35702	YES	YES
56	a	952.20	70.57150	YES	YES
57	a	952.36	1.28813	YES	YES
58	a	999.03	6.37414	YES	YES
59	a	1005.45	1.14438	YES	YES
60	a	1010.31	17.75680	YES	YES
61	a	1020.65	3.45664	YES	YES
62	a	1023.27	3.80186	YES	YES
63	a	1025.47	6.10039	YES	YES
64	a	1026.78	12.31453	YES	YES
65	a	1041.47	3.51836	YES	YES
66	a	1111.75	50.37766	YES	YES
67	a	1114.27	4.26361	YES	YES
68	a	1128.35	14.35804	YES	YES
69	a	1146.98	38.50048	YES	YES
70	a	1161.75	69.47972	YES	YES
71	a	1171.39	0.18080	YES	YES
72	a	1182.87	40.89050	YES	YES
73	a	1228.07	2.01528	YES	YES
74	a	1285.41	2.19881	YES	YES
75	a	1299.37	6.20961	YES	YES
76	a	1309.15	0.11132	YES	YES
77	a	1326.91	1.28213	YES	YES
78	a	1346.35	3.81851	YES	YES
79	a	1349.72	23.95657	YES	YES
80	a	1349.92	4.31179	YES	YES
81	a	1357.78	2.12588	YES	YES
82	a	1362.22	1.23670	YES	YES
83	a	1364.09	7.41052	YES	YES
84	a	1366.74	9.47307	YES	YES
85	a	1369.96	1.21137	YES	YES
86	a	1377.32	33.91287	YES	YES
87	a	1391.21	0.45855	YES	YES
88	a	1399.15	12.41598	YES	YES
89	a	1411.94	11.36514	YES	YES
90	a	1419.39	0.12601	YES	YES
91	a	1421.06	3.41334	YES	YES
92	a	1425.27	0.98620	YES	YES
93	a	1427.09	8.64856	YES	YES
94	a	1428.02	1.10440	YES	YES
95	a	1430.23	2.84840	YES	YES
96	a	1432.36	1.18017	YES	YES
97	a	1438.09	13.21852	YES	YES
98	a	1440.29	2.06809	YES	YES
99	a	1443.45	27.44530	YES	YES
100	a	1447.00	14.04911	YES	YES
101	a	1449.47	12.63865	YES	YES
102	a	1457.32	12.69652	YES	YES
103	a	1565.29	11.15458	YES	YES
104	a	1611.52	25.46726	YES	YES
105	a	2933.55	33.94197	YES	YES
106	a	2938.61	13.42489	YES	YES
107	a	2938.90	11.07879	YES	YES
108	a	2940.38	21.72317	YES	YES
109	a	2943.09	23.67898	YES	YES
110	a	2944.83	21.87742	YES	YES
111	a	2960.47	20.86765	YES	YES
112	a	2977.07	13.96146	YES	YES
113	a	2990.36	0.65617	YES	YES
114	a	3008.00	13.76081	YES	YES
115	a	3011.31	5.00194	YES	YES
116	a	3017.70	1.29733	YES	YES
117	a	3022.02	1.91810	YES	YES
118	a	3026.86	27.08186	YES	YES
119	a	3028.79	88.36895	YES	YES
120	a	3033.02	13.95129	YES	YES
121	a	3038.31	9.63976	YES	YES
122	a	3038.63	15.11060	YES	YES
123	a	3039.57	15.67725	YES	YES
124	a	3040.55	11.33035	YES	YES
125	a	3042.45	26.43907	YES	YES
126	a	3047.38	13.14260	YES	YES
127	a	3050.24	5.05238	YES	YES
128	a	3071.93	27.76282	YES	YES
129	a	3074.06	16.75315	YES	YES

(RI-)MP2/def2-TZVPP level

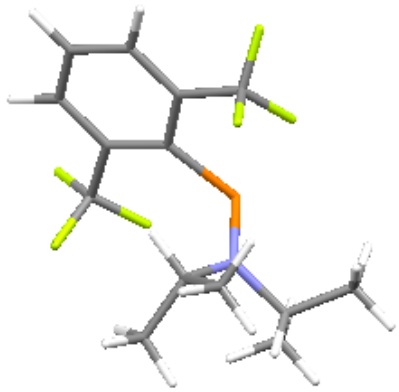
SCF Energy = -1080.6823776790 E_h
Symmetry = C_1

XYZ Coordinates:
43

C	0.91813	0.56988	-0.04354
P	-0.81304	1.18062	-0.04302
N	-1.62496	-0.26803	0.14046
C	-3.01438	-0.21380	0.64579
C	-1.19349	-1.54165	-0.45425
H	-0.17709	-1.37482	-0.80927
C	-2.05035	-1.94536	-1.65026
C	-1.12719	-2.64080	0.59930
H	-3.39975	-1.23041	0.56833
C	-3.90665	0.68926	-0.19996
C	-3.05518	0.18847	2.11396
C	3.61137	-0.23997	0.28866
C	3.04039	-0.11893	-0.97564
C	1.71477	0.27952	-1.17403
C	1.48211	0.45425	1.24874
C	2.80944	0.04967	1.38946
C	5.03145	-0.69950	0.45926
H	3.64536	-0.34241	-1.84766
C	1.22486	0.34448	-2.59876
C	0.68558	0.73356	2.49677
H	3.22634	-0.03132	2.38746
H	-0.10253	-0.00640	2.63732
H	0.20157	1.70956	2.45792
H	1.33724	0.70729	3.36853
H	1.00354	1.36456	-2.90391
H	0.31347	-0.23230	-2.74481
H	1.99063	-0.05615	-3.26061
H	-0.75688	-3.56491	0.15533
H	-2.10862	-2.84870	1.02630
H	-0.45319	-2.34905	1.40361
H	-1.64538	-2.84639	-2.11129
H	-2.06565	-1.15065	-2.39457
H	-3.07758	-2.15957	-1.35397
H	-4.08265	0.18846	2.47869

H	-2.64553	1.18974	2.24298
H	-2.47216	-0.50430	2.71841
H	-3.58230	1.72692	-0.11951
H	-4.93969	0.63003	0.14379
H	-3.86877	0.40216	-1.24896
F	-0.98184	1.56208	-1.61833
H	5.47624	-0.27119	1.35593
H	5.64104	-0.41365	-0.39618
H	5.07963	-1.78536	0.55243

7: $[(CF_3)_2C_6H_3N\{CH(CH_3)_2\}_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -1537.7343159280 E_h
Zero Point Energy 0.2882068 E_h
Symmetry = C_1

XYZ Coordinates:
39

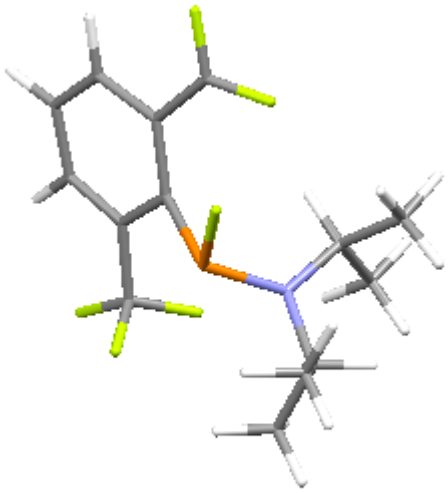
C	0.30092	0.22787	0.89187
P	-0.25318	1.07471	-0.67008
N	-0.58801	-0.13920	-1.73580
C	-1.06288	0.31314	-3.11201
C	-0.48762	-1.62316	-1.51013
H	-0.09551	-1.72839	-0.47719
C	0.51972	-2.26817	-2.47583
C	-1.87743	-2.27906	-1.56943
H	-1.26636	-0.63119	-3.65435
C	0.04971	1.06998	-3.85211
C	-2.37449	1.10576	-3.01262
C	1.20647	-0.63317	3.44476
C	2.12610	-0.40862	2.41098
C	1.68342	0.02764	1.14991
C	-0.61096	0.02236	1.96080
C	-0.15896	-0.41581	3.21889
H	1.55738	-0.96583	4.43405
H	3.20316	-0.55836	2.58493
C	2.72915	0.22662	0.06788
C	-2.10756	0.21369	1.78922
H	-0.88586	-0.57252	4.03117
F	-2.37150	1.03825	0.71087
F	-2.67558	0.77072	2.86078
F	-2.73218	-0.95667	1.53940
F	3.88083	0.69649	0.54770
F	2.27686	1.12968	-0.87586
F	2.98542	-0.92353	-0.59415
H	-1.77155	-3.35190	-1.30058
H	-2.32379	-2.23638	-2.58622
H	-2.57971	-1.81466	-0.84724
H	0.64095	-3.33559	-2.19167
H	1.51562	-1.78504	-2.41309
H	0.17236	-2.24771	-3.53093
H	-2.75382	1.31704	-4.03524
H	-2.22629	2.08435	-2.50313
H	-3.15570	0.53540	-2.46715
H	0.27816	2.04216	-3.36025
H	-0.28085	1.28874	-4.88995
H	0.98403	0.47251	-3.90807

$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a		22.85	0.09669	YES YES
8	a		29.08	0.33594	YES YES
9	a		38.73	2.18445	YES YES
10	a		49.01	0.21084	YES YES
11	a		55.04	0.08159	YES YES
12	a		61.75	0.34638	YES YES
13	a		93.21	0.69611	YES YES
14	a		108.35	0.13146	YES YES
15	a		126.48	11.34295	YES YES
16	a		132.92	0.09729	YES YES
17	a		160.00	4.17997	YES YES
18	a		170.29	2.64402	YES YES
19	a		182.13	2.75128	YES YES
20	a		205.13	17.87238	YES YES
21	a		221.77	1.29945	YES YES
22	a		232.13	0.21836	YES YES
23	a		241.41	0.27454	YES YES
24	a		262.40	0.84413	YES YES
25	a		265.86	1.29997	YES YES
26	a		267.92	2.81899	YES YES
27	a		273.69	1.32683	YES YES
28	a		290.62	0.01013	YES YES
29	a		324.25	0.17220	YES YES
30	a		325.56	1.75507	YES YES
31	a		340.30	4.12301	YES YES
32	a		348.02	5.64783	YES YES
33	a		375.83	0.17816	YES YES
34	a		400.05	1.74736	YES YES
35	a		449.21	5.49223	YES YES
36	a		457.96	0.20934	YES YES
37	a		462.79	1.06810	YES YES
38	a		484.38	0.23998	YES YES
39	a		503.73	6.30631	YES YES
40	a		537.79	10.91773	YES YES
41	a		545.84	3.88966	YES YES
42	a		561.22	0.11212	YES YES
43	a		578.37	13.25096	YES YES
44	a		585.79	0.81909	YES YES
45	a		623.73	1.61082	YES YES
46	a		648.89	3.74227	YES YES
47	a		660.50	43.08754	YES YES
48	a		684.51	4.24380	YES YES
49	a		728.21	7.91881	YES YES
50	a		743.41	14.70574	YES YES

51	a	807.24	30.11903	YES	YES
52	a	822.93	0.95579	YES	YES
53	a	846.02	8.50850	YES	YES
54	a	876.13	5.73199	YES	YES
55	a	910.40	1.50714	YES	YES
56	a	912.51	0.11783	YES	YES
57	a	915.24	25.76282	YES	YES
58	a	927.35	0.06761	YES	YES
59	a	929.19	1.45198	YES	YES
60	a	929.88	0.24171	YES	YES
61	a	995.44	1.85123	YES	YES
62	a	1005.48	15.03054	YES	YES
63	a	1020.94	126.05209	YES	YES
64	a	1033.14	68.37114	YES	YES
65	a	1050.99	5.84929	YES	YES
66	a	1097.12	51.12099	YES	YES
67	a	1103.42	2.07863	YES	YES
68	a	1110.72	34.97508	YES	YES
69	a	1113.28	69.31853	YES	YES
70	a	1119.97	148.33421	YES	YES
71	a	1129.58	3.72835	YES	YES
72	a	1137.23	110.98218	YES	YES
73	a	1149.17	15.07985	YES	YES
74	a	1175.56	21.94366	YES	YES
75	a	1178.29	11.78882	YES	YES
76	a	1202.33	414.18883	YES	YES
77	a	1211.43	133.45635	YES	YES
78	a	1273.51	419.56871	YES	YES
79	a	1288.86	9.80818	YES	YES
80	a	1298.69	3.00740	YES	YES
81	a	1315.71	56.69431	YES	YES
82	a	1335.95	8.04501	YES	YES
83	a	1352.86	2.11794	YES	YES
84	a	1355.14	13.29775	YES	YES
85	a	1356.51	31.57309	YES	YES
86	a	1362.46	6.65729	YES	YES
87	a	1374.18	6.24526	YES	YES
88	a	1378.18	15.43126	YES	YES
89	a	1417.79	0.41525	YES	YES
90	a	1422.97	1.35792	YES	YES
91	a	1424.13	1.23799	YES	YES
92	a	1427.05	1.18439	YES	YES
93	a	1429.69	8.51967	YES	YES
94	a	1437.75	10.86662	YES	YES
95	a	1442.55	20.53708	YES	YES
96	a	1443.08	11.35881	YES	YES
97	a	1450.26	22.04242	YES	YES
98	a	1453.02	1.74343	YES	YES
99	a	1585.93	18.58969	YES	YES
100	a	1594.08	0.44383	YES	YES
101	a	2952.49	2.01925	YES	YES
102	a	2954.17	1.42241	YES	YES
103	a	2965.38	2.99522	YES	YES
104	a	2968.44	6.42056	YES	YES
105	a	3000.94	2.35567	YES	YES
106	a	3022.75	1.13561	YES	YES
107	a	3040.00	2.71597	YES	YES
108	a	3048.55	9.73167	YES	YES
109	a	3049.14	0.04222	YES	YES
110	a	3054.27	15.24246	YES	YES
111	a	3058.83	3.44924	YES	YES
112	a	3060.35	3.43359	YES	YES
113	a	3071.52	2.45568	YES	YES
114	a	3075.75	2.49775	YES	YES
115	a	3123.29	0.56719	YES	YES
116	a	3129.77	2.46119	YES	YES
117	a	3140.09	1.55843	YES	YES

7: $[(CF_3)(CF_2)C_6H_3N\{CH(CH_3)_2\}_2PF]^+$ Isomer



(RI-)BP86/SV(P) level:

SCF Energy = -1537.6908864180 E_h
Zero Point Energy 0.2871725 E_h
Symmetry = C_1

XYZ Coordinates:
39

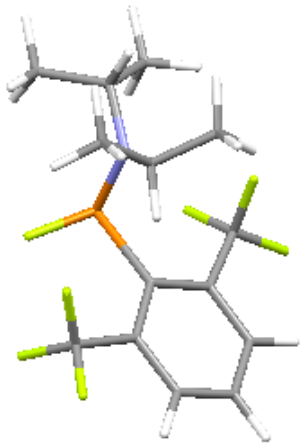
C	0.99408	0.16807	-0.17329
P	-0.57006	1.04701	0.33679
N	-1.74997	-0.11159	0.59163
C	-3.17420	0.37709	0.48652
C	-1.52978	-1.50679	1.10375
H	-0.43313	-1.67003	1.02219
C	-2.21775	-2.57395	0.24040
C	-1.93373	-1.61862	2.58588
H	-3.77844	-0.43863	0.93540
C	-3.61671	0.54599	-0.97378
C	-3.40516	1.64460	1.32148
C	3.68135	-0.07158	-1.24562
C	2.53855	-0.16953	-2.07237
C	1.23516	-0.02451	-1.56684
C	2.18287	0.10397	0.67490
C	3.51386	0.06540	0.11822
H	4.68909	-0.12573	-1.68540
H	2.66980	-0.32878	-3.15301
C	0.09464	-0.08317	-2.59294
C	2.12716	-0.08301	2.06449
H	4.38607	0.09260	0.78845
F	-0.08769	1.59279	1.83164
F	1.07019	-0.35736	2.74398
F	3.18597	-0.06619	2.81000
F	0.56591	-0.25177	-3.83986
F	-0.63692	1.05359	-2.58365
F	-0.73472	-1.11500	-2.32425
H	-1.63452	-2.61387	2.98158
H	-3.03380	-1.53207	2.72034
H	-1.44907	-0.83457	3.20413
H	-1.95557	-3.58192	0.62865

H	-1.89254	-2.51595	-0.81672
H	-3.32538	-2.49085	0.27588
H	-4.47944	1.92909	1.29253
H	-2.83337	2.51281	0.91626
H	-3.11154	1.49713	2.38226
H	-3.05163	1.36639	-1.46818
H	-4.69736	0.80288	-1.01542
H	-3.45916	-0.38444	-1.55741

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.74	0.79058	YES	YES
8	a	24.86	1.80125	YES	YES
9	a	47.18	0.59200	YES	YES
10	a	52.95	1.53196	YES	YES
11	a	59.19	0.22657	YES	YES
12	a	79.78	0.60502	YES	YES
13	a	101.25	2.69043	YES	YES
14	a	104.89	0.11822	YES	YES
15	a	124.81	1.19659	YES	YES
16	a	137.42	0.32994	YES	YES
17	a	144.37	0.70511	YES	YES
18	a	155.16	2.51560	YES	YES
19	a	172.22	0.05001	YES	YES
20	a	205.83	0.66656	YES	YES
21	a	211.32	1.35523	YES	YES
22	a	227.59	0.04901	YES	YES
23	a	229.71	0.43226	YES	YES
24	a	243.58	1.57872	YES	YES
25	a	250.47	1.68783	YES	YES
26	a	266.24	0.12062	YES	YES
27	a	271.12	0.44153	YES	YES
28	a	275.39	0.57383	YES	YES
29	a	304.79	5.97084	YES	YES
30	a	316.80	7.21668	YES	YES
31	a	326.59	0.33514	YES	YES
32	a	344.74	3.85772	YES	YES
33	a	356.80	0.61680	YES	YES
34	a	381.81	1.09484	YES	YES
35	a	395.89	8.45953	YES	YES
36	a	428.48	3.01140	YES	YES
37	a	468.34	2.08288	YES	YES
38	a	481.27	15.69589	YES	YES
39	a	498.40	12.89005	YES	YES
40	a	504.72	14.95238	YES	YES
41	a	520.46	12.76675	YES	YES
42	a	533.52	1.40581	YES	YES
43	a	582.64	1.28648	YES	YES
44	a	585.18	12.02039	YES	YES
45	a	620.56	1.24994	YES	YES
46	a	632.98	14.42828	YES	YES
47	a	670.72	10.96364	YES	YES
48	a	681.31	3.41297	YES	YES
49	a	712.49	44.84257	YES	YES
50	a	730.45	32.29033	YES	YES
51	a	745.27	53.51437	YES	YES
52	a	798.71	20.16571	YES	YES
53	a	840.52	20.07958	YES	YES
54	a	846.16	15.29342	YES	YES
55	a	872.22	4.91162	YES	YES
56	a	900.72	1.53538	YES	YES
57	a	906.71	0.30860	YES	YES
58	a	920.02	2.02635	YES	YES
59	a	922.26	1.01947	YES	YES
60	a	942.57	2.98987	YES	YES
61	a	946.82	9.18581	YES	YES
62	a	982.62	33.94776	YES	YES
63	a	994.77	0.45719	YES	YES
64	a	1013.60	13.16073	YES	YES
65	a	1075.21	14.02542	YES	YES
66	a	1101.12	63.31310	YES	YES
67	a	1105.76	26.50338	YES	YES
68	a	1111.88	29.04703	YES	YES
69	a	1117.89	45.43362	YES	YES
70	a	1128.76	16.65123	YES	YES
71	a	1143.53	39.50652	YES	YES
72	a	1147.38	191.64516	YES	YES
73	a	1157.05	26.24939	YES	YES
74	a	1177.16	18.78302	YES	YES
75	a	1179.39	20.98914	YES	YES
76	a	1193.50	99.94250	YES	YES
77	a	1265.30	243.79122	YES	YES
78	a	1287.85	9.57865	YES	YES
79	a	1297.96	6.72236	YES	YES
80	a	1319.22	20.56683	YES	YES
81	a	1329.91	29.59212	YES	YES
82	a	1346.05	7.48618	YES	YES
83	a	1352.32	8.93559	YES	YES
84	a	1357.01	29.32806	YES	YES
85	a	1370.95	18.57619	YES	YES
86	a	1376.14	20.99309	YES	YES
87	a	1383.81	77.87996	YES	YES
88	a	1410.97	161.64011	YES	YES
89	a	1414.17	1.63143	YES	YES
90	a	1421.83	2.31906	YES	YES
91	a	1426.38	108.80363	YES	YES
92	a	1428.72	3.48838	YES	YES
93	a	1430.98	31.09048	YES	YES
94	a	1438.98	8.38004	YES	YES
95	a	1440.80	14.12418	YES	YES
96	a	1442.84	5.48580	YES	YES
97	a	1453.39	9.99535	YES	YES
98	a	1540.53	533.67738	YES	YES
99	a	1552.18	182.75527	YES	YES
100	a	1591.61	70.40164	YES	YES
101	a	2932.95	21.84120	YES	YES
102	a	2957.25	3.77481	YES	YES
103	a	2958.10	5.76638	YES	YES
104	a	2967.16	4.39266	YES	YES
105	a	2972.38	7.85066	YES	YES
106	a	2999.02	6.71912	YES	YES
107	a	3021.52	20.56638	YES	YES
108	a	3040.35	1.34405	YES	YES
109	a	3044.82	10.79917	YES	YES
110	a	3046.50	24.89010	YES	YES
111	a	3052.77	4.39603	YES	YES
112	a	3058.44	8.67061	YES	YES
113	a	3061.89	6.57294	YES	YES
114	a	3084.80	3.97300	YES	YES
115	a	3132.18	0.71172	YES	YES
116	a	3143.95	5.35787	YES	YES
117	a	3149.53	9.46146	YES	YES

7-F: $(CF_3)_2C_6H_3N\{CH(CH_3)_2\}_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -1637.7640482460 E_h
Zero Point Energy 0.2905453 E_h
Symmetry = C_1

XYZ Coordinates:
40

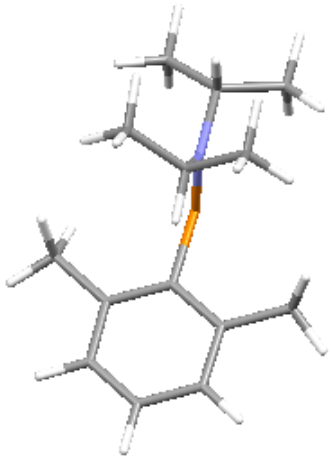
C	0.60643	0.21609	0.70280
P	-0.54511	1.06358	-0.55792
N	-1.34757	-0.25893	-1.26147
C	-2.65157	0.05698	-1.92932
C	-0.74107	-1.58413	-1.55842
H	0.22450	-1.58987	-1.01509
C	-0.41982	-1.77522	-3.05274
C	-1.58384	-2.74307	-0.99606
H	-2.97195	-0.89628	-2.40104
C	-2.50537	1.09999	-3.05383
C	-3.74353	0.45589	-0.92330
C	2.20870	-0.70730	2.90295
C	2.78035	-0.48168	1.65060
C	2.00992	-0.02744	0.55818
C	0.05160	-0.01944	2.00409
C	0.84116	-0.48172	3.07291
H	2.82742	-1.05791	3.74424
H	3.85425	-0.65920	1.50577
C	2.81756	0.16102	-0.73468
C	-1.43080	0.16301	2.33560
H	0.37280	-0.65748	4.05090
F	-2.20040	-0.78032	1.72978
F	-1.91074	1.37441	1.97081
F	-1.66450	0.04636	3.66580
F	3.04663	1.45790	-1.01619
F	2.23662	-0.42888	-1.80561
F	4.04629	-0.41968	-0.62322
H	-1.05113	-3.70825	-1.14833
H	-2.57063	-2.82901	-1.50380
H	-1.76359	-2.60877	0.09022
H	0.13096	-2.73005	-3.20490
H	0.21762	-0.94706	-3.42568
H	-1.34200	-1.82150	-3.67355
H	-4.70366	0.64654	-1.45290
H	-3.46362	1.38330	-0.37732
H	-3.90814	-0.34429	-0.17275
H	-2.23659	2.09836	-2.64061
H	-3.46429	1.21299	-3.60803
H	-1.71554	0.80812	-3.77741
F	0.58525	1.51680	-1.69195

vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	17.20	0.34728	YES YES
8		a	27.57	1.10188	YES YES
9		a	50.84	0.05225	YES YES
10		a	54.85	0.08763	YES YES
11		a	65.33	0.01958	YES YES
12		a	78.09	0.29510	YES YES
13		a	94.36	0.43889	YES YES
14		a	105.50	0.72880	YES YES
15		a	131.57	0.52885	YES YES
16		a	138.05	1.29663	YES YES
17		a	143.39	0.81608	YES YES
18		a	163.36	0.22790	YES YES
19		a	175.66	0.81173	YES YES
20		a	181.47	0.68840	YES YES
21		a	204.86	0.91321	YES YES
22		a	211.66	0.31911	YES YES
23		a	226.58	0.04267	YES YES
24		a	227.83	0.01779	YES YES
25		a	254.75	0.59288	YES YES
26		a	255.61	0.61143	YES YES
27		a	268.24	0.08617	YES YES
28		a	279.74	6.62456	YES YES
29		a	289.46	0.10416	YES YES
30		a	308.45	0.41962	YES YES
31		a	324.60	0.39558	YES YES
32		a	341.49	2.33778	YES YES
33		a	344.80	3.62148	YES YES
34		a	368.78	3.81222	YES YES
35		a	382.50	0.30074	YES YES
36		a	404.29	1.01550	YES YES
37		a	433.02	2.25825	YES YES
38		a	464.41	5.03386	YES YES
39		a	472.94	1.88682	YES YES
40		a	503.89	0.07396	YES YES
41		a	509.99	15.46474	YES YES
42		a	531.67	14.48204	YES YES
43		a	534.82	6.17313	YES YES
44		a	554.45	0.51025	YES YES
45		a	560.08	2.63692	YES YES
46		a	585.05	0.37850	YES YES
47		a	624.00	5.61412	YES YES
48		a	655.12	0.17338	YES YES
49		a	662.55	34.74104	YES YES
50		a	679.07	3.20533	YES YES
51		a	730.14	12.97070	YES YES
52		a	743.20	17.82275	YES YES
53		a	749.27	84.35609	YES YES
54		a	803.28	27.27098	YES YES
55		a	812.47	3.22089	YES YES

56	a	846.15	3.12259	YES	YES
57	a	866.08	15.96399	YES	YES
58	a	898.67	1.73086	YES	YES
59	a	904.44	0.56709	YES	YES
60	a	917.15	0.66755	YES	YES
61	a	920.51	0.33343	YES	YES
62	a	928.70	0.07446	YES	YES
63	a	953.51	55.73483	YES	YES
64	a	981.37	2.48897	YES	YES
65	a	1007.56	15.89293	YES	YES
66	a	1015.42	4.22233	YES	YES
67	a	1055.38	2.75543	YES	YES
68	a	1097.17	214.33637	YES	YES
69	a	1102.46	45.64947	YES	YES
70	a	1112.78	28.41040	YES	YES
71	a	1115.95	20.62583	YES	YES
72	a	1126.20	131.84543	YES	YES
73	a	1131.66	75.91878	YES	YES
74	a	1143.73	74.69746	YES	YES
75	a	1147.60	205.39062	YES	YES
76	a	1157.41	96.33054	YES	YES
77	a	1167.46	245.31589	YES	YES
78	a	1174.21	97.15758	YES	YES
79	a	1181.98	72.22371	YES	YES
80	a	1183.71	67.76982	YES	YES
81	a	1248.92	325.99618	YES	YES
82	a	1288.71	69.38037	YES	YES
83	a	1298.06	4.06839	YES	YES
84	a	1309.50	0.28254	YES	YES
85	a	1325.52	25.29340	YES	YES
86	a	1344.58	6.82658	YES	YES
87	a	1351.20	9.72357	YES	YES
88	a	1352.68	15.37115	YES	YES
89	a	1357.69	4.29344	YES	YES
90	a	1366.46	9.88082	YES	YES
91	a	1375.86	37.82856	YES	YES
92	a	1397.60	24.55065	YES	YES
93	a	1418.39	0.11023	YES	YES
94	a	1425.67	0.36008	YES	YES
95	a	1428.69	1.47296	YES	YES
96	a	1431.31	0.72473	YES	YES
97	a	1437.36	11.44483	YES	YES
98	a	1440.04	3.09746	YES	YES
99	a	1442.78	0.60984	YES	YES
100	a	1444.72	0.96083	YES	YES
101	a	1452.41	11.21797	YES	YES
102	a	1589.24	11.55252	YES	YES
103	a	1598.45	4.30611	YES	YES
104	a	2941.26	12.19309	YES	YES
105	a	2945.21	10.22879	YES	YES
106	a	2949.33	29.21041	YES	YES
107	a	2950.97	18.96225	YES	YES
108	a	2982.84	13.22138	YES	YES
109	a	3011.67	6.83437	YES	YES
110	a	3020.84	16.26793	YES	YES
111	a	3021.33	0.64188	YES	YES
112	a	3033.31	30.11408	YES	YES
113	a	3035.54	57.47061	YES	YES
114	a	3049.11	11.39633	YES	YES
115	a	3057.76	8.16918	YES	YES
116	a	3059.36	11.98358	YES	YES
117	a	3061.14	11.73863	YES	YES
118	a	3115.02	4.21339	YES	YES
119	a	3151.08	0.68687	YES	YES
120	a	3155.48	1.68856	YES	YES

8: [N{CH(CH3)2}2(CH3)2C6H3P]$^+$



(RI-)BP86/SV(P) level:

SCF Energy = -942.687766117 E_h
Zero Point Energy = 0.3315202 E_h
Symmetry = C_1

XYZ Coordinates:
39

C	1.27011	0.42569	-0.03183
P	-0.38560	1.18050	-0.11480
N	-1.47521	-0.06694	0.00166
C	-2.94838	0.30003	-0.03519
C	-1.14522	-1.52522	0.12903
H	-0.03669	-1.56412	0.14581
C	-1.63803	-2.30871	-1.09987
C	-1.67046	-2.10095	1.45534
H	-3.47875	-0.66908	0.04154
C	-3.32322	0.95208	-1.37531
C	-3.33175	1.16068	1.17898
C	3.93815	-0.39860	0.05268
C	3.29757	-0.24073	-1.18634
C	1.95768	0.18334	-1.25593
C	1.91596	0.30932	1.23248
C	3.25749	-0.11652	1.24746
H	4.99047	-0.72363	0.08664
H	3.85009	-0.43565	-2.12042
C	1.27160	0.36000	-2.59277
C	1.19769	0.62968	2.52536
H	3.78129	-0.21042	2.21327
H	0.35016	1.34240	2.37704
H	1.88380	1.09601	3.26399
H	0.77720	-0.28471	3.00305
H	1.98153	0.70917	-3.37207
H	0.44436	1.11191	-2.54863
H	0.82540	-0.59298	-2.95933
H	-1.29854	-3.14307	1.55694
H	-2.77991	-2.14087	1.49674
H	-1.30103	-1.52161	2.32755
H	-1.27496	-3.35558	-1.01778
H	-1.23693	-1.88230	-2.04343
H	-2.74646	-2.34787	-1.16808
H	-4.43192	1.31459	1.18660
H	-2.84977	2.16219	1.13409
H	-3.04982	0.66880	2.13404
H	-2.84298	1.94891	-1.49149

H	-4.42340	1.10131	-1.41462
H	-3.03554	0.31150	-2.23576

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.09	0.12853	YES	YES
8	a	28.97	0.09582	YES	YES
9	a	43.26	0.97501	YES	YES
10	a	56.67	0.04775	YES	YES
11	a	58.25	0.00317	YES	YES
12	a	88.76	0.35307	YES	YES
13	a	112.30	1.64206	YES	YES
14	a	130.51	0.04007	YES	YES
15	a	163.85	0.39161	YES	YES
16	a	166.57	0.55983	YES	YES
17	a	188.73	4.29842	YES	YES
18	a	206.38	0.10691	YES	YES
19	a	219.18	0.94717	YES	YES
20	a	227.08	0.62865	YES	YES
21	a	238.36	0.05346	YES	YES
22	a	248.85	6.71231	YES	YES
23	a	254.02	1.83993	YES	YES
24	a	265.66	0.10502	YES	YES
25	a	287.67	1.61553	YES	YES
26	a	322.69	0.43267	YES	YES
27	a	334.89	3.06530	YES	YES
28	a	369.36	2.65568	YES	YES
29	a	410.28	8.73590	YES	YES
30	a	424.48	0.07689	YES	YES
31	a	464.33	0.92333	YES	YES
32	a	503.13	0.84921	YES	YES
33	a	503.85	0.87053	YES	YES
34	a	513.69	0.23301	YES	YES
35	a	522.96	5.38950	YES	YES
36	a	589.83	11.83481	YES	YES
37	a	590.85	10.01562	YES	YES
38	a	625.29	1.12748	YES	YES
39	a	713.85	4.92433	YES	YES
40	a	750.22	5.55859	YES	YES
41	a	776.04	26.89318	YES	YES
42	a	848.27	5.54725	YES	YES
43	a	873.78	6.23440	YES	YES
44	a	896.34	0.20305	YES	YES
45	a	903.84	0.17237	YES	YES
46	a	911.97	1.53255	YES	YES
47	a	914.78	0.30985	YES	YES
48	a	918.64	23.51076	YES	YES
49	a	926.99	0.36947	YES	YES
50	a	930.68	0.72520	YES	YES
51	a	952.47	2.50504	YES	YES
52	a	984.37	2.42878	YES	YES
53	a	987.64	3.81041	YES	YES
54	a	1000.80	1.00152	YES	YES
55	a	1015.38	10.98398	YES	YES
56	a	1018.74	1.05420	YES	YES
57	a	1039.60	14.55892	YES	YES
58	a	1099.10	46.56361	YES	YES
59	a	1102.73	1.27976	YES	YES
60	a	1103.54	9.19975	YES	YES
61	a	1109.95	37.76483	YES	YES
62	a	1127.72	7.92809	YES	YES
63	a	1145.75	7.48780	YES	YES
64	a	1160.02	2.60330	YES	YES
65	a	1173.71	3.99837	YES	YES
66	a	1234.74	0.14033	YES	YES
67	a	1246.41	8.34032	YES	YES
68	a	1297.26	0.95561	YES	YES
69	a	1316.80	3.49857	YES	YES
70	a	1338.48	0.08794	YES	YES
71	a	1347.52	1.81538	YES	YES
72	a	1348.45	3.59951	YES	YES
73	a	1353.09	18.95047	YES	YES
74	a	1361.95	3.10779	YES	YES
75	a	1364.88	7.68251	YES	YES
76	a	1367.12	3.06364	YES	YES
77	a	1370.06	2.97916	YES	YES
78	a	1375.97	13.59697	YES	YES
79	a	1377.40	11.99811	YES	YES
80	a	1397.58	9.10373	YES	YES
81	a	1403.13	23.84418	YES	YES
82	a	1418.11	0.17533	YES	YES
83	a	1420.33	0.68857	YES	YES
84	a	1422.96	7.49174	YES	YES
85	a	1425.95	1.36078	YES	YES
86	a	1428.66	10.06321	YES	YES
87	a	1436.12	21.59576	YES	YES
88	a	1438.55	6.25016	YES	YES
89	a	1442.54	14.13667	YES	YES
90	a	1443.69	23.17511	YES	YES
91	a	1449.10	11.35063	YES	YES
92	a	1457.39	30.58831	YES	YES
93	a	1578.34	4.41833	YES	YES
94	a	1592.97	18.33845	YES	YES
95	a	2896.31	40.14316	YES	YES
96	a	2908.31	34.62482	YES	YES
97	a	2955.05	2.64564	YES	YES
98	a	2956.83	0.74667	YES	YES
99	a	2961.15	6.10961	YES	YES
100	a	2963.29	5.89308	YES	YES
101	a	2985.29	10.94912	YES	YES
102	a	2989.91	11.64839	YES	YES
103	a	3008.37	2.53065	YES	YES
104	a	3025.63	1.02171	YES	YES
105	a	3039.92	2.70684	YES	YES
106	a	3042.21	2.51428	YES	YES
107	a	3044.60	2.76791	YES	YES
108	a	3050.15	0.11220	YES	YES
109	a	3052.52	6.76051	YES	YES
110	a	3055.58	10.89489	YES	YES
111	a	3056.86	0.22917	YES	YES
112	a	3058.16	9.56651	YES	YES
113	a	3058.75	4.11069	YES	YES
114	a	3059.48	9.28552	YES	YES
115	a	3101.32	0.09670	YES	YES
116	a	3105.80	1.65352	YES	YES
117	a	3125.81	1.32392	YES	YES

(RI-)MP2/def2-TZVPP level

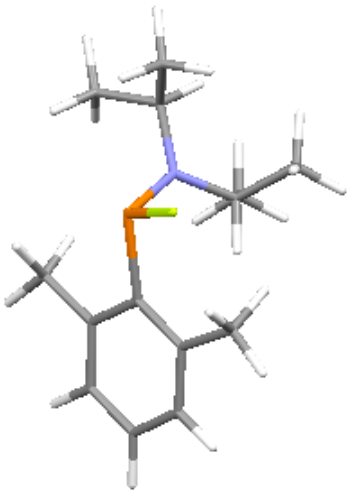
SCF Energy = -941.4442421890 E_h
Symmetry = C_1

XYZ Coordinates:
39

C	1.23202	0.47218	-0.03053
P	-0.40312	1.20374	-0.10695
N	-1.42043	-0.06346	0.00133
C	-2.89846	0.22798	-0.03966
C	-1.03576	-1.49716	0.12859
H	0.05204	-1.50145	0.16814
C	-1.49562	-2.26638	-1.10208
C	-1.58792	-2.07829	1.42293
H	-3.37305	-0.74739	0.01853
C	-3.27402	0.88588	-1.35854
C	-3.30542	1.05532	1.17006
C	3.84589	-0.42257	0.05771
C	3.21478	-0.25133	-1.17159
C	1.90053	0.20961	-1.24246
C	1.85976	0.33503	1.22300
C	3.17508	-0.12753	1.24194
H	4.86842	-0.77215	0.09247
H	3.75029	-0.46186	-2.08836
C	1.21964	0.39413	-2.57062
C	1.13682	0.65315	2.50252
H	3.68106	-0.24012	2.19214
H	0.49358	1.53171	2.40369
H	1.84400	0.86083	3.30261
H	0.51115	-0.18050	2.82434
H	1.95234	0.52638	-3.36378
H	0.57101	1.27467	-2.58108
H	0.60661	-0.47038	-2.82891
H	-1.18410	-3.08202	1.54306
H	-2.67313	-2.15953	1.40817
H	-1.28989	-1.48677	2.28570
H	-1.12136	-3.28585	-1.02724
H	-1.10258	-1.82523	-2.01542
H	-2.58072	-2.31684	-1.17213
H	-4.38884	1.15934	1.18196
H	-2.87021	2.05268	1.11968
H	-2.99524	0.57904	2.09796
H	-2.84640	1.88501	-1.43046
H	-4.35721	0.97790	-1.41321
H	-2.93586	0.29261	-2.20596

C	1.28983	0.37974	0.08099
P	-0.41508	1.14231	0.05565
N	-1.43114	-0.23230	0.09836
C	-2.83729	-0.01057	0.55129
C	-1.13349	-1.51538	-0.58574
H	-0.05488	-1.46128	-0.84287
C	-1.91668	-1.69079	-1.90206
C	-1.30238	-2.72445	0.35285
H	-3.36238	-0.97268	0.36815
C	-3.57002	1.07112	-0.26581
C	-2.91616	0.26890	2.06167
C	3.94350	-0.54363	0.46591
C	3.44848	-0.31875	-0.82391
C	2.13331	0.14603	-1.04969
C	1.79793	0.15913	1.40049
C	3.11717	-0.30494	1.57063
H	4.97658	-0.90197	0.60920
H	4.09772	-0.50715	-1.69603
C	1.71384	0.35564	-2.49236
C	0.95027	0.38887	2.63635
H	3.49788	-0.47470	2.59227
H	0.11076	-0.33847	2.70175
H	0.48832	1.40188	2.63850
H	1.56131	0.28697	3.55863
H	1.49415	1.42174	-2.70777
H	0.79154	-0.20539	-2.75342
H	2.52243	0.01871	-3.17551
H	-0.97944	-3.65691	-0.16115
H	-2.36078	-2.87064	0.66519
H	-0.68285	-2.60390	1.26733
H	-1.57692	-2.60587	-2.43696
H	-1.75857	-0.81675	-2.56897
H	-3.01038	-1.79848	-1.72478
H	-3.97544	0.37336	2.38760
H	-2.38550	1.21290	2.31642
H	-2.45372	-0.55722	2.64376
H	-3.12141	2.07513	-0.09403
H	-4.64213	1.12418	0.02913
H	-3.51615	0.85780	-1.35434
F	-0.49036	1.63570	-1.54809

8-F: N{CH(CH3)2}2(CH3)2C6H3PF



(RI-)BP86/SV(P) level:

SCF Energy = -1042.7212013910 E_h
Zero Point Energy = 0.3348090 E_h
Symmetry = C_1

XYZ Coordinates:
40

vibrational spectrum
mode symmetry wave number IR intensity
selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	33.37	0.02961	YES	YES
8	a	46.84	0.23297	YES	YES
9	a	48.37	0.20560	YES	YES
10	a	60.68	0.08435	YES	YES
11	a	71.83	0.25303	YES	YES
12	a	113.02	1.02328	YES	YES
13	a	128.93	0.63705	YES	YES
14	a	148.61	0.22507	YES	YES
15	a	164.62	0.54798	YES	YES
16	a	185.67	0.53836	YES	YES
17	a	192.76	1.28211	YES	YES
18	a	211.91	0.35021	YES	YES
19	a	226.46	0.13914	YES	YES
20	a	231.26	0.21849	YES	YES
21	a	236.33	2.90976	YES	YES
22	a	249.46	0.02681	YES	YES
23	a	255.87	1.29562	YES	YES
24	a	274.61	1.91058	YES	YES
25	a	283.37	1.13646	YES	YES
26	a	293.55	0.60065	YES	YES
27	a	326.48	0.34507	YES	YES
28	a	326.92	0.47256	YES	YES
29	a	347.51	5.75246	YES	YES
30	a	377.27	6.48889	YES	YES

31	a	412.07	7.43065	YES	YES
32	a	463.02	7.08599	YES	YES
33	a	475.70	2.52808	YES	YES
34	a	508.81	17.07113	YES	YES
35	a	515.50	1.20140	YES	YES
36	a	522.92	0.37636	YES	YES
37	a	528.80	14.09724	YES	YES
38	a	533.67	3.35372	YES	YES
39	a	578.16	9.45798	YES	YES
40	a	624.31	8.72297	YES	YES
41	a	713.77	97.43259	YES	YES
42	a	727.58	5.54938	YES	YES
43	a	752.63	3.89131	YES	YES
44	a	761.96	22.71987	YES	YES
45	a	844.63	3.01197	YES	YES
46	a	861.05	15.54965	YES	YES
47	a	881.23	0.01186	YES	YES
48	a	893.00	0.56309	YES	YES
49	a	899.27	0.69601	YES	YES
50	a	901.24	1.42465	YES	YES
51	a	916.48	0.07403	YES	YES
52	a	922.11	0.01303	YES	YES
53	a	952.48	70.02790	YES	YES
54	a	960.33	0.13850	YES	YES
55	a	976.09	3.69271	YES	YES
56	a	1007.77	15.26843	YES	YES
57	a	1019.89	0.78075	YES	YES
58	a	1023.77	9.92585	YES	YES
59	a	1026.24	2.12113	YES	YES
60	a	1033.70	1.15590	YES	YES
61	a	1112.04	11.36946	YES	YES
62	a	1113.05	40.42768	YES	YES
63	a	1116.45	7.56280	YES	YES
64	a	1128.76	13.12150	YES	YES
65	a	1145.85	41.19996	YES	YES
66	a	1151.97	1.96188	YES	YES
67	a	1160.85	65.56106	YES	YES
68	a	1182.62	41.87366	YES	YES
69	a	1230.27	3.65836	YES	YES
70	a	1237.72	0.60114	YES	YES
71	a	1297.51	4.49401	YES	YES
72	a	1310.13	0.91805	YES	YES
73	a	1325.92	0.75661	YES	YES
74	a	1340.98	13.50986	YES	YES
75	a	1349.14	9.11870	YES	YES
76	a	1350.26	4.22954	YES	YES
77	a	1351.05	9.89327	YES	YES
78	a	1361.44	3.64115	YES	YES
79	a	1364.17	8.00161	YES	YES
80	a	1366.51	4.77904	YES	YES
81	a	1373.95	35.31540	YES	YES
82	a	1389.97	6.08198	YES	YES
83	a	1412.32	12.49233	YES	YES
84	a	1419.15	2.26656	YES	YES
85	a	1421.41	1.57136	YES	YES
86	a	1424.65	0.09324	YES	YES
87	a	1425.20	4.56494	YES	YES
88	a	1429.62	2.91524	YES	YES
89	a	1431.92	1.07334	YES	YES
90	a	1438.30	1.39912	YES	YES
91	a	1439.70	12.85486	YES	YES
92	a	1442.51	20.46433	YES	YES
93	a	1445.87	10.02348	YES	YES
94	a	1449.91	3.63820	YES	YES
95	a	1455.00	28.66049	YES	YES
96	a	1582.67	7.65717	YES	YES
97	a	1596.42	2.03252	YES	YES
98	a	2938.95	11.85835	YES	YES
99	a	2939.66	12.14387	YES	YES
100	a	2940.83	21.57514	YES	YES
101	a	2943.80	22.85221	YES	YES
102	a	2945.22	20.91670	YES	YES
103	a	2959.92	20.62509	YES	YES
104	a	2976.81	14.04882	YES	YES
105	a	2990.93	0.51273	YES	YES
106	a	3011.81	4.78122	YES	YES
107	a	3018.33	1.94836	YES	YES
108	a	3022.26	2.57717	YES	YES
109	a	3027.55	24.01733	YES	YES
110	a	3029.26	87.33122	YES	YES
111	a	3033.67	14.86083	YES	YES
112	a	3039.14	18.54476	YES	YES
113	a	3039.44	11.22333	YES	YES
114	a	3040.32	15.98766	YES	YES
115	a	3044.89	22.69130	YES	YES
116	a	3046.96	12.53764	YES	YES
117	a	3050.29	5.61601	YES	YES
118	a	3080.26	1.11348	YES	YES
119	a	3087.75	23.88630	YES	YES
120	a	3106.90	26.84484	YES	YES

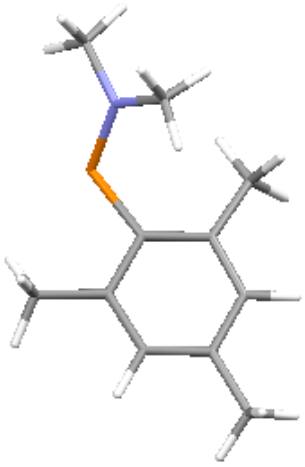
(RI-)MP2/def2-TZVPP level

SCF Energy = 1041.4547520210 E_h
Symmetry = C_1

XYZ Coordinates:
40

C	1.23535	0.44610	0.06658
P	-0.45096	1.17286	0.01385
N	-1.36419	-0.22390	0.08576
C	-2.77231	-0.09765	0.52281
C	-0.98708	-1.49716	-0.54569
H	0.05543	-1.38553	-0.84129
C	-1.80397	-1.78863	-1.80087
C	-1.05038	-2.64317	0.45684
H	-3.22011	-1.07978	0.37211
C	-3.55477	0.90651	-0.31743
C	-2.86495	0.23307	2.00640
C	3.83088	-0.54767	0.48422
C	3.35228	-0.33810	-0.80311
C	2.06563	0.15700	-1.04108
C	1.71911	0.23257	1.37972
C	3.00893	-0.26589	1.56806
H	4.83110	-0.92942	0.63919
H	3.98413	-0.56537	-1.65269
C	1.64771	0.31593	-2.48110
C	0.87386	0.50283	2.59713
H	3.36684	-0.42690	2.57733
H	0.03243	-0.18754	2.65624
H	0.45791	1.51035	2.58513
H	1.47296	0.38849	3.49884
H	1.50908	1.36076	-2.74867
H	0.70811	-0.19074	-2.69283
H	2.41546	-0.10744	-3.12612
H	-0.72017	-3.57036	-0.01155
H	-2.06476	-2.80056	0.82425
H	-0.40173	-2.43523	1.30671
H	-1.43607	-2.69484	-2.28229
H	-1.72642	-0.96352	-2.50728
H	-2.85756	-1.94385	-1.56716
H	-3.90819	0.28038	2.31964
H	-2.40236	1.19864	2.20833
H	-2.35782	-0.52453	2.60143
H	-3.16667	1.91382	-0.16546
H	-4.60644	0.90248	-0.02971
H	-3.47978	0.66990	-1.37700
F	-0.51361	1.63916	-1.54599

9: $[(CH_3)_2C_6H_2N(CH_3)_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -824.8465573318 E_h
Zero Point Energy = 0.2495491 E_h
Symmetry = C_1

XYZ Coordinates:
30

C	0.09970	0.22816	-0.22917
P	-1.57476	0.63142	-0.73366
N	-2.61246	-0.32027	0.16367
C	-4.05657	-0.05096	0.02289
C	-2.28489	-1.43645	1.05452
H	-1.21116	-1.69319	0.97381
H	-2.90472	-2.31394	0.76605
H	-2.52748	-1.17151	2.10728
H	-4.57272	-0.96933	-0.33231
H	-4.22381	0.77223	-0.70173
H	-4.48119	0.24028	1.00883
C	2.87120	-0.13686	0.27721
C	2.36442	-0.19953	-1.04005
C	1.00674	-0.00899	-1.32280
C	0.59649	0.34251	1.11549
C	1.97018	0.15311	1.32590
C	4.33138	-0.37360	0.55518
H	3.05782	-0.40496	-1.87321
C	0.51782	-0.12815	-2.74950
C	-0.25855	0.74028	2.29956
H	2.36544	0.26609	2.35001
H	-1.25376	1.13936	2.01366
H	0.25043	1.53112	2.89174
H	-0.41706	-0.11651	2.99231
H	-0.37069	0.51549	-2.95999
H	0.21815	-1.17407	-2.98929
H	1.30974	0.16330	-3.47075
H	4.67388	0.16975	1.46085
H	4.96872	-0.07470	-0.30369
H	4.51675	-1.45896	0.73583

******* Vibrational Frequencies *******
$vibrational spectrum
mode symmetry wave number IR intensity selection rules
cm**(-1) km/mol IR RAMAN

1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	44.73	0.33587	YES	YES
8	a	51.06	0.48533	YES	YES
9	a	73.01	4.02352	YES	YES
10	a	88.48	0.98015	YES	YES
11	a	117.85	1.59918	YES	YES
12	a	152.60	1.70006	YES	YES
13	a	168.28	0.29407	YES	YES
14	a	174.13	2.67116	YES	YES
15	a	200.96	0.64588	YES	YES
16	a	203.13	0.08434	YES	YES
17	a	227.50	2.06234	YES	YES
18	a	248.64	5.72642	YES	YES
19	a	258.53	0.86363	YES	YES
20	a	277.64	0.26687	YES	YES
21	a	311.39	3.27509	YES	YES
22	a	328.38	1.09197	YES	YES
23	a	367.57	6.78889	YES	YES
24	a	403.79	7.16063	YES	YES
25	a	442.60	6.76384	YES	YES
26	a	487.07	0.88233	YES	YES
27	a	515.05	5.96121	YES	YES
28	a	519.76	2.92885	YES	YES
29	a	542.57	2.72345	YES	YES
30	a	562.50	1.12389	YES	YES
31	a	625.46	8.92103	YES	YES
32	a	689.37	17.90311	YES	YES
33	a	711.78	2.02408	YES	YES
34	a	853.44	11.55026	YES	YES
35	a	890.63	5.62626	YES	YES
36	a	924.62	0.12866	YES	YES
37	a	935.24	7.46367	YES	YES
38	a	968.42	121.28627	YES	YES
39	a	996.14	0.96469	YES	YES
40	a	1003.68	2.86899	YES	YES
41	a	1008.80	5.30974	YES	YES
42	a	1015.96	4.43680	YES	YES
43	a	1016.23	0.12544	YES	YES
44	a	1018.20	2.81808	YES	YES
45	a	1018.98	30.82165	YES	YES
46	a	1056.34	2.29087	YES	YES
47	a	1062.67	53.95562	YES	YES
48	a	1117.27	2.51844	YES	YES
49	a	1160.08	3.08894	YES	YES
50	a	1168.50	13.01362	YES	YES
51	a	1228.01	1.27435	YES	YES
52	a	1259.34	0.50663	YES	YES
53	a	1285.39	54.22753	YES	YES
54	a	1336.83	1.85484	YES	YES
55	a	1357.68	27.26730	YES	YES
56	a	1361.98	16.00696	YES	YES
57	a	1365.93	2.39086	YES	YES
58	a	1379.22	4.75786	YES	YES
59	a	1385.47	13.96635	YES	YES
60	a	1390.61	9.77307	YES	YES
61	a	1405.93	2.15221	YES	YES
62	a	1406.69	2.83565	YES	YES
63	a	1407.91	2.24145	YES	YES
64	a	1414.11	10.37791	YES	YES
65	a	1422.99	27.07210	YES	YES
66	a	1426.99	4.17333	YES	YES

67	a	1427.38	16.58597	YES	YES
68	a	1430.10	17.54735	YES	YES
69	a	1443.88	32.47504	YES	YES
70	a	1448.84	34.42559	YES	YES
71	a	1452.24	36.79740	YES	YES
72	a	1533.10	25.37791	YES	YES
73	a	1604.29	213.68272	YES	YES
74	a	2916.03	13.11400	YES	YES
75	a	2941.58	1.06462	YES	YES
76	a	2951.96	3.56464	YES	YES
77	a	2952.95	0.60135	YES	YES
78	a	2956.86	4.98643	YES	YES
79	a	2992.29	8.93988	YES	YES
80	a	3022.66	8.04382	YES	YES
81	a	3028.51	1.21479	YES	YES
82	a	3034.97	0.82353	YES	YES
83	a	3044.80	0.63916	YES	YES
84	a	3048.28	2.35832	YES	YES
85	a	3050.47	5.62864	YES	YES
86	a	3060.55	2.01044	YES	YES
87	a	3073.76	0.07738	YES	YES
88	a	3091.29	1.83958	YES	YES
89	a	3092.10	2.43004	YES	YES
90	a	3096.40	1.85867	YES	YES

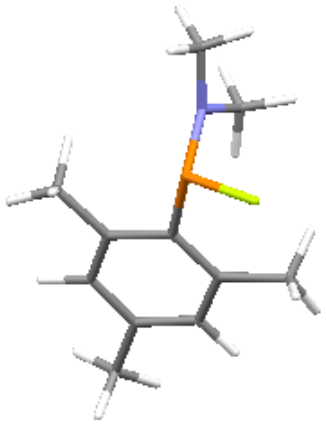
(RI-)MP2/def2-TZVPP level

SCF Energy = -823.7642342434 E_h
Symmetry = C_1

XYZ Coordinates:
30

C	0.09205	0.25514	-0.22286
P	-1.56813	0.66907	-0.69069
N	-2.53435	-0.33252	0.15503
C	-3.99164	-0.13652	0.04240
C	-2.15502	-1.45515	1.01489
H	-1.09015	-1.64418	0.93109
H	-2.72466	-2.32618	0.69694
H	-2.41359	-1.21675	2.04514
H	-4.43853	-1.05538	-0.32959
H	-4.20205	0.68434	-0.63692
H	-4.39102	0.08903	1.02898
C	2.82109	-0.14676	0.25969
C	2.30967	-0.21606	-1.03943
C	0.96510	0.00097	-1.31281
C	0.58265	0.36554	1.10039
C	1.94473	0.15520	1.30331
C	4.27454	-0.39711	0.52373
H	2.98120	-0.43095	-1.86219
C	0.45745	-0.10514	-2.72562
C	-0.26535	0.75239	2.28235
H	2.33886	0.25650	2.30798
H	-1.23955	1.14742	1.99981
H	0.24051	1.52176	2.86282
H	-0.42295	-0.09856	2.94608
H	-0.28076	0.66622	-2.96105
H	-0.00723	-1.07411	-2.91076
H	1.27652	0.01019	-3.43190
H	4.60253	0.10532	1.43057
H	4.88787	-0.05597	-0.30736
H	4.45356	-1.46567	0.65034

9-F: $(CH_3)_2C_6H_2N(CH_3)_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -924.8820041611E_h
Zero Point Energy 0.2518039 E_h
Symmetry = C_1

XYZ Coordinates:

31

C	0.23688	0.30981	-0.04533
P	-1.55362	0.81884	0.01673
N	-2.28945	-0.64957	0.49329
C	-3.63888	-0.57183	1.04575
C	-1.91393	-1.97704	0.02099
H	-0.84763	-1.98483	-0.28474
H	-2.53848	-2.30748	-0.84612
H	-2.04513	-2.72515	0.83833
H	-4.42156	-0.85079	0.29677
H	-3.84353	0.46466	1.39044
H	-3.74288	-1.25853	1.91932
C	3.04329	-0.19817	0.16728
C	2.27706	0.11968	1.30271
C	0.89602	0.37688	1.22158
C	0.99434	-0.01759	-1.21004
C	2.37674	-0.26582	-1.06830
C	4.53406	-0.43330	0.26821
H	2.76862	0.16904	2.29059
C	0.14110	0.68228	2.50150
C	0.40923	-0.13111	-2.60520
H	2.95467	-0.52879	-1.97203
F	-1.88820	0.93598	-1.62004
H	-0.55251	-0.14426	2.77328
H	-0.48587	1.59758	2.40537
H	0.84342	0.83394	3.34892
H	-0.45624	-0.82534	-2.64618
H	1.18137	-0.50013	-3.31336
H	0.03352	0.84548	-2.97555
H	4.81239	-0.88904	1.24338
H	5.09830	0.52477	0.18426
H	4.89934	-1.10019	-0.54241

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#	cm**(-1)	km/mol	IR	RAMAN
1	0.00	0.00000	-	-
2	0.00	0.00000	-	-
3	0.00	0.00000	-	-
4	0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	29.75	0.42957	YES	YES
8	a	47.15	0.37525	YES	YES
9	a	51.13	0.39886	YES	YES
10	a	81.18	0.21588	YES	YES
11	a	106.38	1.74817	YES	YES
12	a	133.79	0.35184	YES	YES
13	a	146.56	0.41540	YES	YES
14	a	179.84	3.94484	YES	YES
15	a	189.93	0.52840	YES	YES
16	a	201.34	1.24465	YES	YES
17	a	211.82	0.73134	YES	YES
18	a	219.23	0.08252	YES	YES
19	a	229.74	1.28029	YES	YES
20	a	262.68	1.63228	YES	YES
21	a	271.55	1.26288	YES	YES
22	a	283.07	0.58372	YES	YES
23	a	324.18	2.10620	YES	YES
24	a	338.44	1.04861	YES	YES
25	a	346.30	6.00128	YES	YES
26	a	399.17	15.20330	YES	YES
27	a	461.48	6.69007	YES	YES
28	a	508.18	1.31719	YES	YES
29	a	516.56	0.06898	YES	YES
30	a	530.10	0.60114	YES	YES
31	a	552.62	1.73843	YES	YES
32	a	569.85	2.56050	YES	YES
33	a	602.83	16.71993	YES	YES
34	a	661.14	44.07379	YES	YES
35	a	725.71	43.91166	YES	YES
36	a	729.71	71.79507	YES	YES
37	a	845.61	6.18597	YES	YES
38	a	874.14	0.04209	YES	YES
39	a	921.69	0.53535	YES	YES
40	a	952.41	0.55586	YES	YES
41	a	972.88	172.14251	YES	YES
42	a	1000.05	4.66465	YES	YES
43	a	1005.37	1.68275	YES	YES
44	a	1022.10	6.33012	YES	YES
45	a	1024.10	4.23370	YES	YES
46	a	1025.89	0.21671	YES	YES
47	a	1027.33	15.17221	YES	YES
48	a	1043.93	7.04312	YES	YES
49	a	1049.08	3.12892	YES	YES
50	a	1087.82	1.90298	YES	YES
51	a	1133.69	2.82372	YES	YES
52	a	1169.00	0.53200	YES	YES
53	a	1202.92	48.68052	YES	YES
54	a	1226.40	1.66578	YES	YES
55	a	1260.76	31.58101	YES	YES
56	a	1285.57	2.02965	YES	YES
57	a	1328.82	1.55954	YES	YES
58	a	1361.34	0.95838	YES	YES
59	a	1364.09	4.99837	YES	YES
60	a	1368.12	0.94907	YES	YES
61	a	1386.87	0.92535	YES	YES
62	a	1391.91	0.42624	YES	YES
63	a	1399.77	10.81345	YES	YES
64	a	1410.95	1.13559	YES	YES
65	a	1413.74	16.01071	YES	YES
66	a	1417.28	4.18195	YES	YES
67	a	1422.86	0.63705	YES	YES
68	a	1426.91	7.33697	YES	YES
69	a	1429.32	9.15915	YES	YES
70	a	1430.78	6.03737	YES	YES
71	a	1442.88	30.57125	YES	YES
72	a	1444.24	26.73791	YES	YES
73	a	1456.34	15.72865	YES	YES
74	a	1467.50	4.69784	YES	YES
75	a	1565.93	13.31808	YES	YES
76	a	1611.31	28.85452	YES	YES
77	a	2891.68	59.21632	YES	YES
78	a	2897.42	134.97558	YES	YES
79	a	2934.89	32.39216	YES	YES
80	a	2937.15	15.44153	YES	YES
81	a	2956.33	62.81283	YES	YES
82	a	2960.03	21.64566	YES	YES
83	a	2964.18	2.33779	YES	YES
84	a	3008.89	9.87746	YES	YES
85	a	3009.12	8.73433	YES	YES
86	a	3030.48	10.15308	YES	YES
87	a	3033.09	14.75251	YES	YES
88	a	3037.93	10.34306	YES	YES
89	a	3041.95	12.36843	YES	YES
90	a	3046.96	7.95155	YES	YES
91	a	3051.00	2.58032	YES	YES
92	a	3071.75	28.83764	YES	YES
93	a	3073.22	14.93955	YES	YES

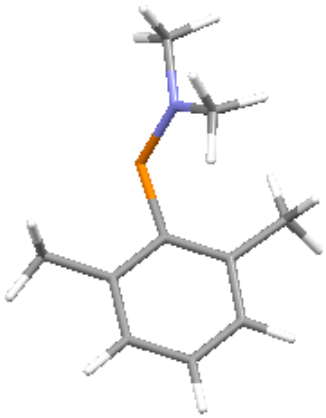
(RI-)MP2/def2-TZVPP level

SCF Energy = -923.7790936709 E_h
Symmetry = C_1

XYZ Coordinates:
31

C	0.21810	0.34406	-0.00996
P	-1.55131	0.80351	0.12020
N	-2.19943	-0.70262	0.44715
C	-3.56936	-0.74828	0.93974
C	-1.76914	-1.95508	-0.15249
H	-0.71115	-1.90687	-0.39723
H	-2.33663	-2.18350	-1.05974
H	-1.92385	-2.76803	0.55895
H	-4.28091	-0.96536	0.13780
H	-3.82855	0.20994	1.38466
H	-3.66298	-1.52630	1.69905
C	2.99026	-0.20894	0.10734
C	2.26964	0.08599	1.26211
C	0.90361	0.36310	1.22721
C	0.92672	0.03277	-1.19118
C	2.29604	-0.23549	-1.09940
C	4.46971	-0.46381	0.15820
H	2.78014	0.09839	2.21885
C	0.19650	0.64529	2.52846
C	0.29801	-0.05756	-2.55861
H	2.83364	-0.48287	-2.00825
F	-1.89154	1.08560	-1.44546
H	-0.53827	-0.12749	2.75554
H	-0.33671	1.59546	2.50059
H	0.91756	0.68037	3.34319
H	-0.58033	-0.69945	-2.56372
H	1.02257	-0.46520	-3.26121
H	-0.02163	0.91714	-2.91994
H	4.75554	-0.92735	1.10096
H	5.02645	0.46976	0.06655
H	4.78293	-1.11669	-0.65469

10: $[(CH_3)_2NP\{C_6H_3(CH_3)_2\}]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -785.5577085137 E_h
Zero Point Energy = 0.2229059 E_h
Symmetry = C_1

XYZ Coordinates:
27

C	0.47376	0.19408	-0.12990
P	-1.14607	0.71286	-0.72558
N	-2.27457	-0.27452	0.00202
C	-3.69683	0.04286	-0.23412
C	-2.04425	-1.45819	0.83551
H	-0.97210	-1.73277	0.83003
H	-2.65254	-2.29896	0.43521
H	-2.37339	-1.25695	1.87898
H	-4.19648	-0.82867	-0.70999
H	-3.78732	0.92957	-0.89419
H	-4.19701	0.25618	0.73607
C	3.14907	-0.30579	0.54790
C	2.76206	-0.32570	-0.80148
C	1.43213	-0.06680	-1.16904
C	0.86791	0.25316	1.24987
C	2.21533	-0.01003	1.55378
H	4.19859	-0.50459	0.81909
H	3.50580	-0.54755	-1.58448
C	1.02483	-0.13495	-2.62366
C	-0.06450	0.64260	2.37670
H	2.54622	0.04628	2.60404
H	-1.00216	1.12589	2.02993
H	0.43638	1.36066	3.06114
H	-0.34103	-0.23965	2.99743
H	0.15240	0.52350	-2.86124
H	0.72971	-1.16939	-2.91392
H	1.85652	0.17308	-3.29177

Vibrational Spectrum:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

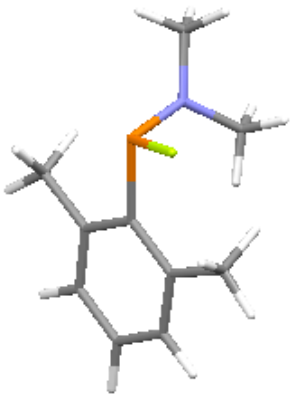
(RI-)MP2/def2-TZVPP level

SCF Energy = -784.5335019575 E_h
Symmetry = C_1

XYZ Coordinates:
27

C	0.46139	0.22333	-0.12911
P	-1.14527	0.74344	-0.68866
N	-2.20208	-0.28381	0.00084
C	-3.64063	-0.03666	-0.21343
C	-1.92186	-1.47040	0.81278
H	-0.85831	-1.68319	0.80702
H	-2.48140	-2.30346	0.39200
H	-2.26411	-1.28846	1.83015
H	-4.07435	-0.90854	-0.69720
H	-3.77525	0.84340	-0.83534
H	-4.11462	0.11692	0.75366
C	3.09580	-0.33599	0.52571
C	2.69879	-0.35447	-0.80890
C	1.38735	-0.05599	-1.16592
C	0.85266	0.27438	1.22978
C	2.18399	-0.01651	1.52673
H	4.12220	-0.55623	0.78500
H	3.41592	-0.59124	-1.58380
C	0.96517	-0.10344	-2.60923
C	-0.07097	0.65925	2.35371
H	2.51149	0.02802	2.55757
H	-0.98431	1.14359	2.01146
H	0.43160	1.35330	3.02460
H	-0.35071	-0.21326	2.94545
H	0.26840	0.69983	-2.86515
H	0.48091	-1.05000	-2.85150
H	1.82875	0.00391	-3.26163

10-F: $(CH_3)_2NP\{C_6H_3(CH_3)_2\}F$



(RI-)BP86/SV(P) level:
SCF Energy = -885.5971548721 E_h

Zero Point Energy = 0.2254900 E_h
Symmetry = C_1

XYZ Coordinates:
28

C	0.58228	0.24366	0.00777
P	-1.18248	0.84646	-0.00684
N	-2.01490	-0.58919	0.40286
C	-3.38163	-0.45173	0.89873
C	-1.68576	-1.92735	-0.07440
H	-0.60854	-1.98614	-0.33268
H	-2.28599	-2.21220	-0.97425
H	-1.89190	-2.67958	0.72324
H	-4.14354	-0.67968	0.11219
H	-3.54940	0.58817	1.25272
H	-3.55730	-1.14603	1.75457
C	3.32171	-0.39386	0.33888
C	2.54182	-0.05718	1.45203
C	1.17781	0.26401	1.30815
C	1.37173	-0.10467	-1.13056
C	2.73494	-0.41930	-0.93184
H	4.38999	-0.63902	0.46114
H	2.99403	-0.03976	2.45847
C	0.37478	0.58941	2.55289
C	0.84392	-0.16940	-2.55121
H	3.34670	-0.69380	-1.80824
F	-1.42491	1.01396	-1.65449
H	-0.35688	-0.21526	2.78774
H	-0.21671	1.52541	2.43424
H	1.04225	0.71334	3.43236
H	-0.05689	-0.81188	-2.63951
H	1.62514	-0.57561	-3.22839
H	0.54269	0.83122	-2.92580

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

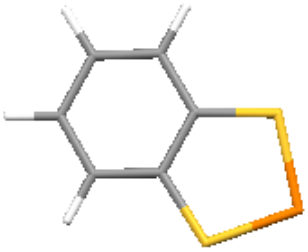
(RI-)MP2/def2-TZVPP level

SCF Energy = -884.5514073916 E_h
Symmetry = C_1

XYZ Coordinates:
28

C	0.56045	0.27535	0.02106
P	-1.18485	0.83489	0.10532
N	-1.92502	-0.63560	0.39399
C	-3.30690	-0.61055	0.85420
C	-1.55096	-1.90377	-0.21082
H	-0.48516	-1.91589	-0.42383
H	-2.10343	-2.08680	-1.13733
H	-1.77438	-2.71482	0.48424
H	-4.00928	-0.78629	0.03437
H	-3.52597	0.35824	1.29768
H	-3.45967	-1.38546	1.60700
C	3.27193	-0.42733	0.21056
C	2.55375	-0.10504	1.35548
C	1.20598	0.24797	1.28028
C	1.28189	-0.06168	-1.14644
C	2.63162	-0.40826	-1.02208
H	4.31796	-0.69484	0.27742
H	3.03830	-0.12448	2.32360
C	0.47487	0.56154	2.56076
C	0.68624	-0.09853	-2.53084
H	3.18283	-0.67222	-1.91601
F	-1.46141	1.15453	-1.46513
H	-0.30641	-0.17226	2.75984
H	-0.00575	1.53891	2.52320
H	1.17148	0.55349	3.39704
H	-0.22689	-0.68851	-2.56806
H	1.40520	-0.53866	-3.21930
H	0.43332	0.89742	-2.88675

11: $[PS_2C_2(C_6H_4)]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -1368.1799115260 E_h
Zero Point Energy = 0.0824079 E_h
Symmetry = C_{2V}

XYZ Coordinates:
13

S	-1.56019	0.00000	0.99919
P	0.00000	0.00000	2.36811
S	1.56019	0.00000	0.99919
C	-0.71459	0.00000	-0.53598
C	0.71459	0.00000	-0.53598
C	1.42940	0.00000	-1.75640
C	-1.42940	0.00000	-1.75640
H	-2.53056	0.00000	-1.76101
C	-0.70839	0.00000	-2.95249
C	0.70839	0.00000	-2.95249
H	2.53056	0.00000	-1.76101
H	-1.25428	0.00000	-3.90938
H	1.25428	0.00000	-3.90938

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN

1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.66	0.12888	YES	YES
8	a	30.57	0.12557	YES	YES
9	a	40.65	0.17456	YES	YES
10	a	88.17	0.03953	YES	YES
11	a	121.18	0.01303	YES	YES
12	a	132.90	0.28272	YES	YES
13	a	147.20	0.07963	YES	YES
14	a	161.90	1.11528	YES	YES
15	a	183.03	1.97686	YES	YES
16	a	201.20	0.25088	YES	YES
17	a	232.31	0.17361	YES	YES
18	a	262.57	0.07299	YES	YES
19	a	266.57	0.11650	YES	YES
20	a	301.12	1.67660	YES	YES
21	a	307.43	2.38793	YES	YES
22	a	328.94	7.37375	YES	YES
23	a	373.79	2.50256	YES	YES
24	a	384.03	7.28597	YES	YES
25	a	385.76	15.81145	YES	YES
26	a	395.20	0.70132	YES	YES
27	a	421.06	18.01500	YES	YES
28	a	432.96	5.92777	YES	YES
29	a	480.62	3.67693	YES	YES
30	a	488.46	9.66577	YES	YES
31	a	503.70	30.92937	YES	YES
32	a	566.52	0.94818	YES	YES
33	a	607.76	0.20035	YES	YES
34	a	622.13	8.35296	YES	YES
35	a	627.61	0.26013	YES	YES
36	a	682.30	3.27772	YES	YES
37	a	698.91	36.47011	YES	YES
38	a	736.77	22.23096	YES	YES
39	a	752.56	8.21784	YES	YES
40	a	790.92	71.63465	YES	YES
41	a	817.60	0.97977	YES	YES
42	a	835.72	0.41256	YES	YES
43	a	903.82	1.12480	YES	YES
44	a	957.19	0.54002	YES	YES
45	a	982.48	2.27337	YES	YES
46	a	985.09	8.82753	YES	YES
47	a	987.44	145.78461	YES	YES
48	a	1022.49	1.60674	YES	YES
49	a	1072.43	4.16028	YES	YES
50	a	1079.85	24.40550	YES	YES
51	a	1099.05	194.36722	YES	YES
52	a	1143.40	0.07736	YES	YES
53	a	1158.66	5.59585	YES	YES
54	a	1163.42	1.40165	YES	YES
55	a	1288.33	35.84153	YES	YES
56	a	1291.68	4.43757	YES	YES
57	a	1347.75	3.07779	YES	YES
58	a	1362.48	1.66469	YES	YES
59	a	1384.55	29.99692	YES	YES
60	a	1430.44	10.67474	YES	YES
61	a	1471.95	4.57679	YES	YES
62	a	1486.40	396.86941	YES	YES
63	a	1515.06	213.54415	YES	YES
64	a	1589.52	0.52817	YES	YES
65	a	1601.70	0.78501	YES	YES
66	a	1614.60	12.77237	YES	YES
67	a	1622.66	50.06897	YES	YES
68	a	3071.64	2.92299	YES	YES
69	a	3093.65	0.34226	YES	YES
70	a	3103.72	14.16686	YES	YES
71	a	3115.56	17.55188	YES	YES

(RI-)MP2/def2-TZVPP level

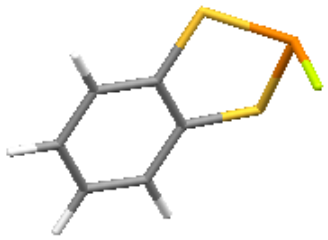
SCF Energy = -1366.6444439349 E_h

Symmetry = C_{2V}

XYZ Coordinates:
13

S	-1.52769	0.00000	0.98542
P	0.00000	0.00000	2.33145
S	1.52769	0.00000	0.98542
C	-0.70916	0.00000	-0.51921
C	0.70916	0.00000	-0.51921
C	1.42125	0.00000	-1.73441
C	-1.42125	0.00000	-1.73441
H	-2.50231	0.00000	-1.73465
C	-0.70512	0.00000	-2.91402
C	0.70512	0.00000	-2.91402
H	2.50231	0.00000	-1.73465
H	-1.23745	0.00000	-3.85476
H	1.23745	0.00000	-3.85476

11-F: $PS_2C_2(C_6H_4)F$



(RI-)BP86/SV(P) level:

SCF Energy = -1468.2337172270 E_h
Zero Point Energy = 0.0842839 E_h
Symmetry = C_s

XYZ Coordinates:
14

S	0.46135	0.71226	-1.57725
P	0.19121	2.14129	0.00000
S	0.46135	0.71226	1.57725
C	0.12555	-0.80578	-0.70776
C	0.12555	-0.80578	0.70776
C	-0.09885	-2.00634	1.41108
C	-0.09885	-2.00634	-1.41108
H	-0.10808	-2.00157	-2.51270
C	-0.31271	-3.19910	-0.70350
C	-0.31271	-3.19910	0.70350
H	-0.10808	-2.00157	2.51270
H	-0.49055	-4.13445	-1.25830
H	-0.49055	-4.13445	1.25830
F	-1.44383	2.35669	0.00000

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.66	0.12888	YES	YES
8	a	30.57	0.12557	YES	YES
9	a	40.65	0.17456	YES	YES

10	a	88.17	0.03953	YES	YES
11	a	121.18	0.01303	YES	YES
12	a	132.90	0.28272	YES	YES
13	a	147.20	0.07963	YES	YES
14	a	161.90	1.11528	YES	YES
15	a	183.03	1.97686	YES	YES
16	a	201.20	0.25088	YES	YES
17	a	232.31	0.17361	YES	YES
18	a	262.57	0.07299	YES	YES
19	a	266.57	0.11650	YES	YES
20	a	301.12	1.67660	YES	YES
21	a	307.43	2.38793	YES	YES
22	a	328.94	7.37375	YES	YES
23	a	373.79	2.50256	YES	YES
24	a	384.03	7.28597	YES	YES
25	a	385.76	15.81145	YES	YES
26	a	395.20	0.70132	YES	YES
27	a	421.06	18.01500	YES	YES
28	a	432.96	5.92777	YES	YES
29	a	480.62	3.67693	YES	YES
30	a	488.46	9.66577	YES	YES
31	a	503.70	30.92937	YES	YES
32	a	566.52	0.94818	YES	YES
33	a	607.76	0.20035	YES	YES
34	a	622.13	8.35296	YES	YES
35	a	627.61	0.26013	YES	YES
36	a	682.30	3.27772	YES	YES
37	a	698.91	36.47011	YES	YES
38	a	736.77	22.23096	YES	YES
39	a	752.56	8.21784	YES	YES
40	a	790.92	71.63465	YES	YES
41	a	817.60	0.97977	YES	YES
42	a	835.72	0.41256	YES	YES
43	a	903.82	1.12480	YES	YES
44	a	957.19	0.54002	YES	YES
45	a	982.48	2.27337	YES	YES
46	a	985.09	8.82753	YES	YES
47	a	987.44	145.78461	YES	YES
48	a	1022.49	1.60674	YES	YES
49	a	1072.43	4.16028	YES	YES
50	a	1079.85	24.40550	YES	YES
51	a	1099.05	194.36722	YES	YES
52	a	1143.40	0.07736	YES	YES
53	a	1158.66	5.59585	YES	YES
54	a	1163.42	1.40165	YES	YES
55	a	1288.33	35.84153	YES	YES
56	a	1291.68	4.43757	YES	YES
57	a	1347.75	3.07779	YES	YES
58	a	1362.48	1.66469	YES	YES
59	a	1384.55	29.99692	YES	YES
60	a	1430.44	10.67474	YES	YES
61	a	1471.95	4.57679	YES	YES
62	a	1486.40	396.86941	YES	YES
63	a	1515.06	213.54415	YES	YES
64	a	1589.52	0.52817	YES	YES
65	a	1601.70	0.78501	YES	YES
66	a	1614.60	12.77237	YES	YES
67	a	1622.66	50.06897	YES	YES
68	a	3071.64	2.92299	YES	YES
69	a	3093.65	0.34226	YES	YES
70	a	3103.72	14.16686	YES	YES
71	a	3115.56	17.55188	YES	YES

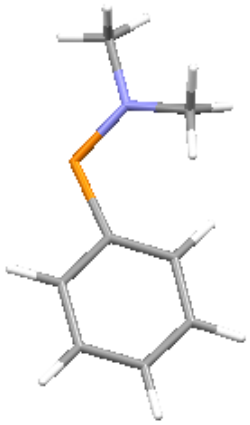
(RI-)MP2/def2-TZVPP level

SCF Energy = -1466.6704722080 E_h
Symmetry = C_1

XYZ Coordinates:
14

S	0.47484	0.72441	-1.54611
P	0.15185	2.09532	-0.00000
S	0.47484	0.72441	1.54611
C	0.13053	-0.77587	-0.70012
C	0.13053	-0.77587	0.70012
C	-0.09261	-1.96567	1.40027
C	-0.09261	-1.96567	-1.40027
H	-0.10187	-1.95917	-2.48169
C	-0.30524	-3.14643	-0.69836
C	-0.30524	-3.14643	0.69836
H	-0.10188	-1.95917	2.48169
H	-0.48016	-4.06495	-1.24084
H	-0.48016	-4.06495	1.24084
F	-1.45060	2.22292	0.00000

12: $[(CH_3)_2NP(C_6H_5)]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -706.9896338396 E_h
Zero Point Energy = 0.1703579 E_h
Symmetry = C_1

XYZ Coordinates:
21

C	0.55118	0.25960	0.08854
P	-1.08244	0.97092	0.22934
N	-2.22349	-0.19783	-0.09124
C	-3.63192	0.19773	0.12342
C	-2.05219	-1.56505	-0.60022
H	-1.05979	-1.68461	-1.07553
H	-2.84536	-1.76004	-1.35305
H	-2.16747	-2.30455	0.22373
H	-4.19402	0.10341	-0.83083
H	-3.68733	1.24516	0.48500
H	-4.09264	-0.47245	0.88236
C	3.28584	-0.40205	-0.07076
C	2.87332	0.91174	-0.36101
C	1.51969	1.25215	-0.25730
C	0.98770	-1.06204	0.39975
C	2.34674	-1.37885	0.32502
H	4.35417	-0.66616	-0.13184
H	3.61157	1.67563	-0.65204
H	1.20521	2.29220	-0.45529
H	0.27805	-1.82867	0.74472
H	2.68578	-2.39447	0.58422

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES

11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

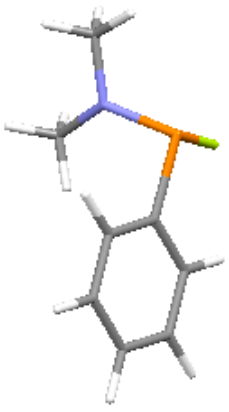
(RI-)MP2/def2-TZVPP level

SCF Energy = -706.0770290616 E_h
Symmetry = C_1

XYZ Coordinates:
21

C	0.53570	0.26784	0.11385
P	-1.08140	0.96203	0.26849
N	-2.16376	-0.19440	-0.09677
C	-3.58884	0.15445	0.07725
C	-1.95440	-1.54400	-0.63476
H	-0.96440	-1.62445	-1.06867
H	-2.71141	-1.71483	-1.39637
H	-2.07914	-2.27766	0.15957
H	-4.08531	0.07773	-0.88693
H	-3.67895	1.16451	0.46623
H	-4.03503	-0.54922	0.77655
C	3.22940	-0.40000	-0.09501
C	2.81795	0.89482	-0.40774
C	1.47958	1.24335	-0.27412
C	0.96088	-1.03159	0.45039
C	2.30767	-1.35169	0.34956
H	4.27424	-0.66565	-0.17747
H	3.53842	1.63247	-0.73086
H	1.16209	2.25924	-0.48144
H	0.26289	-1.76719	0.82268
H	2.64407	-2.34202	0.62247

12-F: $(CH_3)_2NP(C_6H_5)F$



(RI-)BP86/SV(P) level:
SCF Energy = -807.0369303972 E_h
Zero Point Energy = 0.1719870 E_h
Symmetry = C_1

XYZ Coordinates:
22

C	0.65648	0.13159	0.26839
P	-1.09361	0.52617	0.73240
N	-1.92531	-0.65743	-0.17100
C	-3.27479	-1.01252	0.26274
C	-1.63932	-0.98759	-1.56450
H	-0.58603	-0.74113	-1.80776
H	-2.30452	-0.42703	-2.26632
H	-1.79475	-2.07772	-1.74143
H	-4.06404	-0.51049	-0.35065
H	-3.41731	-0.71741	1.32411
H	-3.42957	-2.11443	0.18193
C	3.38502	-0.45600	-0.17344
C	2.87689	0.81638	-0.48630
C	1.52059	1.11222	-0.26338
C	1.17686	-1.14233	0.59019
C	2.53123	-1.43597	0.36542
H	4.44972	-0.68515	-0.34691
H	3.54252	1.58800	-0.90850
H	1.12053	2.10790	-0.51026
H	0.51000	-1.91383	1.01273
H	2.92406	-2.43658	0.61260
F	-1.20863	1.92784	-0.18053

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.03	0.03297	YES	YES
8		a	54.03	0.12061	YES	YES
9		a	108.47	0.65451	YES	YES
10		a	143.10	1.87741	YES	YES
11		a	161.89	3.23946	YES	YES
12		a	220.77	0.84890	YES	YES
13		a	258.07	0.23833	YES	YES
14		a	261.93	0.25719	YES	YES
15		a	331.59	0.65752	YES	YES
16		a	431.69	25.51929	YES	YES
17		a	435.65	24.98526	YES	YES
18		a	505.39	1.25012	YES	YES
19		a	523.48	2.22561	YES	YES
20		a	528.83	0.84803	YES	YES
21		a	549.42	11.99635	YES	YES
22		a	726.13	1.43402	YES	YES
23		a	729.50	5.41704	YES	YES
24		a	820.34	66.34508	YES	YES
25		a	1102.54	231.73283	YES	YES
26		a	1125.45	315.13040	YES	YES
27		a	1148.81	88.79335	YES	YES
28		a	1154.27	19.36874	YES	YES
29		a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

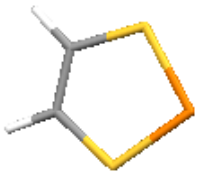
SCF Energy = -806.1029571853 E_h
Symmetry = C_1

XYZ Coordinates:
22

C	0.63493	0.16024	0.29095
P	-1.09898	0.53237	0.72265
N	-1.85352	-0.66901	-0.15399
C	-3.22470	-1.01213	0.19740
C	-1.51464	-1.01540	-1.52660
H	-0.47634	-0.76836	-1.73002

H	-2.15035	-0.47858	-2.23557
H	-1.65615	-2.08627	-1.68015
H	-3.94378	-0.53062	-0.47113
H	-3.43043	-0.69696	1.21745
H	-3.36366	-2.09190	0.12800
C	3.32714	-0.45061	-0.17975
C	2.82691	0.80741	-0.50846
C	1.48889	1.11631	-0.26792
C	1.14838	-1.09756	0.63199
C	2.48454	-1.40390	0.39199
H	4.36577	-0.68729	-0.36639
H	3.47803	1.54962	-0.95057
H	1.10209	2.09155	-0.52806
H	0.49443	-1.84034	1.07261
H	2.86878	-2.38136	0.65115
F	-1.23185	1.87619	-0.19155

13: $[S_2(CH)_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -1214.6238981160 E_h
Zero Point Energy 0.0360429E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

S	-1.55462	0.00000	-0.02065
P	0.00000	0.00000	1.37403
S	1.55462	0.00000	-0.02065
C	-0.68642	0.00000	-1.51222
C	0.68642	0.00000	-1.51222
H	1.29606	0.00000	-2.43450
H	-1.29606	0.00000	-2.43450

$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b2	252.72	1.61021	YES	YES
8	a1	376.33	0.40712	YES	YES
9	a2	423.30	0.00000	NO	YES
10	b1	487.36	3.85415	YES	YES
11	a1	506.07	6.42921	YES	YES
12	b1	610.12	1.21855	YES	YES
13	b2	723.98	74.83425	YES	YES
14	a1	736.00	0.07781	YES	YES
15	b1	822.30	8.89252	YES	YES
16	a2	856.97	0.00000	NO	YES
17	a1	1093.30	0.31197	YES	YES
18	b1	1240.36	12.24556	YES	YES
19	a1	1460.52	16.57981	YES	YES
20	b1	3109.14	33.43748	YES	YES
21	a1	3122.56	66.46664	YES	YES

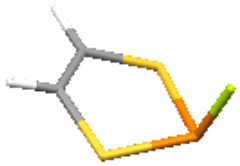
(RI-)MP2/def2-TZVPP level

SCF Energy = -1213.3109727785 E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

S	-1.51999	0.00000	-0.02024
P	0.00000	0.00000	1.35166
S	1.51999	0.00000	-0.02024
C	-0.68655	0.00000	-1.48783
C	0.68655	0.00000	-1.48783
H	1.27932	0.00000	-2.39433
H	-1.27932	0.00000	-2.39433

13-F: $S_2(CH)_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -1314.6840609080 E_h
Zero Point Energy 0.0360429E_h
Symmetry = C_s

XYZ Coordinates:
8

S	0.24679	-0.35763	-1.58099
P	0.49426	1.08618	0.00000
S	0.24679	-0.35763	1.58099
C	-0.45788	-1.69978	-0.67668
C	-0.45788	-1.69978	0.67668
H	-0.86746	-2.52668	1.28110
H	-0.86746	-2.52668	-1.28110
F	-0.96781	1.85369	0.00000

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	124.50	1.29397	YES	YES
8	a"	184.74	0.70699	YES	YES
9	a'	229.83	2.29427	YES	YES
10	a'	365.63	0.72114	YES	YES
11	a"	378.41	1.34458	YES	YES

12	a"	437.32	6.08578	YES	YES
13	a'	466.01	47.77045	YES	YES
14	a"	599.29	0.82755	YES	YES
15	a'	626.34	65.89870	YES	YES
16	a'	698.60	1.93982	YES	YES
17	a'	757.09	145.28607	YES	YES
18	a"	764.32	30.93731	YES	YES
19	a"	805.11	0.01642	YES	YES
20	a'	1078.36	0.14523	YES	YES
21	a"	1217.94	1.34268	YES	YES
22	a'	1554.05	18.89440	YES	YES
23	a"	3109.15	3.88497	YES	YES
24	a'	3127.06	0.46171	YES	YES

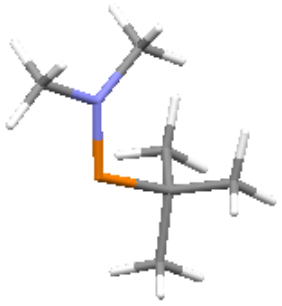
(RI-)MP2/def2-TZVPP level

SCF Energy = -1313.3381787393 E_h
Symmetry = C_s

XYZ Coordinates:
8

S	0.27416	-0.33907	-1.54357
P	0.46777	1.06228	0.00000
S	0.27416	-0.33907	1.54357
C	-0.47939	-1.64459	-0.67184
C	-0.47939	-1.64459	0.67184
H	-0.90228	-2.44660	1.25965
H	-0.90228	-2.44660	-1.25965
F	-0.98614	1.75173	0.00000

14: $[Me_2NPC(CH_3)_3]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -633.2140998207 E_h
Zero Point Energy = 0.1988215 E_h
Symmetry = C_1

XYZ Coordinates:
23

C	1.35602	-0.00067	-0.09716
P	-0.22658	0.00375	0.91681
N	-1.57271	0.00215	-0.05130
C	-1.70568	0.00237	-1.51525
C	-2.87868	-0.00361	0.65011
H	-2.72639	-0.00696	1.74822
H	-3.44970	-0.90933	0.35073
H	-3.45517	0.90046	0.35653
H	-2.25617	-0.91262	-1.82740
H	-0.72201	0.03017	-2.01057
H	-2.30385	0.88874	-1.82159
C	1.49736	-1.28715	-0.94715
C	2.41073	-0.01735	1.04805
C	1.51658	1.29751	-0.92636
H	1.34093	-2.20949	-0.34542
H	2.53824	-1.32875	-1.34065
H	0.81509	-1.32041	-1.82190
H	0.80659	1.37471	-1.77604
H	2.54484	1.30795	-1.35402
H	1.41443	2.21104	-0.30031
H	2.33072	-0.92499	1.68683
H	2.34024	0.87961	1.70285
H	3.42721	-0.01914	0.59634

Vibrational Spectrum:

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

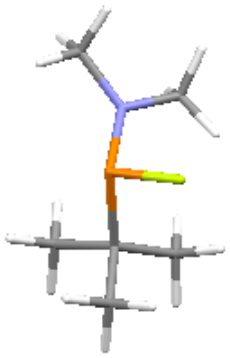
SCF Energy = -632.4106483780 E_h
Symmetry = C_1

XYZ Coordinates:
23

C	1.31025	-0.00017	-0.09072
P	-0.21809	0.00239	0.91430
N	-1.52781	0.00100	-0.04394
C	-1.66078	0.00181	-1.50576
C	-2.84146	-0.00276	0.63887
H	-2.69988	-0.00816	1.71519
H	-3.38618	-0.89110	0.32818
H	-3.38717	0.88791	0.33690
H	-2.19956	-0.89783	-1.79717
H	-0.69417	0.02822	-1.98375
H	-2.24422	0.87507	-1.79088
C	1.45700	-1.27315	-0.93440
C	2.38884	-0.01706	1.01416
C	1.47225	1.28596	-0.91150
H	1.31337	-2.17400	-0.33730
H	2.47534	-1.29936	-1.32405
H	0.77777	-1.31122	-1.78158
H	0.77955	1.35732	-1.74574
H	2.48419	1.29627	-1.31829

H	1.35924	2.17732	-0.29405
H	2.32285	-0.90929	1.63762
H	2.32946	0.86041	1.65891
H	3.36638	-0.01487	0.53348

14-F: $Me_2NPC(CH_3)_3F$



(RI-)BP86/SV(P) level:
SCF Energy = -733.2662290576 E_h
Zero Point Energy = 0.2010776 E_h
Symmetry = C_1

XYZ Coordinates:
24

C	1.36170	0.04505	-0.38052
P	-0.18780	-0.70462	0.45306
N	-1.55508	0.02473	-0.26973
C	-1.87653	1.44613	-0.26917
C	-2.66512	-0.84259	-0.64534
H	-2.36595	-1.90644	-0.53078
H	-2.96217	-0.68124	-1.71000
H	-3.56761	-0.66071	-0.00849
H	-1.96562	1.85896	-1.30408
H	-1.10750	2.02234	0.27967
H	-2.85206	1.61956	0.24801
C	1.32343	-0.42358	-1.84801
C	2.54405	-0.62340	0.36065
C	1.49949	1.57418	-0.29329
H	1.21346	-1.53004	-1.92660
H	2.27063	-0.14649	-2.36722
H	0.47909	0.04161	-2.40309
H	0.76014	2.09935	-0.93479
H	2.51289	1.88426	-0.64232
H	1.38026	1.93213	0.75247
H	2.47325	-1.73462	0.33324
H	2.58117	-0.30996	1.42697
H	3.50971	-0.33382	-0.11529
F	-0.05520	0.16674	1.87705

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -732.4396031856 E_h
Symmetry = C_1

XYZ Coordinates:
24

C	1.31749	0.02587	-0.36543
P	-0.17938	-0.67397	0.48261
N	-1.50673	0.00929	-0.26450
C	-1.82317	1.42627	-0.32719
C	-2.63136	-0.84749	-0.60023
H	-2.35684	-1.88873	-0.45119
H	-2.91751	-0.71123	-1.64528
H	-3.50020	-0.61818	0.02376
H	-1.90064	1.77337	-1.36044
H	-1.06881	2.01065	0.18737
H	-2.78169	1.60877	0.16489
C	1.31788	-0.57157	-1.77202
C	2.51548	-0.51958	0.41979
C	1.42317	1.54508	-0.44304
H	1.24784	-1.66055	-1.74478
H	2.24611	-0.30855	-2.28339
H	0.48250	-0.19193	-2.36078
H	0.69432	1.96617	-1.13278
H	2.41611	1.81535	-0.81044
H	1.29371	2.00804	0.53490
H	2.46942	-1.60530	0.51693
H	2.55944	-0.08914	1.41978
H	3.44015	-0.26564	-0.10201
F	-0.05997	0.21880	1.84035

15: $[(H_2N)_2P]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -452.8706814948 E_h
Zero Point Energy = 0.0523396 E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

N	1.29650	0.00000	-0.47815
P	0.00000	0.00000	0.53464
N	-1.29650	0.00000	-0.47815
H	1.30129	0.00000	-1.51180
H	2.24045	0.00000	-0.05829
H	-2.24045	0.00000	-0.05829

H	-1.30129	0.00000	-1.51180

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -452.3751114525 E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

N	1.27389	0.00000	-0.46681
P	0.00000	0.00000	0.52168
N	-1.27389	0.00000	-0.46681
H	1.27181	0.00000	-1.47932
H	2.19645	0.00000	-0.04919
H	-2.19645	0.00000	-0.04919
H	-1.27181	0.00000	-1.47932

15-F: $(H_2N)_2PF$

(RI-)BP86/SV(P) level:

SCF Energy = -552.9191711261 E_h
Zero Point Energy = 0.0542138 E_h
Symmetry = C_1

XYZ Coordinates:
8

N	-0.59682	-0.32617	-1.42030
P	-0.07695	0.51449	-0.04312
N	1.48304	-0.27782	0.00705
F	-0.64424	-0.31599	1.28236
H	-1.47383	-0.03349	-1.86558
H	-0.39560	-1.33395	-1.50003
H	1.95798	-0.13521	0.91057
H	2.10391	0.04160	-0.75143

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

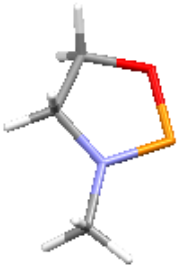
(RI-)MP2/def2-TZVPP level

SCF Energy = -552.4068364160 E_h
Symmetry = C_1

XYZ Coordinates:
8

N	-0.59925	-0.30570	-1.38465
P	-0.06139	0.50235	-0.03034
N	1.46346	-0.28407	0.00694
F	-0.64843	-0.31033	1.23424
H	-1.46177	0.00583	-1.79847
H	-0.44857	-1.30280	-1.44633
H	1.98082	-0.07071	0.84972
H	2.02866	-0.02449	-0.79107

16: $[(CH_2)_2N(CH_3)OP]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -589.3649422356 E_h
Zero Point Energy = 0.1035755 E_h
Symmetry = C_1

XYZ Coordinates:
13

N	0.83586	-0.14973	-0.01170
P	-0.15195	1.17504	0.00372
O	-1.53206	0.34468	0.03786
C	0.11547	-1.44646	0.08849
C	-1.38641	-1.11520	-0.09126
H	-1.77726	-1.37658	-1.09568
H	-2.03376	-1.56804	0.68425
H	0.34662	-1.89775	1.07958
H	0.48948	-2.13356	-0.70076
C	2.30376	-0.13388	-0.03169
H	2.67515	0.91117	-0.04590
H	2.67077	-0.66445	-0.93695
H	2.69402	-0.64842	0.87336

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -588.6938530453 E_h
Symmetry = C_1

XYZ Coordinates:
13

N	0.82298	-0.13976	-0.01870
P	-0.15821	1.14433	0.00418
O	-1.51705	0.34894	0.05791
C	0.11333	-1.42878	0.12977
C	-1.35789	-1.10387	-0.13517
H	-1.65288	-1.30285	-1.16053
H	-2.03750	-1.58589	0.55668
H	0.29138	-1.80028	1.13782
H	0.50618	-2.14026	-0.59272
C	2.29003	-0.11801	-0.04343
H	2.63969	0.90944	-0.08801
H	2.63610	-0.66106	-0.91858
H	2.66457	-0.59389	0.85939

16-F: $(CH_2)_2N(CH_3)OPF$

(RI-)BP86/SV(P) level:
SCF Energy = -689.4204715250
Zero Point Energy = 0.1053066
Symmetry = C_1

XYZ Coordinates:
14

N	0.08600	-1.00779	-0.01705
P	0.69442	0.49269	0.53901
O	-0.84367	1.14093	0.62154
C	-1.33320	-0.98851	-0.36033
C	-1.71828	0.50411	-0.33093
H	-1.57881	0.97262	-1.33197
H	-2.76265	0.67235	0.00332
H	-1.92114	-1.58571	0.38271
H	-1.52442	-1.42583	-1.36946
C	0.79259	-2.26934	0.05387
H	1.79911	-2.11126	0.49890
H	0.93639	-2.73155	-0.95324
H	0.24786	-3.00732	0.69371
F	1.19792	1.20890	-0.87650

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

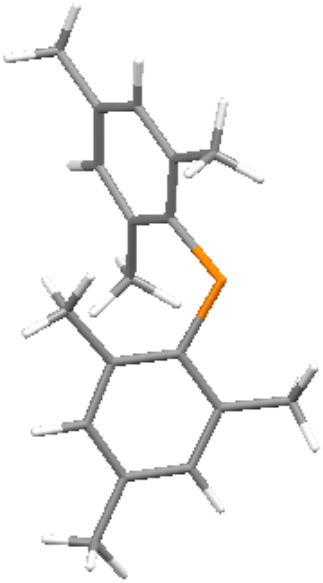
(RI-)MP2/def2-TZVPP level

SCF Energy = -688.7251329337 E_h
Symmetry = C_1

XYZ Coordinates:
14

N	0.12167	-0.97822	-0.08149
P	0.67483	0.48955	0.51315
O	-0.83215	1.10199	0.63259
C	-1.30698	-1.00467	-0.34418
C	-1.70883	0.46415	-0.31831
H	-1.56544	0.92355	-1.29558
H	-2.72885	0.62105	0.01664
H	-1.82544	-1.57764	0.43195
H	-1.53185	-1.45075	-1.31465
C	0.81688	-2.23605	0.07275
H	1.81988	-2.05555	0.45392
H	0.90596	-2.75881	-0.88045
H	0.29446	-2.88999	0.77631
F	1.14681	1.23791	-0.84028

17: $[\{(CH_3)_3C_6H_2\}_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -1039.6877315900 E_h
Zero Point Energy = 0.3361339 E_h
Symmetry = C_1

XYZ Coordinates:
41

C	1.48416	0.03155	0.37693
P	0.02657	0.03710	1.40437
C	-1.47086	0.03884	0.42899
C	1.63865	-0.72559	-0.85441
C	2.92796	-0.87397	-1.37462
C	4.07614	-0.29240	-0.77947
C	3.91012	0.44905	0.41054
C	2.65667	0.61763	1.00745
C	-1.73085	0.92168	-0.69062
C	-3.02990	0.96270	-1.20838
C	-4.09144	0.17602	-0.69557
C	-3.82951	-0.65682	0.41448
C	-2.55936	-0.73761	0.99512
C	0.50515	-1.41294	-1.58085
H	3.05924	-1.47754	-2.28848
C	5.43440	-0.49437	-1.38719
H	4.79236	0.91443	0.88044
C	2.54887	1.46878	2.24904
C	-0.72858	1.91541	-1.23594
H	-3.24225	1.65557	-2.03989
C	-5.45489	0.21914	-1.32547
H	-4.64773	-1.26627	0.83307
C	-2.33925	-1.68974	2.14623
H	-0.78000	2.86417	-0.65218
H	-0.96928	2.17647	-2.28762
H	0.32022	1.56686	-1.19718
H	-1.92553	-2.66186	1.79266
H	-3.29131	-1.90615	2.67366
H	-1.61243	-1.29057	2.89257
H	-5.66721	1.20679	-1.78635
H	-6.25551	-0.01924	-0.59413
H	-5.52331	-0.54049	-2.14097
H	1.79809	1.07339	2.97239
H	2.22540	2.50452	1.99592
H	3.52571	1.54199	2.76988
H	-0.08867	-0.69566	-2.18924
H	-0.20745	-1.91463	-0.89387
H	0.90503	-2.17870	-2.27708
H	6.15930	0.27770	-1.05580
H	5.39100	-0.49930	-2.49764
H	5.84409	-1.48666	-1.08031

vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.88	0.06728	-	-
8	a	29.99	0.35289	YES	YES
9	a	32.07	0.76668	YES	YES
10	a	39.16	0.75838	YES	YES
11	a	50.04	0.52700	YES	YES
12	a	72.61	2.18122	YES	YES
13	a	79.04	7.66299	YES	YES
14	a	115.31	0.71452	YES	YES
15	a	125.43	0.31521	YES	YES
16	a	128.27	3.20160	YES	YES
17	a	139.06	1.47538	YES	YES
18	a	169.57	1.90323	YES	YES
19	a	176.44	1.15872	YES	YES
20	a	188.60	1.15671	YES	YES
21	a	196.13	0.43727	YES	YES
22	a	201.75	0.31274	YES	YES
23	a	225.55	11.37938	YES	YES
24	a	270.87	0.00819	YES	YES
25	a	281.39	1.38703	YES	YES
26	a	289.29	3.85949	YES	YES
27	a	291.20	2.66359	YES	YES
28	a	324.08	0.51318	YES	YES
29	a	339.68	8.82201	YES	YES
30	a	396.79	54.66923	YES	YES
31	a	401.28	4.35387	YES	YES
32	a	487.42	3.71094	YES	YES
33	a	499.95	3.06523	YES	YES
34	a	505.50	0.35650	YES	YES
35	a	510.93	17.54629	YES	YES
36	a	522.67	7.53371	YES	YES
37	a	528.56	1.78471	YES	YES
38	a	541.66	3.34134	YES	YES
39	a	546.70	3.69908	YES	YES
40	a	565.60	5.06236	YES	YES
41	a	569.50	1.16687	YES	YES
42	a	612.04	3.91367	YES	YES
43	a	643.23	5.85352	YES	YES
44	a	710.87	24.44395	YES	YES
45	a	722.27	3.36871	YES	YES
46	a	852.67	7.57695	YES	YES

47	a	853.01	17.26285	YES	YES
48	a	886.12	12.10476	YES	YES
49	a	886.97	0.48188	YES	YES
50	a	913.46	3.52770	YES	YES
51	a	922.88	2.03441	YES	YES
52	a	942.12	5.49770	YES	YES
53	a	948.30	5.82592	YES	YES
54	a	987.65	132.72563	YES	YES
55	a	998.93	3.59127	YES	YES
56	a	1001.71	2.62824	YES	YES
57	a	1002.10	5.47639	YES	YES
58	a	1007.77	42.52407	YES	YES
59	a	1008.78	13.76970	YES	YES
60	a	1013.73	5.81894	YES	YES
61	a	1014.29	10.43133	YES	YES
62	a	1017.14	8.68065	YES	YES
63	a	1018.25	15.71377	YES	YES
64	a	1021.43	12.47582	YES	YES
65	a	1023.90	3.29295	YES	YES
66	a	1060.44	195.33508	YES	YES
67	a	1065.19	7.34168	YES	YES
68	a	1158.82	8.64477	YES	YES
69	a	1161.93	0.74601	YES	YES
70	a	1223.06	5.49523	YES	YES
71	a	1229.86	4.19087	YES	YES
72	a	1271.07	290.16218	YES	YES
73	a	1282.54	7.61790	YES	YES
74	a	1321.04	3.06931	YES	YES
75	a	1327.92	2.02500	YES	YES
76	a	1350.19	75.99361	YES	YES
77	a	1350.92	26.93529	YES	YES
78	a	1358.55	14.87365	YES	YES
79	a	1359.98	11.87099	YES	YES
80	a	1362.89	1.83095	YES	YES
81	a	1367.87	5.99272	YES	YES
82	a	1379.32	23.82313	YES	YES
83	a	1381.92	4.93516	YES	YES
84	a	1387.66	7.68345	YES	YES
85	a	1387.86	9.11205	YES	YES
86	a	1403.03	25.64376	YES	YES
87	a	1407.01	0.33676	YES	YES
88	a	1416.95	12.15445	YES	YES
89	a	1420.18	6.63118	YES	YES
90	a	1424.81	26.47900	YES	YES
91	a	1425.61	19.15711	YES	YES
92	a	1427.17	10.79761	YES	YES
93	a	1428.76	3.44092	YES	YES
94	a	1437.37	8.61583	YES	YES
95	a	1441.34	9.85704	YES	YES
96	a	1452.57	59.27052	YES	YES
97	a	1456.93	55.61226	YES	YES
98	a	1506.43	50.39623	YES	YES
99	a	1513.52	52.72796	YES	YES
100	a	1600.29	700.47678	YES	YES
101	a	1609.44	65.62178	YES	YES
102	a	2928.67	1.74398	YES	YES
103	a	2933.89	0.81818	YES	YES
104	a	2935.99	13.04526	YES	YES
105	a	2936.28	7.27429	YES	YES
106	a	2949.29	1.65180	YES	YES
107	a	2961.65	1.67965	YES	YES
108	a	2997.41	5.47230	YES	YES
109	a	3001.42	2.19262	YES	YES
110	a	3017.41	10.44026	YES	YES
111	a	3019.67	11.84116	YES	YES
112	a	3033.39	3.31017	YES	YES
113	a	3037.98	2.92712	YES	YES
114	a	3052.16	7.06704	YES	YES
115	a	3054.41	7.27215	YES	YES
116	a	3059.95	3.17915	YES	YES
117	a	3061.64	1.64840	YES	YES
118	a	3061.98	5.89814	YES	YES
119	a	3091.89	5.00087	YES	YES
120	a	3097.05	3.76986	YES	YES
121	a	3097.71	4.28617	YES	YES
122	a	3100.28	6.27473	YES	YES
123	a	3102.57	6.24609	YES	YES

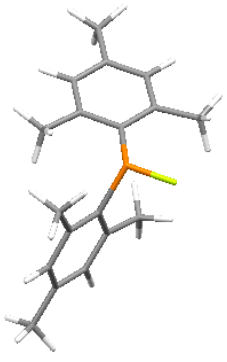
(RI-)MP2/def2-TZVPP level

SCF Energy = -1038.2687442102 E_h
Symmetry = C_1

XYZ Coordinates:
41

C	1.39835	-0.09188	0.51832
P	0.00192	-0.00368	1.57749
C	-1.39877	0.09238	0.52413
C	1.44808	-0.86992	-0.68365
C	2.66011	-0.93180	-1.35322
C	3.80839	-0.25341	-0.91852
C	3.74442	0.47361	0.27236
C	2.57939	0.54606	1.02125
C	-1.45406	0.88686	-0.66624
C	-2.66799	0.95531	-1.33188
C	-3.81210	0.26423	-0.90591
C	-3.74358	-0.47613	0.27671
C	-2.57695	-0.55399	1.02255
C	0.31161	-1.70094	-1.22132
H	2.72783	-1.54332	-2.24558
C	5.08548	-0.36202	-1.68830
H	4.62977	0.98754	0.62631
C	2.57113	1.36276	2.28268
C	-0.32142	1.72925	-1.19477
H	-2.74150	1.58507	-2.21088
C	-5.07533	0.33003	-1.70294
H	-4.62878	-0.99061	0.63017
C	-2.56498	-1.38071	2.27741
H	0.30094	2.14253	-0.40412
H	-0.73439	2.55928	-1.76470
H	0.33100	1.16407	-1.86059
H	-2.16126	-2.37654	2.09196
H	-3.57780	-1.49806	2.65603
H	-1.95928	-0.92531	3.06224
H	-5.22609	1.32602	-2.11481
H	-5.93924	0.06029	-1.10075
H	-5.01984	-0.36602	-2.54208
H	1.96673	0.90203	3.06541
H	2.16791	2.36038	2.10590
H	3.58486	1.47595	2.66005
H	-0.35146	-1.12183	-1.86399
H	-0.29844	-2.13682	-0.43301
H	0.72010	-2.51455	-1.81752
H	5.75825	0.46043	-1.45878
H	4.89620	-0.37892	-2.75983
H	5.59376	-1.29323	-1.43072

17-F: $[\{(CH_3)_3C_6H_2\}_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -1139.7331424620 E_h
Zero Point Energy = 0.3397841E_h
Symmetry = C_1

XYZ Coordinates:
42

C	1.47817	0.35391	0.23411
P	0.00952	1.16006	1.05131
C	-1.48451	0.27282	0.36377
C	1.62240	0.22377	-1.18352
C	2.79555	-0.35514	-1.69938
C	3.84592	-0.80243	-0.87273
C	3.70069	-0.63461	0.51291
C	2.54405	-0.06262	1.08584
C	-2.57357	0.91078	-0.30609
C	-3.70661	0.13859	-0.63831
C	-3.82701	-1.22587	-0.32113
C	-2.76862	-1.81697	0.38917
C	-1.61326	-1.09639	0.74536
F	-0.00318	2.57384	0.17510
C	0.58119	0.72282	-2.16045
H	2.89732	-0.45177	-2.79485
C	5.07911	-1.44581	-1.46635
H	4.51989	-0.95197	1.18203
C	2.50551	0.05138	2.59878
C	-2.60624	2.38063	-0.68359
H	-4.54008	0.63863	-1.16309
C	-5.04416	-2.02380	-0.73193
H	-2.84393	-2.87666	0.69191
C	-0.54275	-1.80490	1.54933
H	-2.36404	3.04400	0.17234
H	-3.61714	2.65356	-1.05443
H	-1.87479	2.62488	-1.48316
H	0.34748	-2.05943	0.93166
H	-0.93578	-2.74879	1.98426
H	-0.17965	-1.17516	2.39553
H	-5.95507	-1.38813	-0.77814
H	-5.24262	-2.86038	-0.02744
H	-4.90839	-2.47315	-1.74374
H	1.84460	0.87098	2.94844
H	3.52671	0.22426	3.00201
H	2.12895	-0.88910	3.06442
H	0.48666	1.82833	-2.10636
H	-0.42417	0.30226	-1.94286
H	0.85349	0.44844	-3.20144
H	5.91837	-1.47342	-0.73900
H	5.42587	-0.90471	-2.37414
H	4.87250	-2.49673	-1.77585

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.86	0.28987	YES	YES
8	a	31.21	0.08745	YES	YES
9	a	33.32	0.03125	YES	YES
10	a	39.90	0.31663	YES	YES
11	a	46.50	0.13895	YES	YES
12	a	63.14	0.23329	YES	YES
13	a	89.63	0.51697	YES	YES
14	a	113.39	0.28128	YES	YES
15	a	141.75	0.36852	YES	YES
16	a	163.77	0.55125	YES	YES
17	a	174.37	4.74933	YES	YES
18	a	181.12	1.62597	YES	YES
19	a	189.75	1.07231	YES	YES
20	a	199.09	0.14441	YES	YES
21	a	206.63	1.71077	YES	YES
22	a	212.03	0.24206	YES	YES
23	a	219.82	0.45209	YES	YES
24	a	228.83	0.10722	YES	YES
25	a	253.08	0.54294	YES	YES
26	a	274.81	0.58460	YES	YES
27	a	280.47	0.39866	YES	YES
28	a	294.21	1.27936	YES	YES
29	a	319.40	0.16071	YES	YES
30	a	335.10	0.09213	YES	YES
31	a	353.66	1.01063	YES	YES
32	a	393.04	37.21307	YES	YES
33	a	418.57	7.96871	YES	YES
34	a	497.71	1.22877	YES	YES
35	a	505.42	0.62246	YES	YES
36	a	516.31	0.28102	YES	YES
37	a	519.65	0.59972	YES	YES
38	a	529.28	1.60408	YES	YES
39	a	531.54	1.69790	YES	YES
40	a	547.89	1.77238	YES	YES
41	a	551.43	3.84934	YES	YES
42	a	564.36	0.23318	YES	YES
43	a	569.01	3.94722	YES	YES
44	a	596.19	12.93101	YES	YES
45	a	606.48	27.68514	YES	YES
46	a	720.26	3.30478	YES	YES
47	a	730.93	1.37507	YES	YES
48	a	756.19	85.20939	YES	YES
49	a	846.37	9.92062	YES	YES
50	a	847.17	4.22305	YES	YES
51	a	873.78	0.06506	YES	YES
52	a	875.34	0.12724	YES	YES
53	a	922.32	2.54054	YES	YES
54	a	924.83	2.14076	YES	YES
55	a	946.68	2.41290	YES	YES
56	a	952.17	0.22590	YES	YES
57	a	1002.95	11.49060	YES	YES
58	a	1003.23	1.32753	YES	YES
59	a	1003.73	2.62558	YES	YES
60	a	1005.14	2.26240	YES	YES
61	a	1017.74	2.83495	YES	YES
62	a	1022.51	3.47718	YES	YES
63	a	1023.32	5.79757	YES	YES
64	a	1025.50	1.91795	YES	YES
65	a	1025.73	9.75324	YES	YES
66	a	1026.46	0.93426	YES	YES
67	a	1027.57	11.90396	YES	YES
68	a	1029.11	5.95529	YES	YES
69	a	1036.40	2.47919	YES	YES
70	a	1038.62	9.37985	YES	YES
71	a	1165.08	0.34244	YES	YES
72	a	1167.78	0.11796	YES	YES
73	a	1224.43	1.03911	YES	YES
74	a	1225.83	1.59428	YES	YES
75	a	1284.42	6.46277	YES	YES
76	a	1287.24	3.42959	YES	YES
77	a	1326.84	0.89534	YES	YES
78	a	1333.24	0.60945	YES	YES
79	a	1359.18	6.88743	YES	YES
80	a	1360.76	2.34871	YES	YES
81	a	1362.08	0.12713	YES	YES
82	a	1366.76	1.16165	YES	YES
83	a	1367.11	2.92820	YES	YES
84	a	1372.42	1.40423	YES	YES
85	a	1391.61	3.20118	YES	YES
86	a	1394.33	6.62389	YES	YES
87	a	1395.52	10.50304	YES	YES
88	a	1403.15	6.63255	YES	YES
89	a	1417.04	17.41557	YES	YES
90	a	1419.83	8.23077	YES	YES
91	a	1423.06	8.26707	YES	YES
92	a	1424.36	8.33536	YES	YES
93	a	1426.57	6.98300	YES	YES
94	a	1428.41	7.35180	YES	YES

95	a	1430.19	4.60985	YES	YES
96	a	1434.61	8.46252	YES	YES
97	a	1444.30	22.63746	YES	YES
98	a	1446.88	45.94024	YES	YES
99	a	1454.95	34.82826	YES	YES
100	a	1458.33	16.30818	YES	YES
101	a	1564.68	14.59536	YES	YES
102	a	1566.27	12.27392	YES	YES
103	a	1608.88	43.06107	YES	YES
104	a	1611.28	13.67169	YES	YES
105	a	2926.92	15.85425	YES	YES
106	a	2932.84	36.02294	YES	YES
107	a	2936.37	29.49895	YES	YES
108	a	2937.61	16.83713	YES	YES
109	a	2956.60	16.09173	YES	YES
110	a	2959.57	22.63425	YES	YES
111	a	3001.90	5.90376	YES	YES
112	a	3007.04	14.39496	YES	YES
113	a	3009.67	11.45765	YES	YES
114	a	3011.77	14.64682	YES	YES
115	a	3030.69	14.05269	YES	YES
116	a	3037.32	10.06850	YES	YES
117	a	3038.76	12.25758	YES	YES
118	a	3039.60	3.01206	YES	YES
119	a	3040.06	10.05773	YES	YES
120	a	3045.56	8.46749	YES	YES
121	a	3048.35	7.88327	YES	YES
122	a	3050.17	6.23487	YES	YES
123	a	3070.01	25.90916	YES	YES
124	a	3071.56	20.29881	YES	YES
125	a	3072.87	24.54105	YES	YES
126	a	3074.58	17.66716	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1138.3026856572E_h
Symmetry = C_1

XYZ Coordinates:
42

C	1.39966	0.51086	0.01087
P	0.02621	1.61460	0.51395
C	-1.39930	0.47748	0.32335
C	1.34665	-0.33918	-1.11606
C	2.43333	-1.17602	-1.37523
C	3.56689	-1.20268	-0.56407
C	3.61081	-0.33199	0.52232
C	2.55459	0.52939	0.82281
C	-2.54981	0.76669	-0.44173
C	-3.57471	-0.18094	-0.49248
C	-3.52292	-1.38683	0.20420
C	-2.41379	-1.61338	1.01487
C	-1.36111	-0.70160	1.09904
F	-0.07917	2.51328	-0.82802
C	0.17911	-0.39328	-2.06608
H	2.39319	-1.82232	-2.24559
C	4.69972	-2.14639	-0.85095
H	4.49525	-0.31377	1.14942
C	2.69828	1.43885	2.01719
C	-2.75254	2.04806	-1.20993
H	-4.45172	0.04340	-1.09009
C	-4.62619	-2.39960	0.08907
H	-2.36710	-2.51690	1.61357
C	-0.22534	-1.01638	2.03840
H	-2.51689	2.92401	-0.60915
H	-3.79354	2.11906	-1.51980
H	-2.12959	2.09451	-2.10139
H	0.61424	-1.48412	1.52261
H	-0.57202	-1.69671	2.81555
H	0.15344	-0.11948	2.53211
H	-5.58518	-1.91573	-0.08886
H	-4.70620	-2.99655	0.99603
H	-4.44142	-3.08234	-0.74146
H	2.46696	2.47329	1.77125
H	3.72073	1.39555	2.38895
H	2.03442	1.14889	2.83209
H	-0.22806	0.59429	-2.26605
H	-0.62855	-1.00990	-1.66895
H	0.50142	-0.82703	-3.01197
H	5.63384	-1.77578	-0.43282
H	4.83298	-2.28404	-1.92273
H	4.50586	-3.12698	-0.41410

18: $[P(SCH_3)_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -1217.0302855600 E_h
Zero Point Energy = 0.0767794 E_h
Symmetry = C_1

XYZ Coordinates:
11

S	1.23861	-0.00853	-0.67418
P	0.09285	-0.00229	1.03243
S	-1.85095	0.00151	0.36921
C	2.94237	0.01291	0.03390
C	-1.88724	0.00574	-1.46314
H	-1.36106	0.90053	-1.85877
H	-2.96518	0.05227	-1.72428
H	-1.44044	-0.93176	-1.85717
H	2.92673	-0.00726	1.14354
H	3.42954	0.94021	-0.33243
H	3.46288	-0.88264	-0.36411

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.03	0.03297	YES	YES
8		a	54.03	0.12061	YES	YES
9		a	108.47	0.65451	YES	YES
10		a	143.10	1.87741	YES	YES
11		a	161.89	3.23946	YES	YES
12		a	220.77	0.84890	YES	YES
13		a	258.07	0.23833	YES	YES
14		a	261.93	0.25719	YES	YES
15		a	331.59	0.65752	YES	YES
16		a	431.69	25.51929	YES	YES
17		a	435.65	24.98526	YES	YES
18		a	505.39	1.25012	YES	YES
19		a	523.48	2.22561	YES	YES
20		a	528.83	0.84803	YES	YES
21		a	549.42	11.99635	YES	YES
22		a	726.13	1.43402	YES	YES
23		a	729.50	5.41704	YES	YES
24		a	820.34	66.34508	YES	YES
25		a	1102.54	231.73283	YES	YES

26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1215.6971685876 E_h
Symmetry = C_s

XYZ Coordinates:
11

S	1.19860	0.67034	0.00000
P	0.09037	-1.00062	0.00000
S	-1.81280	-0.36894	0.00000
C	2.86712	-0.06479	0.00000
C	-1.80336	1.43966	0.00000
H	-1.30804	1.80297	0.89715
H	-2.84974	1.73200	0.00000
H	-1.30804	1.80297	-0.89715
H	2.81432	-1.14973	0.00000
H	3.36845	0.29444	0.89319
H	3.36845	0.29444	-0.89319

18-F: $P(SCH_3)_2F$

(RI-)BP86/SV(P) level:
SCF Energy = -1317.0909826210 E_h
Zero Point Energy = 0.0789686 E_h
Symmetry = C_1

XYZ Coordinates:
12

S	1.27015	0.00862	-0.94870
P	0.07751	-0.54598	0.75031
S	-1.83832	-0.56505	-0.18151
C	2.92233	0.02768	-0.13828
C	-1.98168	1.08658	-0.98400
H	-1.62322	1.87322	-0.28985
H	-3.06379	1.23433	-1.18349
H	-1.41670	1.12215	-1.93695
H	3.13400	-0.94104	0.36246
H	2.99771	0.86202	0.58894
H	3.66275	0.18360	-0.95033
F	0.04204	0.89481	1.57463

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1315.7352254076 E_h
Symmetry = C_1

XYZ Coordinates:
12

S	1.20517	0.00481	-0.94039
P	0.08539	-0.48854	0.75797
S	-1.81189	-0.53559	-0.09341
C	2.84502	-0.05433	-0.16092
C	-1.88618	0.96173	-1.11948
H	-1.47286	1.80622	-0.57685
H	-2.93985	1.13842	-1.31868
H	-1.35534	0.81599	-2.05419
H	2.97663	-0.98925	0.37706
H	2.98311	0.78970	0.50751
H	3.57256	0.00147	-0.96615
F	0.07885	0.92960	1.53239

19: $[S_2(CH_2)_2P]^+$

(RI-)BP86/SV(P) level:

SCF Energy = -1215.8319658550 E_h

Zero Point Energy 0.0587489 E_h
Symmetry = C_2

XYZ Coordinates:
9

S	-0.06561	1.58317	0.04834
P	0.00000	0.00000	1.36239
S	0.06561	-1.58317	0.04834

C	0.30179	0.69546	-1.54943
C	-0.30179	-0.69546	-1.54943
H	-1.40928	-0.69805	-1.65111
H	0.13607	-1.32527	-2.35562
H	1.40928	0.69805	-1.65111
H	-0.13607	1.32527	-2.35562

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b	194.20	3.25941	YES	YES
8	a	214.00	0.58732	YES	YES
9	a	354.16	1.95583	YES	YES
10	b	430.28	0.35602	YES	YES
11	a	530.77	12.68777	YES	YES
12	b	535.64	28.39918	YES	YES
13	a	598.20	4.63554	YES	YES
14	b	600.88	1.47593	YES	YES
15	b	804.69	6.93545	YES	YES
16	a	926.02	1.22672	YES	YES
17	a	997.95	1.03723	YES	YES
18	b	1083.34	0.52876	YES	YES
19	a	1149.12	6.60270	YES	YES
20	b	1221.17	12.92366	YES	YES
21	a	1279.94	7.33604	YES	YES
22	b	1390.82	26.20580	YES	YES
23	a	1405.22	9.70514	YES	YES
24	b	2983.01	8.72604	YES	YES
25	a	2984.00	10.75444	YES	YES
26	a	3047.22	8.99214	YES	YES
27	b	3057.17	11.78664	YES	YES

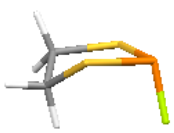
(RI-)MP2/def2-TZVPP level

SCF Energy = --1214.5062954978 E_h
Symmetry = C_2

XYZ Coordinates:
9

S	-0.06787	1.55159	0.05015
P	0.00000	0.00000	1.32456
S	0.06787	-1.55159	0.05015
C	0.31393	0.68407	-1.51427
C	-0.31393	-0.68407	-1.51427
H	-1.40060	-0.64901	-1.58779
H	0.09056	-1.30383	-2.31430
H	1.40060	0.64901	-1.58779
H	-0.09056	1.30383	-2.31430

19-F: $S_2(CH_2)_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -1315.9022080350 E_h

Zero Point Energy 0.0610044 E_h
Symmetry = C_1

XYZ Coordinates:
10

S	0.37731	-0.03723	1.60211
P	0.49284	-1.07897	-0.26201
S	0.22211	0.66335	-1.50232
C	-0.78479	1.28274	1.03094
C	-0.23304	1.93471	-0.22791
H	-0.99526	2.59380	-0.69985
H	0.67659	2.53235	-0.00626
H	-0.86154	2.01593	1.86437
H	-1.78272	0.82699	0.85820
F	-1.01445	-1.75456	-0.35592

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	84.08	2.39913	YES	YES
8	a	200.55	2.08502	YES	YES
9	a	218.13	2.18107	YES	YES
10	a	267.63	2.54024	YES	YES
11	a	362.38	1.06973	YES	YES
12	a	418.65	16.18279	YES	YES
13	a	449.97	14.11022	YES	YES
14	a	466.37	41.03087	YES	YES
15	a	628.51	1.86698	YES	YES
16	a	643.79	2.16462	YES	YES
17	a	754.07	119.68663	YES	YES
18	a	820.91	12.88954	YES	YES
19	a	925.41	4.25265	YES	YES
20	a	986.91	1.01985	YES	YES
21	a	1087.39	1.51217	YES	YES
22	a	1132.95	0.18643	YES	YES
23	a	1215.75	2.27884	YES	YES
24	a	1271.23	12.53318	YES	YES
25	a	1398.34	10.33529	YES	YES
26	a	1413.49	2.78206	YES	YES
27	a	2971.58	7.71418	YES	YES
28	a	2978.37	12.13237	YES	YES
29	a	3033.28	0.58225	YES	YES
30	a	3048.08	3.84919	YES	YES

(RI-)MP2/def2-TZVPP level

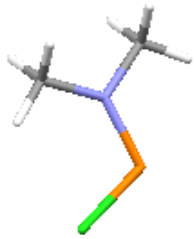
SCF Energy = -1314.5525244239 E_h
Symmetry = C_1

XYZ Coordinates:
10

S	0.38607	-0.13589	1.55625
P	0.47297	-1.03481	-0.32333
S	0.22431	0.73286	-1.42896
C	-0.78040	1.17981	1.09067

C	-0.23793	1.91245	-0.11394
H	-0.99255	2.57568	-0.53593
H	0.64835	2.48635	0.14856
H	-0.86138	1.84551	1.94992
H	-1.75257	0.73669	0.88402
F	-1.00047	-1.68098	-0.43501

20: $[(CH_3)_2N\}PCl]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -935.6172626112 E_h
Zero Point Energy = 0.0824883 E_h
Symmetry = C_1

XYZ Coordinates:
11

Cl	1.82383	-0.24471	0.00130
P	0.16859	0.91093	-0.00170
N	-1.10450	-0.14672	-0.00192
C	-2.44135	0.49496	0.00310
C	-1.10604	-1.61473	-0.00154
H	-0.07608	-2.01174	-0.06883
H	-1.70799	-1.97108	-0.86626
H	-1.58777	-1.97251	0.93581
H	-2.99524	0.18662	-0.90980
H	-2.34459	1.60192	0.01752
H	-2.99842	0.16412	0.90619

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES
15	a	331.59	0.65752	YES YES
16	a	431.69	25.51929	YES YES
17	a	435.65	24.98526	YES YES
18	a	505.39	1.25012	YES YES
19	a	523.48	2.22561	YES YES
20	a	528.83	0.84803	YES YES
21	a	549.42	11.99635	YES YES
22	a	726.13	1.43402	YES YES
23	a	729.50	5.41704	YES YES
24	a	820.34	66.34508	YES YES
25	a	1102.54	231.73283	YES YES
26	a	1125.45	315.13040	YES YES
27	a	1148.81	88.79335	YES YES
28	a	1154.27	19.36874	YES YES
29	a	1170.73	346.92142	YES YES

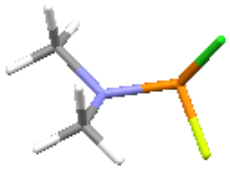
(RI-)MP2/def2-TZVPP level

SCF Energy = -934.6419671053 E_h
Symmetry = C_1

XYZ Coordinates:
11

Cl	1.79118	-0.24131	-0.00004
P	0.17619	0.88992	0.00008
N	-1.07440	-0.13532	-0.00015
C	-2.41139	0.50549	-0.00004
C	-1.10521	-1.60273	0.00008
H	-0.10063	-2.00580	-0.00374
H	-1.64603	-1.92661	-0.88643
H	-1.63923	-1.92658	0.89075
H	-2.94192	0.18438	-0.89243
H	-2.31000	1.58847	0.00090
H	-2.94250	0.18289	0.89147

20-F: $(CH_3)_2N\}PClF$



(RI-)BP86/SV(P) level:

Energy = -1035.6880718470 E_h
Zero Point Energy = 0.0847407 E_h
Symmetry = C_1

XYZ Coordinates:
12

Cl	1.66378	0.13106	-0.86589
P	0.16383	-0.70289	0.43379
N	-1.27175	0.05014	-0.05141
C	-2.26264	-0.76824	-0.74149
C	-1.42653	1.49502	-0.17706
H	-0.64428	2.00855	0.41634
H	-2.42295	1.80525	0.21365
H	-1.34449	1.82553	-1.24067
H	-3.28124	-0.56680	-0.33490
H	-2.03589	-1.84584	-0.58544
H	-2.27897	-0.56940	-1.84072
F	0.53516	0.26394	1.70614

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES

15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

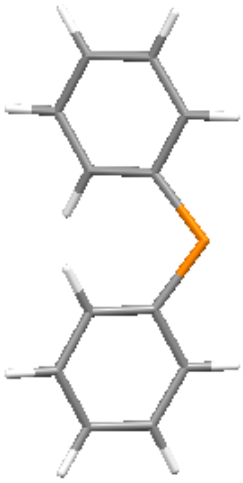
(RI-)MP2/def2-TZVPP level

SCF Energy = -1034.6886601199 E_h
Symmetry = C_1

XYZ Coordinates:
12

Cl	1.54416	0.14517	-0.91189
P	0.18386	-0.69054	0.44851
N	-1.25548	0.02986	0.05331
C	-2.16527	-0.75489	-0.76951
C	-1.39103	1.46899	-0.11609
H	-0.69840	1.98506	0.54130
H	-2.40695	1.76515	0.14223
H	-1.18638	1.76243	-1.14827
H	-3.19317	-0.53517	-0.48313
H	-1.98148	-1.81637	-0.61516
H	-2.04167	-0.52860	-1.83168
F	0.60323	0.24177	1.67116

21: $[P(C_6H_5)_2]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -803.9774516355 E_h
Zero Point Energy = 0.1779319 E_h
Symmetry = C_1

XYZ Coordinates:
23

C	1.06413	-1.59938	1.71159
P	-0.01300	-0.54398	2.65250
C	-0.90060	0.54138	1.56028
C	0.96469	-1.96532	0.33060
C	1.89856	-2.83819	-0.22682
C	2.94697	-3.35986	0.56707
C	3.04429	-3.04004	1.93635
C	2.09892	-2.18977	2.51382
C	-0.55492	0.93982	0.22883
C	-1.36741	1.83861	-0.46178
C	-2.53292	2.35796	0.14902
C	-2.87605	2.00342	1.46940
C	-2.05800	1.12329	2.18068
H	0.12484	-1.60392	-0.28259
H	1.81204	-3.13540	-1.28405
H	3.68180	-4.04493	0.11339
H	3.84971	-3.47158	2.55154
H	2.15640	-1.95487	3.59051
H	0.37710	0.58231	-0.23498
H	-1.09414	2.15787	-1.47991
H	-3.16600	3.06889	-0.40740
H	-3.77360	2.42991	1.94332
H	-2.30942	0.85987	3.22232

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	52.25	3.37204	YES YES
8		a	62.01	1.60483	YES YES
9		a	180.47	17.14319	YES YES
10		a	402.06	0.51145	YES YES
11		a	404.01	0.50696	YES YES
12		a	447.22	2.83071	YES YES
13		a	739.84	3.69086	YES YES
14		a	757.66	5.46120	YES YES
15		a	817.70	1.30369	YES YES
16		a	949.16	9.83394	YES YES
17		a	960.51	14.98237	YES YES
18		a	965.91	19.76635	YES YES
19		a	1068.40	43.33553	YES YES
20		a	1240.65	148.20902	YES YES
21		a	1243.50	116.67886	YES YES
22		a	1271.64	1.23740	YES YES
23		a	1300.94	86.08384	YES YES
24		a	1309.93	85.86253	YES YES
25		a	1346.87	3.06878	YES YES
26		a	1357.59	1.06744	YES YES
27		a	1379.25	53.29733	YES YES
28		a	1436.77	1.46522	YES YES
29		a	1453.20	37.25682	YES YES
30		a	1457.25	35.36943	YES YES
31		a	2868.91	117.74263	YES YES
32		a	2877.64	84.28624	YES YES
33		a	2893.34	29.20329	YES YES
34		a	2963.18	21.64613	YES YES
35		a	2973.98	22.67130	YES YES
36		a	2979.38	17.20698	YES YES
37		a	3081.87	6.77553	YES YES
38		a	3085.00	4.78460	YES YES

(RI-)MP2/def2-TZVPP level

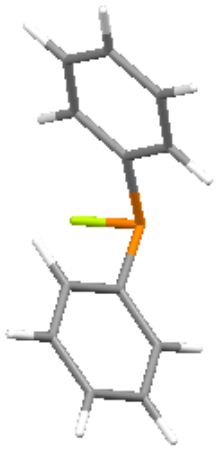
SCF Energy = -802.8968049830 E_h
Symmetry = C_2

XYZ Coordinates:
23

C	1.40789	-0.05389	0.40862

P	0.00000	0.00000	1.44620
C	-1.40789	0.05389	0.40862
C	1.46315	-0.53755	-0.92180
C	2.67571	-0.54771	-1.58984
C	3.83104	-0.06590	-0.96257
C	3.79456	0.39092	0.35740
C	2.59985	0.36511	1.05785
C	-1.46315	0.53755	-0.92180
C	-2.67571	0.54771	-1.58984
C	-3.83104	0.06590	-0.96257
C	-3.79456	-0.39092	0.35740
C	-2.59985	-0.36511	1.05785
H	0.57972	-0.94942	-1.38821
H	2.73367	-0.93865	-2.59595
H	4.77030	-0.07313	-1.49908
H	4.69864	0.73787	0.83684
H	2.56298	0.68640	2.09202
H	-0.57972	0.94942	-1.38821
H	-2.73367	0.93865	-2.59595
H	-4.77030	0.07313	-1.49908
H	-4.69864	-0.73787	0.83684
H	-2.56298	-0.68640	2.09202

21-F: $P(C_6H_5)_2F$



(RI-)BP86/SV(P) level:
SCF Energy = -904.0412520899 E_h
Zero Point Energy = 0.1799682 E_h
Symmetry = C_1

XYZ Coordinates:
24

C	1.43173	0.27259	0.18249
P	0.02143	1.34483	0.71803
C	-1.40746	0.24453	0.29403
C	1.51056	-0.30038	-1.10692
C	2.62165	-1.07710	-1.46626
C	3.65827	-1.29996	-0.53870
C	3.58725	-0.73517	0.74530
C	2.48111	0.05772	1.10079
C	-2.32348	0.58396	-0.72369
C	-3.44404	-0.23082	-0.96579
C	-3.66535	-1.38173	-0.19118
C	-2.76025	-1.71824	0.83244
C	-1.64207	-0.90646	1.07917
F	-0.06615	2.34828	-0.60091
H	0.69531	-0.13311	-1.83038
H	2.68046	-1.51843	-2.47531
H	4.52784	-1.91563	-0.82320
H	4.40063	-0.90331	1.47059
H	2.43305	0.52083	2.10179
H	-2.15450	1.48798	-1.32982
H	-4.15241	0.04071	-1.76651
H	-4.54577	-2.01759	-0.38144
H	-2.92767	-2.61947	1.44560
H	-0.93962	-1.17915	1.88671

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	52.25	3.37204	YES	YES
8		a	62.01	1.60483	YES	YES
9		a	180.47	17.14319	YES	YES
10		a	402.06	0.51145	YES	YES
11		a	404.01	0.50696	YES	YES
12		a	447.22	2.83071	YES	YES
13		a	739.84	3.69086	YES	YES
14		a	757.66	5.46120	YES	YES
15		a	817.70	1.30369	YES	YES
16		a	949.16	9.83394	YES	YES
17		a	960.51	14.98237	YES	YES
18		a	965.91	19.76635	YES	YES
19		a	1068.40	43.33553	YES	YES
20		a	1240.65	148.20902	YES	YES
21		a	1243.50	116.67886	YES	YES
22		a	1271.64	1.23740	YES	YES
23		a	1300.94	86.08384	YES	YES
24		a	1309.93	85.86253	YES	YES
25		a	1346.87	3.06878	YES	YES
26		a	1357.59	1.06744	YES	YES
27		a	1379.25	53.29733	YES	YES
28		a	1436.77	1.46522	YES	YES
29		a	1453.20	37.25682	YES	YES
30		a	1457.25	35.36943	YES	YES
31		a	2868.91	117.74263	YES	YES
32		a	2877.64	84.28624	YES	YES
33		a	2893.34	29.20329	YES	YES
34		a	2963.18	21.64613	YES	YES
35		a	2973.98	22.67130	YES	YES
36		a	2979.38	17.20698	YES	YES
37		a	3081.87	6.77553	YES	YES
38		a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -902.9442804529 E_h
Symmetry = C_1

XYZ Coordinates:
24

C	1.37988	0.28780	0.14843
P	0.04014	1.44103	0.59023
C	-1.36741	0.32660	0.28398
C	1.29890	-0.58389	-0.94552
C	2.36363	-1.42638	-1.24617
C	3.51111	-1.41674	-0.45050
C	3.59747	-0.55629	0.64130
C	2.53788	0.30105	0.93392
C	-2.27341	0.52737	-0.76127
C	-3.34832	-0.34504	-0.93134
C	-3.53140	-1.41353	-0.05690
C	-2.63517	-1.61136	0.99413
C	-1.56298	-0.74229	1.16749
F	-0.04333	2.31344	-0.76802
H	0.40055	-0.60459	-1.55014
H	2.29935	-2.09642	-2.09301
H	4.33339	-2.08029	-0.68172
H	4.48691	-0.54837	1.25656
H	2.60194	0.98006	1.77534
H	-2.13207	1.35495	-1.44259

H	-4.04239	-0.18750	-1.74607
H	-4.36617	-2.08768	-0.19131
H	-2.77392	-2.43860	1.67708
H	-0.86903	-0.90243	1.98518

22: $[P\{OCH_3\}_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -571.1195933475 E_h
Zero Point Energy = 0.0830436 E_h
Symmetry = C_1

XYZ Coordinates:
11

O	0.95142	0.00071	-0.45296
P	0.04638	0.00054	0.86155
O	-1.42735	-0.00140	0.31171
C	2.41630	-0.00072	-0.53785
C	-2.04132	0.00126	-1.01968
H	-1.27494	0.18309	-1.79707
H	-2.80849	0.79960	-0.99460
H	-2.52339	-0.98964	-1.14060
H	2.87728	0.03970	0.47081
H	2.69330	0.88595	-1.14093
H	2.69721	-0.93074	-1.07017

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

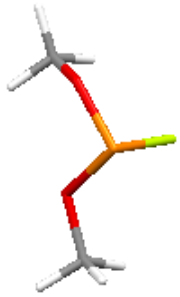
(RI-)MP2/def2-TZVPP level

SCF Energy = -570.5163111006 E_h
Symmetry = C_1

XYZ Coordinates:
11

O	0.91197	-0.00199	-0.49520
P	0.06434	-0.00050	0.80925
O	-1.40066	0.00159	0.35489
C	2.38994	0.00152	-0.48442
C	-2.03707	0.00022	-0.97556
H	-1.28430	0.16611	-1.73551
H	-2.76886	0.79621	-0.94330
H	-2.51029	-0.96809	-1.07600
H	2.75660	0.00227	0.53763
H	2.68891	0.89698	-1.01268
H	2.69265	-0.89255	-1.01285

22-F: $P\{OCH_3\}_2F$



(RI-)BP86/SV(P) level:

SCF Energy = -671.1981583453 E_h
Zero Point Energy = 0.0854721 E_h
Symmetry = C_1

XYZ Coordinates:
12

O	0.92975	0.07697	-0.79271
P	0.04096	-0.62526	0.43705
O	-1.43456	-0.53329	-0.26277
C	2.34148	0.20302	-0.63165
C	-1.91977	0.63514	-0.94412
H	-1.69817	1.55715	-0.36439
H	-3.01819	0.51379	-1.04060
H	-1.46190	0.71471	-1.95350
H	2.79623	-0.71959	-0.19596
H	2.59563	1.06951	0.02114
H	2.77763	0.37050	-1.63871
F	-0.01391	0.68775	1.44696

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES

11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

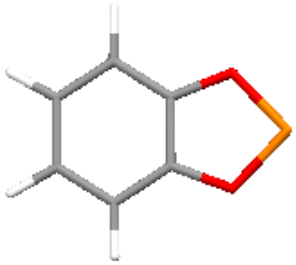
(RI-)MP2/def2-TZVPP level

SCF Energy = -670.5717204554 E_h
Symmetry = C_1

XYZ Coordinates:
12

O	0.89090	0.07044	-0.80101
P	0.04772	-0.60576	0.41743
O	-1.41277	-0.53945	-0.22803
C	2.30195	0.19918	-0.60078
C	-1.89416	0.63410	-0.90531
H	-1.74372	1.51697	-0.28997
H	-2.95358	0.47703	-1.07166
H	-1.37858	0.75344	-1.85304
H	2.70693	-0.67259	-0.08572
H	2.51987	1.09308	-0.02053
H	2.75864	0.27933	-1.58105
F	0.00256	0.67286	1.39831

23: $[C_6H_4O_2P]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -722.2637447902 E_h
Zero Point Energy = 0.0872097 E_h
Symmetry = C_{2V}

XYZ Coordinates:
13

O	-1.19539	0.00000	1.12613
P	0.00000	0.00000	2.27081
O	1.19539	0.00000	1.12613
C	-0.71051	0.00000	-0.15792
C	0.71051	0.00000	-0.15792
C	1.45925	0.00000	-1.33997
C	-1.45925	0.00000	-1.33997
H	-2.55888	0.00000	-1.32660
C	-0.71225	0.00000	-2.52585
C	0.71225	0.00000	-2.52585
H	2.55888	0.00000	-1.32660
H	-1.24421	0.00000	-3.49061
H	1.24421	0.00000	-3.49061

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b2	178.57	6.11111	YES	YES
8	a2	230.06	0.00000	NO	YES
9	b1	365.87	6.47734	YES	YES
10	b2	388.96	9.33329	YES	YES
11	b2	475.82	0.09772	YES	YES
12	a1	479.30	2.52602	YES	YES
13	a2	537.94	0.00000	NO	YES
14	b1	579.56	1.06770	YES	YES
15	a1	605.48	0.12201	YES	YES
16	a2	738.41	0.00000	NO	YES
17	b2	754.37	70.97278	YES	YES
18	b1	765.42	43.66283	YES	YES
19	a1	773.03	12.17702	YES	YES
20	a1	827.99	4.88334	YES	YES
21	a2	858.07	0.00000	NO	YES
22	b1	862.54	1.07645	YES	YES
23	b2	953.77	1.17023	YES	YES
24	a1	994.04	0.00922	YES	YES
25	a2	996.98	0.00000	NO	YES
26	b1	1094.63	4.64597	YES	YES
27	a1	1132.40	16.43813	YES	YES
28	b1	1167.45	0.29368	YES	YES
29	a1	1214.60	9.11538	YES	YES
30	b1	1261.60	0.71047	YES	YES
31	a1	1400.83	0.00246	YES	YES
32	a1	1426.59	2.77220	YES	YES
33	b1	1472.46	10.20975	YES	YES
34	b1	1579.61	0.03051	YES	YES
35	a1	1594.44	70.78688	YES	YES
36	b1	3127.64	0.00157	YES	YES
37	a1	3136.70	3.96713	YES	YES
38	b1	3151.94	17.52590	YES	YES
39	a1	3153.56	1.20910	YES	YES

(RI-)MP2/def2-TZVPP level

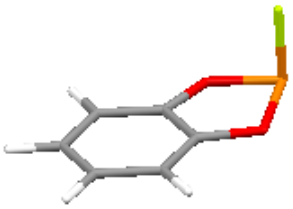
SCF Energy = -721.4349050845 E_h
Symmetry = C_{2v}

XYZ Coordinates:
13

O	-1.18105	0.00000	1.13544
P	0.00000	0.00000	2.21947
O	1.18105	0.00000	1.13544
C	-0.69765	0.00000	-0.15651
C	0.69765	0.00000	-0.15651
C	1.44795	0.00000	-1.32281
C	-1.44795	0.00000	-1.32281
H	-2.52738	0.00000	-1.30802
C	-0.70573	0.00000	-2.49616

C	0.70573	0.00000	-2.49616
H	2.52738	0.00000	-1.30802
H	-1.22623	0.00000	-3.44303
H	1.22623	0.00000	-3.44303

23-F: $C_6H_4O_2PF$



(RI-)BP86/SV(P) level:

SCF Energy = -822.3480134567 E_h
Zero Point Energy = 0.0893779E_h
Symmetry = C_s

XYZ Coordinates:
14

O	-0.41983	-0.78885	-1.23083
P	-0.39742	-1.95603	0.00000
O	-0.41983	-0.78885	1.23083
C	-0.17386	0.46805	-0.70381
C	-0.17386	0.46805	0.70381
C	0.02816	1.64087	1.43277
C	0.02816	1.64087	-1.43277
H	0.02455	1.62221	-2.53290
C	0.23093	2.83149	-0.70369
C	0.23093	2.83149	0.70369
H	0.02455	1.62221	2.53290
H	0.39303	3.77481	-1.24972
H	0.39303	3.77481	1.24972
F	1.20298	-2.30189	0.00000

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a'	87.39	0.75990	YES	YES
8	a"	170.28	0.22709	YES	YES
9	a'	253.01	2.46471	YES	YES
10	a"	286.28	1.19898	YES	YES
11	a"	364.74	9.20243	YES	YES
12	a'	388.51	6.75923	YES	YES
13	a'	439.63	0.95338	YES	YES
14	a'	501.25	18.24240	YES	YES
15	a"	556.49	0.21300	YES	YES
16	a"	583.61	0.57092	YES	YES
17	a'	604.84	16.12518	YES	YES
18	a"	691.66	33.71678	YES	YES
19	a"	722.98	6.42853	YES	YES
20	a'	735.21	53.32931	YES	YES
21	a'	746.50	26.13517	YES	YES
22	a'	792.07	176.40973	YES	YES
23	a"	840.03	0.87932	YES	YES
24	a"	840.89	3.93980	YES	YES
25	a'	841.34	257.49651	YES	YES
26	a'	910.55	3.91876	YES	YES
27	a"	953.51	0.00071	YES	YES
28	a'	1008.87	8.15552	YES	YES
29	a"	1082.75	8.36193	YES	YES
30	a'	1133.21	6.04462	YES	YES
31	a"	1152.54	1.23882	YES	YES
32	a'	1249.53	225.80214	YES	YES
33	a"	1253.50	0.30314	YES	YES
34	a'	1391.22	0.26197	YES	YES
35	a"	1458.72	3.27019	YES	YES
36	a'	1474.58	179.07671	YES	YES
37	a"	1610.51	0.73192	YES	YES
38	a'	1618.27	2.05688	YES	YES
39	a"	3103.23	1.52947	YES	YES
40	a'	3116.87	10.03034	YES	YES
41	a"	3132.45	4.97458	YES	YES
42	a'	3135.37	1.26405	YES	YES

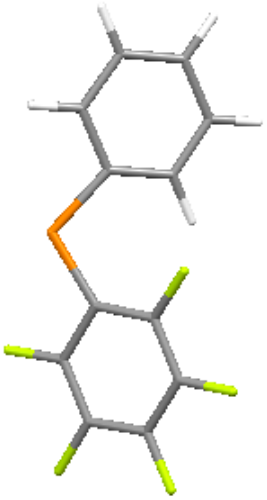
(RI-)MP2/def2-TZVPP level

SCF Energy = -821.5002629579 E_h
Symmetry = C_s

XYZ Coordinates:
14

O	-0.45030	-0.80831	-1.21014
P	-0.35679	-1.92704	0.00000
O	-0.45030	-0.80831	1.21014
C	-0.18896	0.44786	-0.69455
C	-0.18896	0.44786	0.69455
C	0.01902	1.60359	1.42271
C	0.01902	1.60359	-1.42271
H	0.01486	1.58634	-2.50249
C	0.23163	2.77979	-0.69808
C	0.23163	2.77979	0.69808
H	0.01486	1.58634	2.50249
H	0.40025	3.70390	-1.23217
H	0.40025	3.70390	1.23217
F	1.21805	-2.16699	0.00000

24: $[P(C_6H_5)(C_6F_5)]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -1299.7777553790 E_h
Zero Point Energy = 0.1379301 E_h
Symmetry = C_1

XYZ Coordinates:
23

C	1.68217	-0.00001	1.91787
P	0.95254	1.62521	1.72097
C	-0.61232	1.45588	0.90910

C	1.60700	-1.11361	1.02022
C	2.39454	-2.25435	1.20169
C	3.28132	-2.32197	2.30568
C	3.39976	-1.24273	3.21220
C	2.61914	-0.10265	3.00089
C	-1.09645	2.70094	0.37452
C	-2.34935	2.76652	-0.23606
C	-3.16193	1.61417	-0.27998
C	-2.72394	0.39172	0.28528
C	-1.46273	0.30306	0.86796
F	2.33328	-3.26724	0.35304
F	0.83467	-1.06841	-0.06137
F	4.00531	-3.40250	2.48466
F	4.23180	-1.32726	4.23527
F	2.73283	0.90888	3.85448
H	-0.46768	3.60583	0.43727
H	-2.70756	3.71508	-0.66574
H	-4.16041	1.66906	-0.74441
H	-3.38569	-0.48877	0.26718
H	-1.14044	-0.64303	1.32644

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	31.72	0.11897	YES YES
8	a	40.72	0.77102	YES YES
9	a	57.83	0.40207	YES YES
10	a	114.57	0.57026	YES YES
11	a	124.58	0.40996	YES YES
12	a	136.97	0.86780	YES YES
13	a	152.56	0.01197	YES YES
14	a	189.26	9.01027	YES YES
15	a	210.84	1.21552	YES YES
16	a	218.07	4.83642	YES YES
17	a	261.90	0.17150	YES YES
18	a	268.33	0.94263	YES YES
19	a	307.32	1.59017	YES YES
20	a	330.76	3.22105	YES YES
21	a	372.11	0.99723	YES YES
22	a	384.34	1.11344	YES YES
23	a	389.09	1.35151	YES YES
24	a	405.26	52.63370	YES YES
25	a	415.29	2.35456	YES YES
26	a	422.98	8.03935	YES YES
27	a	449.69	10.43991	YES YES
28	a	503.79	4.43362	YES YES
29	a	510.35	6.82970	YES YES
30	a	566.59	0.09520	YES YES
31	a	593.47	0.45636	YES YES
32	a	625.97	8.50837	YES YES
33	a	638.46	2.57794	YES YES
34	a	659.38	29.65747	YES YES
35	a	704.38	2.33061	YES YES
36	a	753.41	18.63681	YES YES
37	a	760.76	14.32872	YES YES
38	a	820.00	3.78025	YES YES
39	a	866.01	3.21373	YES YES
40	a	941.32	0.36361	YES YES
41	a	974.17	14.80774	YES YES
42	a	975.76	14.56007	YES YES
43	a	999.90	116.15102	YES YES
44	a	1010.38	1.25195	YES YES
45	a	1013.75	10.12958	YES YES
46	a	1078.96	111.15324	YES YES
47	a	1095.68	176.48736	YES YES
48	a	1128.74	170.21344	YES YES
49	a	1155.43	1.30088	YES YES
50	a	1176.47	7.81424	YES YES
51	a	1182.23	13.17763	YES YES
52	a	1283.49	12.42972	YES YES
53	a	1304.70	247.23674	YES YES
54	a	1355.38	3.02139	YES YES
55	a	1363.05	64.81017	YES YES
56	a	1371.90	4.58942	YES YES
57	a	1436.88	37.39445	YES YES
58	a	1449.68	11.57546	YES YES
59	a	1468.72	378.44916	YES YES
60	a	1511.65	820.76399	YES YES
61	a	1543.77	1.50007	YES YES
62	a	1582.09	114.10473	YES YES
63	a	1596.21	182.46133	YES YES
64	a	1628.59	104.56696	YES YES
65	a	3100.90	1.03558	YES YES
66	a	3118.63	0.26784	YES YES
67	a	3128.59	0.42482	YES YES
68	a	3136.46	0.25009	YES YES

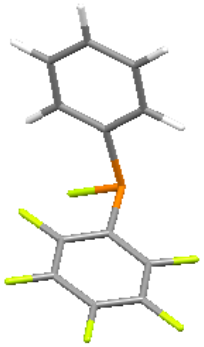
(RI-)MP2/def2-TZVPP level

SCF Energy = -1298.5064834576 E_h
Symmetry = C_1

XYZ Coordinates:
23

C	0.33263	0.53195	-0.20645
P	-1.13569	1.43896	-0.58849
C	-2.46853	0.44672	-0.07288
C	0.52919	-0.85898	-0.36742
C	1.78236	-1.42557	-0.22302
C	2.87501	-0.61494	0.10006
C	2.72592	0.76564	0.25043
C	1.47278	1.32050	0.07359
C	-3.71421	0.86920	-0.61905
C	-4.87744	0.21119	-0.26148
C	-4.82272	-0.81782	0.68340
C	-3.60898	-1.19975	1.27412
C	-2.43066	-0.58516	0.89846
F	1.96226	-2.71794	-0.40019
F	-0.46461	-1.64932	-0.75355
F	4.05581	-1.15887	0.25413
F	3.76687	1.51024	0.55250
F	1.32936	2.63148	0.21422
H	-3.73985	1.68952	-1.32679
H	-5.82436	0.50413	-0.69139
H	-5.73622	-1.31540	0.98115
H	-3.59903	-1.97357	2.02854
H	-1.49651	-0.85804	1.36825

24-F:P(C_6H_5)(C_6F_5)F



(RI-)BP86/SV(P) level:
Energy = -1399.8551779830 E_h
Zero Point Energy = 0.1401102 E_h
Symmetry = C_1

XYZ Coordinates:

24

C	0.39827	0.54908	0.37966
P	-1.18697	1.27541	1.04800
C	-2.39436	0.04611	0.37503
C	0.69445	0.42843	-0.99316
C	1.92796	-0.07366	-1.43995
C	2.89071	-0.48236	-0.49809
C	2.62019	-0.38548	0.87798
C	1.38366	0.13557	1.29688
C	-3.14178	0.27058	-0.79920
C	-4.08902	-0.67987	-1.21634
C	-4.29662	-1.85271	-0.46948
C	-3.56030	-2.07304	0.70829
C	-2.62030	-1.12185	1.13596
F	-1.38811	2.48200	-0.05756
F	2.19391	-0.17654	-2.74583
F	-0.20089	0.78841	-1.91975
F	4.06066	-0.96644	-0.91492
F	3.53319	-0.78543	1.76845
F	1.15701	0.21928	2.61745
H	-2.97915	1.18790	-1.38559
H	-4.66963	-0.50271	-2.13704
H	-5.04053	-2.59549	-0.80183
H	-3.72574	-2.98574	1.30442
H	-2.05834	-1.29158	2.07207

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	15.66	0.12888	YES YES
8	a	30.57	0.12557	YES YES
9	a	40.65	0.17456	YES YES
10	a	88.17	0.03953	YES YES
11	a	121.18	0.01303	YES YES
12	a	132.90	0.28272	YES YES
13	a	147.20	0.07963	YES YES
14	a	161.90	1.11528	YES YES
15	a	183.03	1.97686	YES YES
16	a	201.20	0.25088	YES YES
17	a	232.31	0.17361	YES YES
18	a	262.57	0.07299	YES YES
19	a	266.57	0.11650	YES YES
20	a	301.12	1.67660	YES YES
21	a	307.43	2.38793	YES YES
22	a	328.94	7.37375	YES YES
23	a	373.79	2.50256	YES YES
24	a	384.03	7.28597	YES YES
25	a	385.76	15.81145	YES YES
26	a	395.20	0.70132	YES YES
27	a	421.06	18.01500	YES YES
28	a	432.96	5.92777	YES YES
29	a	480.62	3.67693	YES YES
30	a	488.46	9.66577	YES YES
31	a	503.70	30.92937	YES YES
32	a	566.52	0.94818	YES YES
33	a	607.76	0.20035	YES YES
34	a	622.13	8.35296	YES YES
35	a	627.61	0.26013	YES YES
36	a	682.30	3.27772	YES YES
37	a	698.91	36.47011	YES YES
38	a	736.77	22.23096	YES YES
39	a	752.56	8.21784	YES YES
40	a	790.92	71.63465	YES YES
41	a	817.60	0.97977	YES YES
42	a	835.72	0.41256	YES YES
43	a	903.82	1.12480	YES YES
44	a	957.19	0.54002	YES YES
45	a	982.48	2.27337	YES YES
46	a	985.09	8.82753	YES YES
47	a	987.44	145.78461	YES YES
48	a	1022.49	1.60674	YES YES
49	a	1072.43	4.16028	YES YES
50	a	1079.85	24.40550	YES YES
51	a	1099.05	194.36722	YES YES
52	a	1143.40	0.07736	YES YES
53	a	1158.66	5.59585	YES YES
54	a	1163.42	1.40165	YES YES
55	a	1288.33	35.84153	YES YES
56	a	1291.68	4.43757	YES YES
57	a	1347.75	3.07779	YES YES
58	a	1362.48	1.66469	YES YES
59	a	1384.55	29.99692	YES YES
60	a	1430.44	10.67474	YES YES
61	a	1471.95	4.57679	YES YES
62	a	1486.40	396.86941	YES YES
63	a	1515.06	213.54415	YES YES
64	a	1589.52	0.52817	YES YES
65	a	1601.70	0.78501	YES YES
66	a	1614.60	12.77237	YES YES
67	a	1622.66	50.06897	YES YES
68	a	3071.64	2.92299	YES YES
69	a	3093.65	0.34226	YES YES
70	a	3103.72	14.16686	YES YES
71	a	3115.56	17.55188	YES YES

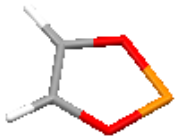
(RI-)MP2/def2-TZVPP level

SCF Energy = -1398.5732224704 E_h
Symmetry = C_1

XYZ Coordinates:
24

C	0.36912	0.56364	0.44972
P	-1.19140	1.18511	1.20329
C	-2.32093	0.00926	0.39714
C	0.62492	0.54731	-0.92210
C	1.81676	0.06288	-1.44157
C	2.78689	-0.43354	-0.57751
C	2.56310	-0.43860	0.79333
C	1.36568	0.06286	1.28619
C	-3.05926	0.30450	-0.75187
C	-3.92087	-0.65223	-1.28388
C	-4.04647	-1.90194	-0.67942
C	-3.31674	-2.19495	0.47204
C	-2.46695	-1.23737	1.01773
F	-1.42117	2.48090	0.28471
F	2.03961	0.06047	-2.75213
F	-0.28305	1.00386	-1.78429
F	3.92759	-0.90498	-1.06493
F	3.49341	-0.91597	1.61425
F	1.18686	0.03965	2.61068
H	-2.95637	1.27042	-1.22551
H	-4.49269	-0.42173	-2.17257
H	-4.71469	-2.64127	-1.09902
H	-3.42024	-3.15935	0.95033
H	-1.91764	-1.45893	1.92633

25: [(CH)$_2$O$_2$P]$^+$



(RI-)BP86/SV(P) level:
SCF Energy = -568.7004117234 E_h
Zero Point Energy = 0.0411612 E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

O	-1.17615	0.00000	-0.01705
P	0.00000	0.00000	1.15104
O	1.17615	0.00000	-0.01705
C	-0.68676	0.00000	-1.28472
C	0.68676	0.00000	-1.28472
H	1.41892	0.00000	-2.10546
H	-1.41892	0.00000	-2.10546

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.03	0.03297	YES	YES
8		a	54.03	0.12061	YES	YES
9		a	108.47	0.65451	YES	YES
10		a	143.10	1.87741	YES	YES
11		a	161.89	3.23946	YES	YES
12		a	220.77	0.84890	YES	YES
13		a	258.07	0.23833	YES	YES
14		a	261.93	0.25719	YES	YES
15		a	331.59	0.65752	YES	YES
16		a	431.69	25.51929	YES	YES
17		a	435.65	24.98526	YES	YES
18		a	505.39	1.25012	YES	YES
19		a	523.48	2.22561	YES	YES
20		a	528.83	0.84803	YES	YES
21		a	549.42	11.99635	YES	YES
22		a	726.13	1.43402	YES	YES
23		a	729.50	5.41704	YES	YES
24		a	820.34	66.34508	YES	YES
25		a	1102.54	231.73283	YES	YES
26		a	1125.45	315.13040	YES	YES
27		a	1148.81	88.79335	YES	YES
28		a	1154.27	19.36874	YES	YES
29		a	1170.73	346.92142	YES	YES

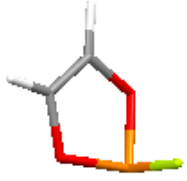
(RI-)MP2/def2-TZVPP level

SCF Energy = -568.0973052601 E_h
Symmetry = C_{2V}

XYZ Coordinates:
7

O	-1.16378	0.00000	0.00486
P	0.00000	0.00000	1.11476
O	1.16378	0.00000	0.00486
C	-0.67697	0.00000	-1.26990
C	0.67697	0.00000	-1.26990
H	1.39358	0.00000	-2.07241
H	-1.39358	0.00000	-2.07241

25-F: (CH)-O-PF



(RI-)BP86/SV(P) level:
SCF Energy = -668.7895398831 E_h
Zero Point Energy = 0.0430627 E_h
Symmetry = C_s

XYZ Coordinates:
8

O	0.26182	-0.37614	-1.21971
P	0.57019	0.75632	0.00000
O	0.26182	-0.37614	1.21971
C	-0.33537	-1.50562	-0.67433
C	-0.33537	-1.50562	0.67433
H	-0.70773	-2.25227	1.38688
H	-0.70773	-2.25227	-1.38688
F	-0.87143	1.54323	0.00000

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.03	0.03297	YES	YES
8		a	54.03	0.12061	YES	YES
9		a	108.47	0.65451	YES	YES
10		a	143.10	1.87741	YES	YES
11		a	161.89	3.23946	YES	YES
12		a	220.77	0.84890	YES	YES
13		a	258.07	0.23833	YES	YES
14		a	261.93	0.25719	YES	YES
15		a	331.59	0.65752	YES	YES
16		a	431.69	25.51929	YES	YES
17		a	435.65	24.98526	YES	YES
18		a	505.39	1.25012	YES	YES
19		a	523.48	2.22561	YES	YES
20		a	528.83	0.84803	YES	YES
21		a	549.42	11.99635	YES	YES
22		a	726.13	1.43402	YES	YES
23		a	729.50	5.41704	YES	YES
24		a	820.34	66.34508	YES	YES
25		a	1102.54	231.73283	YES	YES
26		a	1125.45	315.13040	YES	YES
27		a	1148.81	88.79335	YES	YES
28		a	1154.27	19.36874	YES	YES
29		a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -668.1647939942 E_h
Symmetry = C_s

XYZ Coordinates:
8

O	0.28998	-0.35164	-1.19962
P	0.54650	0.74658	0.00000
O	0.28998	-0.35164	1.19962
C	-0.33673	-1.46949	-0.66653
C	-0.33673	-1.46949	0.66653
H	-0.71810	-2.19528	1.35946
H	-0.71810	-2.19528	-1.35946
F	-0.87743	1.46610	0.00000

26: $[(CH)-O-P]^+$

(RI-)BP86/SV(P) level:

SCF Energy = -569.9150966857 E_h
Zero Point Energy = 0.0640614 E_h
Symmetry = C_{2v}

XYZ Coordinates:
9

O	0.00000	1.19970	0.09751
P	0.00000	0.00000	1.15432
O	0.00000	-1.19970	0.09751
C	0.00000	0.77874	-1.32066
C	0.00000	-0.77874	-1.32066
H	-0.90667	-1.22731	-1.77299
H	0.90667	-1.22731	-1.77299
H	0.90667	1.22731	-1.77299
H	-0.90667	1.22731	-1.77299

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

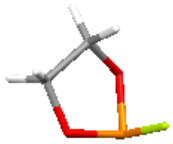
(RI-)MP2/def2-TZVPP level

SCF Energy = -569.3175753514 E_h
Symmetry = C_{2v}

XYZ Coordinates:
9

O	0.00000	1.18971	0.11452
P	0.00000	0.00000	1.12096
O	0.00000	-1.18971	0.11452
C	0.00000	0.77031	-1.30539
C	0.00000	-0.77031	-1.30539
H	-0.89290	-1.20064	-1.74269
H	0.89290	-1.20064	-1.74269
H	0.89290	1.20064	-1.74269
H	-0.89290	1.20064	-1.74269

26-F: $(CH_2)_2O_2PF$



(RI-)BP86/SV(P) level:
SCF Energy = -670.0086916848 E_h
Zero Point Energy = 0.0667498 E_h
Symmetry = C_1

XYZ Coordinates:
10

O	0.49794	0.29250	1.16674
P	0.56725	-0.79015	-0.10220
O	0.15043	0.35468	-1.24426
C	-0.43127	1.34993	0.85465
C	-0.27501	1.60151	-0.65963
H	-1.22953	1.91681	-1.13216
H	0.50419	2.36745	-0.87326
H	-0.16049	2.23386	1.46774
H	-1.46452	1.02666	1.11474
F	-0.89962	-1.52306	0.07798

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -669.3857649548 E_h
Symmetry = C_1

XYZ Coordinates:
10

O	0.51387	0.26554	1.14177
P	0.54528	-0.77665	-0.10767
O	0.15355	0.33734	-1.22855
C	-0.42321	1.32195	0.85176

C	-0.27121	1.58371	-0.64232
H	-1.20660	1.88647	-1.10399
H	0.49888	2.32458	-0.84478
H	-0.15417	2.18057	1.45761
H	-1.42841	0.98868	1.10245
F	-0.89053	-1.47009	0.08378

27: $[P(PH_2)_3]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -1025.9484184440 E_h
Zero Point Energy = 0.0352392 E_h
Symmetry = C_2

XYZ Coordinates:
7

P	1.68641	0.05746	-0.39751
P	0.00000	0.00000	0.89479
P	-1.68641	-0.05746	-0.39751
H	1.36620	-0.45797	-1.69733
H	2.57948	-0.91187	0.16428
H	-2.57948	0.91187	0.16428
H	-1.36620	0.45797	-1.69733

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	157.97	0.10297	YES	YES
8	b	192.72	204.70589	YES	YES
9	a	265.98	14.60931	YES	YES
10	b	323.49	5.88158	YES	YES
11	a	432.61	9.29590	YES	YES
12	a	551.59	4.02451	YES	YES
13	b	582.34	3.33948	YES	YES
14	b	634.32	5.35083	YES	YES
15	a	724.06	0.13218	YES	YES
16	a	1033.48	1.08206	YES	YES
17	b	1034.20	99.26931	YES	YES
18	a	2357.59	0.00987	YES	YES
19	b	2362.65	13.83589	YES	YES
20	a	2406.76	1.25370	YES	YES
21	b	2408.47	4.49758	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1024.7206898416 E_h
Symmetry = C_2

XYZ Coordinates:
7

P	1.61854	0.05425	-0.39800
P	0.00000	0.00000	0.89994
P	-1.61854	-0.05425	-0.39800
H	1.26901	-0.36553	-1.68757
H	2.53684	-0.88075	0.09072
H	-2.53684	0.88075	0.09072
H	-1.26901	0.36553	-1.68757

27-F: $P(PH_2)_2F$

(RI-)BP86/SV(P) level:
SCF Energy = -1126.0405389050 E_h
Zero Point Energy = 0.0379469 E_h
Symmetry = C_1

XYZ Coordinates:
8

P	-1.66792	-0.11693	-0.76830
P	-0.00774	0.63356	0.56260
P	1.62084	-0.19036	-0.79435
F	0.09098	-0.53242	1.73341
H	-2.69048	0.11595	0.22414
H	-1.49149	-1.50263	-0.40816
H	2.67618	0.46843	-0.05522
H	1.47561	0.92771	-1.70196

vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	127.13	3.47118	YES	YES
8	a	135.09	0.59479	YES	YES
9	a	181.18	2.98573	YES	YES
10	a	195.40	8.09241	YES	YES
11	a	229.95	4.10360	YES	YES
12	a	390.31	8.45933	YES	YES
13	a	412.26	8.00926	YES	YES
14	a	659.49	24.61435	YES	YES
15	a	675.04	0.86084	YES	YES
16	a	697.81	25.60041	YES	YES
17	a	777.90	61.51299	YES	YES
18	a	790.57	2.83450	YES	YES
19	a	1068.36	7.51543	YES	YES
20	a	1085.41	23.60847	YES	YES
21	a	2287.90	37.77539	YES	YES
22	a	2304.78	49.17727	YES	YES
23	a	2309.25	36.84966	YES	YES
24	a	2328.94	31.89101	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1124.7899840021 E_h
Symmetry = C_1

XYZ Coordinates:
8

P	-1.61109	-0.10679	-0.76614
P	-0.00888	0.61383	0.55631
P	1.58470	-0.18604	-0.76492
F	0.06315	-0.51836	1.71055
H	-2.62104	0.01998	0.20727
H	-1.39215	-1.48062	-0.54367
H	2.61518	0.59137	-0.19553
H	1.29134	0.77543	-1.75572

28: $[PI_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -363.9235055808 E_h
Zero Point Energy = 0.0018864 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	1.22581
I	1.95815	0.00000	-0.14959
I	-1.95815	0.00000	-0.14959

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	15.66	0.12888	YES	YES
8		a	30.57	0.12557	YES	YES
9		a	40.65	0.17456	YES	YES
10		a	88.17	0.03953	YES	YES
11		a	121.18	0.01303	YES	YES
12		a	132.90	0.28272	YES	YES
13		a	147.20	0.07963	YES	YES
14		a	161.90	1.11528	YES	YES
15		a	183.03	1.97686	YES	YES
16		a	201.20	0.25088	YES	YES
17		a	232.31	0.17361	YES	YES
18		a	262.57	0.07299	YES	YES
19		a	266.57	0.11650	YES	YES
20		a	301.12	1.67660	YES	YES
21		a	307.43	2.38793	YES	YES
22		a	328.94	7.37375	YES	YES
23		a	373.79	2.50256	YES	YES
24		a	384.03	7.28597	YES	YES
25		a	385.76	15.81145	YES	YES
26		a	395.20	0.70132	YES	YES
27		a	421.06	18.01500	YES	YES
28		a	432.96	5.92777	YES	YES
29		a	480.62	3.67693	YES	YES
30		a	488.46	9.66577	YES	YES
31		a	503.70	30.92937	YES	YES
32		a	566.52	0.94818	YES	YES
33		a	607.76	0.20035	YES	YES
34		a	622.13	8.35296	YES	YES
35		a	627.61	0.26013	YES	YES
36		a	682.30	3.27772	YES	YES
37		a	698.91	36.47011	YES	YES
38		a	736.77	22.23096	YES	YES
39		a	752.56	8.21784	YES	YES
40		a	790.92	71.63465	YES	YES
41		a	817.60	0.97977	YES	YES
42		a	835.72	0.41256	YES	YES
43		a	903.82	1.12480	YES	YES
44		a	957.19	0.54002	YES	YES
45		a	982.48	2.27337	YES	YES
46		a	985.09	8.82753	YES	YES
47		a	987.44	145.78461	YES	YES
48		a	1022.49	1.60674	YES	YES
49		a	1072.43	4.16028	YES	YES
50		a	1079.85	24.40550	YES	YES
51		a	1099.05	194.36722	YES	YES
52		a	1143.40	0.07736	YES	YES
53		a	1158.66	5.59585	YES	YES
54		a	1163.42	1.40165	YES	YES
55		a	1288.33	35.84153	YES	YES
56		a	1291.68	4.43757	YES	YES
57		a	1347.75	3.07779	YES	YES
58		a	1362.48	1.66469	YES	YES
59		a	1384.55	29.99692	YES	YES
60		a	1430.44	10.67474	YES	YES
61		a	1471.95	4.57679	YES	YES
62		a	1486.40	396.86941	YES	YES
63		a	1515.06	213.54415	YES	YES
64		a	1589.52	0.52817	YES	YES
65		a	1601.70	0.78501	YES	YES
66		a	1614.60	12.77237	YES	YES
67		a	1622.66	50.06897	YES	YES
68		a	3071.64	2.92299	YES	YES
69		a	3093.65	0.34226	YES	YES
70		a	3103.72	14.16686	YES	YES
71		a	3115.56	17.55188	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -934.9207190862 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	1.20797
I	1.87197	0.00000	-0.14742
I	-1.87197	0.00000	-0.14742

28-F: I-PF

(RI-)BP86/SV(P) level:
SCF Energy = -464.0348303674 E_h
Zero Point Energy = 0.0043127 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	1.10508	0.63260	0.00000
F	2.18971	-0.58183	0.00000
I	-0.29877	-0.03365	1.98982
I	-0.29877	-0.03365	-1.98982

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES
15	a	331.59	0.65752	YES YES
16	a	431.69	25.51929	YES YES
17	a	435.65	24.98526	YES YES
18	a	505.39	1.25012	YES YES
19	a	523.48	2.22561	YES YES
20	a	528.83	0.84803	YES YES
21	a	549.42	11.99635	YES YES
22	a	726.13	1.43402	YES YES
23	a	729.50	5.41704	YES YES
24	a	820.34	66.34508	YES YES
25	a	1102.54	231.73283	YES YES
26	a	1125.45	315.13040	YES YES
27	a	1148.81	88.79335	YES YES
28	a	1154.27	19.36874	YES YES
29	a	1170.73	346.92142	YES YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1035.0052650757 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	1.09356	0.62323	0.00000
F	2.13070	-0.58127	0.00000
I	-0.29294	-0.03255	1.88587
I	-0.29294	-0.03255	-1.88587

29: $[P(CH_3)_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -420.7113740203 E_h
Zero Point Energy = 0.0692113 E_h
Symmetry = C_2

XYZ Coordinates:
9

C	0.01459	1.41492	-0.54174
P	0.00000	0.00000	0.56626
C	-0.01459	-1.41492	-0.54174
H	0.50992	2.29661	-0.07308
H	-1.08264	1.70066	-0.58207
H	0.34311	1.23601	-1.58964
H	1.08264	-1.70066	-0.58207
H	-0.34311	-1.23601	-1.58964
H	-0.50992	-2.29661	-0.07308

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	22.03	0.03297	YES YES
8	a	54.03	0.12061	YES YES
9	a	108.47	0.65451	YES YES
10	a	143.10	1.87741	YES YES
11	a	161.89	3.23946	YES YES
12	a	220.77	0.84890	YES YES
13	a	258.07	0.23833	YES YES
14	a	261.93	0.25719	YES YES
15	a	331.59	0.65752	YES YES
16	a	431.69	25.51929	YES YES
17	a	435.65	24.98526	YES YES
18	a	505.39	1.25012	YES YES
19	a	523.48	2.22561	YES YES
20	a	528.83	0.84803	YES YES
21	a	549.42	11.99635	YES YES
22	a	726.13	1.43402	YES YES
23	a	729.50	5.41704	YES YES
24	a	820.34	66.34508	YES YES
25	a	1102.54	231.73283	YES YES
26	a	1125.45	315.13040	YES YES
27	a	1148.81	88.79335	YES YES
28	a	1154.27	19.36874	YES YES
29	a	1170.73	346.92142	YES YES

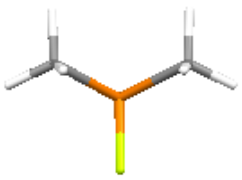
(RI-)MP2/def2-TZVPP level

SCF Energy = -420.1864158257 E_h
Symmetry = C_2

XYZ Coordinates:
9

C	0.01545	1.38436	-0.53771
P	0.00000	0.00000	0.56203
C	-0.01545	-1.38436	-0.53771
H	0.43487	2.27751	-0.08162
H	-1.08314	1.55768	-0.59764
H	0.36900	1.19745	-1.54850
H	1.08314	-1.55768	-0.59764
H	-0.36900	-1.19745	-1.54850
H	-0.43487	-2.27751	-0.08162

29-F: $P(CH_3)_2F$



(RI-)BP86/SV(P) level:

SCF Energy = -520.8336710270 E_h
Zero Point Energy = 0.0749795 E_h

Symmetry = C_s

XYZ Coordinates:
10

C	-0.84746	-0.32087	1.41218
P	-0.00416	0.54544	0.00000
C	-0.84746	-0.32087	-1.41218
F	1.40436	-0.32931	0.00000
H	-0.34010	-0.05082	2.36399
H	-0.82844	-1.42714	1.29294
H	-1.90393	0.02452	1.47853
H	-0.34010	-0.05082	-2.36399
H	-1.90393	0.02452	-1.47853
H	-0.82844	-1.42714	-1.29294

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -520.2870024434 E_h
Symmetry = C_s

XYZ Coordinates:
10

C	-0.84021	-0.31015	1.38115
P	0.00599	0.53239	0.00000
C	-0.84021	-0.31015	-1.38115
F	1.37765	-0.32741	0.00000
H	-0.35484	-0.05570	2.32074
H	-0.83908	-1.39124	1.25059
H	-1.86901	0.04843	1.42366
H	-0.35484	-0.05570	-2.32074
H	-1.86901	0.04843	-1.42366
H	-0.83908	-1.39124	-1.25059

30: $[PBr_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -5489.2667946170 E_h
Zero Point Energy = 0.0023550 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	-1.06358
Br	1.74134	0.00000	0.20613
Br	-1.74134	0.00000	0.20613

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	52.25	3.37204	YES	YES
8	a	62.01	1.60483	YES	YES
9	a	180.47	17.14319	YES	YES
10	a	402.06	0.51145	YES	YES
11	a	404.01	0.50696	YES	YES
12	a	447.22	2.83071	YES	YES
13	a	739.84	3.69086	YES	YES
14	a	757.66	5.46120	YES	YES
15	a	817.70	1.30369	YES	YES
16	a	949.16	9.83394	YES	YES
17	a	960.51	14.98237	YES	YES
18	a	965.91	19.76635	YES	YES
19	a	1068.40	43.33553	YES	YES
20	a	1240.65	148.20902	YES	YES
21	a	1243.50	116.67886	YES	YES
22	a	1271.64	1.23740	YES	YES
23	a	1300.94	86.08384	YES	YES
24	a	1309.93	85.86253	YES	YES
25	a	1346.87	3.06878	YES	YES
26	a	1357.59	1.06744	YES	YES
27	a	1379.25	53.29733	YES	YES
28	a	1436.77	1.46522	YES	YES
29	a	1453.20	37.25682	YES	YES
30	a	1457.25	35.36943	YES	YES
31	a	2868.91	117.74263	YES	YES
32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -5485.7517124181 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	-1.04856
Br	1.69360	0.00000	0.20322
Br	-1.69360	0.00000	0.20322

30-F: Br_2PF

(RI-)BP86/SV(P) level:
SCF Energy = -5589.3932381060 E_h
Zero Point Energy = 0.0048685 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	0.84515	0.62805	0.00000
F	1.98276	-0.53497	0.00000
Br	-0.39950	-0.05813	1.76528
Br	-0.39950	-0.05813	-1.76528

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -5585.8553222819 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	0.84456	0.61800	0.00000
F	1.92723	-0.53736	0.00000
Br	-0.39278	-0.05589	1.71169
Br	-0.39278	-0.05589	-1.71169

31: $[PCl_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -1261.1983970530 E_h
Zero Point Energy = 0.0031388 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	0.83005
Cl	0.00000	1.59493	-0.36259
Cl	0.00000	-1.59493	-0.36259

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	52.25	3.37204	YES	YES
8	a	62.01	1.60483	YES	YES
9	a	180.47	17.14319	YES	YES
10	a	402.06	0.51145	YES	YES
11	a	404.01	0.50696	YES	YES
12	a	447.22	2.83071	YES	YES
13	a	739.84	3.69086	YES	YES
14	a	757.66	5.46120	YES	YES
15	a	817.70	1.30369	YES	YES
16	a	949.16	9.83394	YES	YES
17	a	960.51	14.98237	YES	YES
18	a	965.91	19.76635	YES	YES
19	a	1068.40	43.33553	YES	YES
20	a	1240.65	148.20902	YES	YES
21	a	1243.50	116.67886	YES	YES
22	a	1271.64	1.23740	YES	YES
23	a	1300.94	86.08384	YES	YES
24	a	1309.93	85.86253	YES	YES
25	a	1346.87	3.06878	YES	YES
26	a	1357.59	1.06744	YES	YES
27	a	1379.25	53.29733	YES	YES
28	a	1436.77	1.46522	YES	YES
29	a	1453.20	37.25682	YES	YES
30	a	1457.25	35.36943	YES	YES
31	a	2868.91	117.74263	YES	YES
32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1259.9935261063 E_h
Symmetry = C_{2V}

XYZ Coordinates:

3

P	0.00000	0.00000	0.81010
Cl	-1.54911	0.00000	-0.35388
Cl	1.54911	0.00000	-0.35388

31-F: ClPF

(RI-)BP86/SV(P) level:
SCF Energy = 1361.3371557480 E_h
Zero Point Energy = 0.0057037 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	0.45323	0.60556	0.00000
F	1.67316	-0.46801	0.00000
Cl	-0.64629	-0.13913	1.61613
Cl	-0.64629	-0.13913	-1.61613

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	22.03	0.03297	YES YES
8		a	54.03	0.12061	YES YES
9		a	108.47	0.65451	YES YES
10		a	143.10	1.87741	YES YES
11		a	161.89	3.23946	YES YES
12		a	220.77	0.84890	YES YES
13		a	258.07	0.23833	YES YES
14		a	261.93	0.25719	YES YES
15		a	331.59	0.65752	YES YES
16		a	431.69	25.51929	YES YES
17		a	435.65	24.98526	YES YES
18		a	505.39	1.25012	YES YES
19		a	523.48	2.22561	YES YES
20		a	528.83	0.84803	YES YES
21		a	549.42	11.99635	YES YES
22		a	726.13	1.43402	YES YES
23		a	729.50	5.41704	YES YES
24		a	820.34	66.34508	YES YES
25		a	1102.54	231.73283	YES YES
26		a	1125.45	315.13040	YES YES
27		a	1148.81	88.79335	YES YES
28		a	1154.27	19.36874	YES YES
29		a	1170.73	346.92142	YES YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -1360.1076909101 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	0.45082	0.59449	0.00000
F	1.62422	-0.46518	0.00000
Cl	-0.63212	-0.13505	1.56668
Cl	-0.63212	-0.13505	-1.56668

32: $[PF_2]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -540.5038179068 E_h
Zero Point Energy = 0.0052685 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	0.53661
F	-1.21448	0.00000	-0.43743
F	1.21448	0.00000	-0.43743

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	52.25	3.37204	YES YES
8		a	62.01	1.60483	YES YES
9		a	180.47	17.14319	YES YES
10		a	402.06	0.51145	YES YES
11		a	404.01	0.50696	YES YES
12		a	447.22	2.83071	YES YES
13		a	739.84	3.69086	YES YES
14		a	757.66	5.46120	YES YES
15		a	817.70	1.30369	YES YES
16		a	949.16	9.83394	YES YES
17		a	960.51	14.98237	YES YES
18		a	965.91	19.76635	YES YES
19		a	1068.40	43.33553	YES YES
20		a	1240.65	148.20902	YES YES
21		a	1243.50	116.67886	YES YES
22		a	1271.64	1.23740	YES YES
23		a	1300.94	86.08384	YES YES
24		a	1309.93	85.86253	YES YES
25		a	1346.87	3.06878	YES YES
26		a	1357.59	1.06744	YES YES
27		a	1379.25	53.29733	YES YES
28		a	1436.77	1.46522	YES YES
29		a	1453.20	37.25682	YES YES
30		a	1457.25	35.36943	YES YES
31		a	2868.91	117.74263	YES YES
32		a	2877.64	84.28624	YES YES
33		a	2893.34	29.20329	YES YES
34		a	2963.18	21.64613	YES YES
35		a	2973.98	22.67130	YES YES
36		a	2979.38	17.20698	YES YES
37		a	3081.87	6.77553	YES YES
38		a	3085.00	4.78460	YES YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -540.0607352233 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	0.51542
F	-1.18051	0.00000	-0.42015
F	1.18051	0.00000	-0.42015

32-F: $[PF_3]^+$

(RI-)BP86/SV(P) level:

SCF Energy = -640.6764731844 E_h
Zero Point Energy = 0.0082026 E_h
Symmetry = C_{3V}

XYZ Coordinates:
4

P	0.00000	0.00000	0.51868
F	-1.40640	0.00000	-0.28188
F	0.70320	-1.21798	-0.28188
F	0.70320	1.21798	-0.28188

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	52.25	3.37204	YES	YES
8		a	62.01	1.60483	YES	YES
9		a	180.47	17.14319	YES	YES
10		a	402.06	0.51145	YES	YES
11		a	404.01	0.50696	YES	YES
12		a	447.22	2.83071	YES	YES
13		a	739.84	3.69086	YES	YES
14		a	757.66	5.46120	YES	YES
15		a	817.70	1.30369	YES	YES
16		a	949.16	9.83394	YES	YES
17		a	960.51	14.98237	YES	YES
18		a	965.91	19.76635	YES	YES
19		a	1068.40	43.33553	YES	YES
20		a	1240.65	148.20902	YES	YES
21		a	1243.50	116.67886	YES	YES
22		a	1271.64	1.23740	YES	YES
23		a	1300.94	86.08384	YES	YES
24		a	1309.93	85.86253	YES	YES
25		a	1346.87	3.06878	YES	YES
26		a	1357.59	1.06744	YES	YES
27		a	1379.25	53.29733	YES	YES
28		a	1436.77	1.46522	YES	YES
29		a	1453.20	37.25682	YES	YES
30		a	1457.25	35.36943	YES	YES
31		a	2868.91	117.74263	YES	YES
32		a	2877.64	84.28624	YES	YES
33		a	2893.34	29.20329	YES	YES
34		a	2963.18	21.64613	YES	YES
35		a	2973.98	22.67130	YES	YES
36		a	2979.38	17.20698	YES	YES
37		a	3081.87	6.77553	YES	YES
38		a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -640.2067235987 E_h
Symmetry = C_{3V}

XYZ Coordinates:
4

P	0.00000	0.00000	0.50228
F	0.68361	-1.18404	-0.27296
F	0.68361	1.18404	-0.27296
F	-1.36721	0.00000	-0.27296

33: $[PH_2]^+$

(RI-)BP86/SV(P) level:

SCF Energy = -342.0641992940 E_h
Zero Point Energy = 0.0131189 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	0.06165
H	-1.04384	0.00000	-0.94722
H	1.04384	0.00000	-0.94722

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	52.25	3.37204	YES	YES
8		a	62.01	1.60483	YES	YES
9		a	180.47	17.14319	YES	YES
10		a	402.06	0.51145	YES	YES
11		a	404.01	0.50696	YES	YES
12		a	447.22	2.83071	YES	YES
13		a	739.84	3.69086	YES	YES
14		a	757.66	5.46120	YES	YES
15		a	817.70	1.30369	YES	YES
16		a	949.16	9.83394	YES	YES
17		a	960.51	14.98237	YES	YES
18		a	965.91	19.76635	YES	YES
19		a	1068.40	43.33553	YES	YES
20		a	1240.65	148.20902	YES	YES
21		a	1243.50	116.67886	YES	YES
22		a	1271.64	1.23740	YES	YES
23		a	1300.94	86.08384	YES	YES

24	a	1309.93	85.86253	YES	YES
25	a	1346.87	3.06878	YES	YES
26	a	1357.59	1.06744	YES	YES
27	a	1379.25	53.29733	YES	YES
28	a	1436.77	1.46522	YES	YES
29	a	1453.20	37.25682	YES	YES
30	a	1457.25	35.36943	YES	YES
31	a	2868.91	117.74263	YES	YES
32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -341.6615817780 E_h
Symmetry = C_{2V}

XYZ Coordinates:
3

P	0.00000	0.00000	0.05970
H	-1.02158	0.00000	-0.91730
H	1.02158	0.00000	-0.91730

33-F: PH_2F

(RI-)BP86/SV(P) level:
SCF Energy = -442.2470385794 E_h
Zero Point Energy = 0.0187519 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	-0.58938	0.06923	0.00000
H	-0.84910	-0.91835	-1.03532
H	-0.84910	-0.91835	1.03532
F	1.05099	-0.01543	0.00000

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	52.25	3.37204	YES	YES
8		a	62.01	1.60483	YES	YES
9		a	180.47	17.14319	YES	YES
10		a	402.06	0.51145	YES	YES
11		a	404.01	0.50696	YES	YES
12		a	447.22	2.83071	YES	YES
13		a	739.84	3.69086	YES	YES
14		a	757.66	5.46120	YES	YES
15		a	817.70	1.30369	YES	YES
16		a	949.16	9.83394	YES	YES
17		a	960.51	14.98237	YES	YES
18		a	965.91	19.76635	YES	YES
19		a	1068.40	43.33553	YES	YES
20		a	1240.65	148.20902	YES	YES
21		a	1243.50	116.67886	YES	YES
22		a	1271.64	1.23740	YES	YES
23		a	1300.94	86.08384	YES	YES
24		a	1309.93	85.86253	YES	YES
25		a	1346.87	3.06878	YES	YES
26		a	1357.59	1.06744	YES	YES
27		a	1379.25	53.29733	YES	YES
28		a	1436.77	1.46522	YES	YES
29		a	1453.20	37.25682	YES	YES
30		a	1457.25	35.36943	YES	YES
31		a	2868.91	117.74263	YES	YES
32		a	2877.64	84.28624	YES	YES
33		a	2893.34	29.20329	YES	YES
34		a	2963.18	21.64613	YES	YES
35		a	2973.98	22.67130	YES	YES
36		a	2979.38	17.20698	YES	YES
37		a	3081.87	6.77553	YES	YES
38		a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -441.8152222953 E_h
Symmetry = C_s

XYZ Coordinates:
4

P	-0.57732	0.06621	0.00000
H	-0.82376	-0.88189	-1.01713
H	-0.82376	-0.88189	1.01713
F	1.02864	-0.01436	0.00000

34: $[SbF_5]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -504.3407252152 E_h
Zero Point Energy = 0.0103519 E_h
Symmetry = D_{3h}

XYZ Coordinates:
6

Sb	0.00000	0.00000	0.00000
F	0.00000	0.00000	1.92574
F	0.00000	0.00000	-1.92574
F	0.95718	-1.65789	0.00000
F	0.95718	1.65789	0.00000
F	-1.91436	0.00000	0.00000

Vibrational Spectrum:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.66	0.12888	YES	YES
8	a	30.57	0.12557	YES	YES
9	a	40.65	0.17456	YES	YES
10	a	88.17	0.03953	YES	YES
11	a	121.18	0.01303	YES	YES
12	a	132.90	0.28272	YES	YES
13	a	147.20	0.07963	YES	YES
14	a	161.90	1.11528	YES	YES
15	a	183.03	1.97686	YES	YES
16	a	201.20	0.25088	YES	YES
17	a	232.31	0.17361	YES	YES
18	a	262.57	0.07299	YES	YES
19	a	266.57	0.11650	YES	YES
20	a	301.12	1.67660	YES	YES
21	a	307.43	2.38793	YES	YES
22	a	328.94	7.37375	YES	YES
23	a	373.79	2.50256	YES	YES
24	a	384.03	7.28597	YES	YES
25	a	385.76	15.81145	YES	YES
26	a	395.20	0.70132	YES	YES
27	a	421.06	18.01500	YES	YES
28	a	432.96	5.92777	YES	YES
29	a	480.62	3.67693	YES	YES
30	a	488.46	9.66577	YES	YES
31	a	503.70	30.92937	YES	YES
32	a	566.52	0.94818	YES	YES
33	a	607.76	0.20035	YES	YES
34	a	622.13	8.35296	YES	YES
35	a	627.61	0.26013	YES	YES
36	a	682.30	3.27772	YES	YES
37	a	698.91	36.47011	YES	YES
38	a	736.77	22.23096	YES	YES
39	a	752.56	8.21784	YES	YES
40	a	790.92	71.63465	YES	YES
41	a	817.60	0.97977	YES	YES
42	a	835.72	0.41256	YES	YES
43	a	903.82	1.12480	YES	YES
44	a	957.19	0.54002	YES	YES
45	a	982.48	2.27337	YES	YES
46	a	985.09	8.82753	YES	YES
47	a	987.44	145.78461	YES	YES
48	a	1022.49	1.60674	YES	YES
49	a	1072.43	4.16028	YES	YES
50	a	1079.85	24.40550	YES	YES
51	a	1099.05	194.36722	YES	YES
52	a	1143.40	0.07736	YES	YES
53	a	1158.66	5.59585	YES	YES
54	a	1163.42	1.40165	YES	YES
55	a	1288.33	35.84153	YES	YES
56	a	1291.68	4.43757	YES	YES
57	a	1347.75	3.07779	YES	YES
58	a	1362.48	1.66469	YES	YES
59	a	1384.55	29.99692	YES	YES
60	a	1430.44	10.67474	YES	YES
61	a	1471.95	4.57679	YES	YES
62	a	1486.40	396.86941	YES	YES
63	a	1515.06	213.54415	YES	YES
64	a	1589.52	0.52817	YES	YES
65	a	1601.70	0.78501	YES	YES
66	a	1614.60	12.77237	YES	YES
67	a	1622.66	50.06897	YES	YES
68	a	3071.64	2.92299	YES	YES
69	a	3093.65	0.34226	YES	YES
70	a	3103.72	14.16686	YES	YES
71	a	3115.56	17.55188	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -738.3567708992 E_h
Symmetry = D_{3h}

XYZ Coordinates:

6

Sb	0.00000	0.00000	0.00000
F	0.00000	0.00000	1.85463
F	0.00000	0.00000	-1.85463
F	0.92197	-1.59690	0.00000
F	0.92197	1.59690	0.00000
F	-1.84394	0.00000	0.00000

34-F:SbF_6

(RI-)BP86/SV(P) level:
SCF Energy = -604.2814774278 E_h
Zero Point Energy = 0.0124628 E_h
Symmetry = O_h

XYZ Coordinates:
7

Sb	0.00000	0.00000	0.00000
F	0.00000	1.95611	0.00000
F	0.00000	-1.95611	0.00000
F	0.00000	0.00000	1.95611
F	0.00000	0.00000	-1.95611
F	1.95611	0.00000	0.00000
F	-1.95611	0.00000	0.00000

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.66	0.12888	YES	YES
8	a	30.57	0.12557	YES	YES
9	a	40.65	0.17456	YES	YES
10	a	88.17	0.03953	YES	YES
11	a	121.18	0.01303	YES	YES
12	a	132.90	0.28272	YES	YES
13	a	147.20	0.07963	YES	YES
14	a	161.90	1.11528	YES	YES
15	a	183.03	1.97686	YES	YES
16	a	201.20	0.25088	YES	YES
17	a	232.31	0.17361	YES	YES
18	a	262.57	0.07299	YES	YES
19	a	266.57	0.11650	YES	YES
20	a	301.12	1.67660	YES	YES
21	a	307.43	2.38793	YES	YES
22	a	328.94	7.37375	YES	YES
23	a	373.79	2.50256	YES	YES
24	a	384.03	7.28597	YES	YES
25	a	385.76	15.81145	YES	YES
26	a	395.20	0.70132	YES	YES
27	a	421.06	18.01500	YES	YES
28	a	432.96	5.92777	YES	YES
29	a	480.62	3.67693	YES	YES
30	a	488.46	9.66577	YES	YES
31	a	503.70	30.92937	YES	YES

32	a	566.52	0.94818	YES	YES
33	a	607.76	0.20035	YES	YES
34	a	622.13	8.35296	YES	YES
35	a	627.61	0.26013	YES	YES
36	a	682.30	3.27772	YES	YES
37	a	698.91	36.47011	YES	YES
38	a	736.77	22.23096	YES	YES
39	a	752.56	8.21784	YES	YES
40	a	790.92	71.63465	YES	YES
41	a	817.60	0.97977	YES	YES
42	a	835.72	0.41256	YES	YES
43	a	903.82	1.12480	YES	YES
44	a	957.19	0.54002	YES	YES
45	a	982.48	2.27337	YES	YES
46	a	985.09	8.82753	YES	YES
47	a	987.44	145.78461	YES	YES
48	a	1022.49	1.60674	YES	YES
49	a	1072.43	4.16028	YES	YES
50	a	1079.85	24.40550	YES	YES
51	a	1099.05	194.36722	YES	YES
52	a	1143.40	0.07736	YES	YES
53	a	1158.66	5.59585	YES	YES
54	a	1163.42	1.40165	YES	YES
55	a	1288.33	35.84153	YES	YES
56	a	1291.68	4.43757	YES	YES
57	a	1347.75	3.07779	YES	YES
58	a	1362.48	1.66469	YES	YES
59	a	1384.55	29.99692	YES	YES
60	a	1430.44	10.67474	YES	YES
61	a	1471.95	4.57679	YES	YES
62	a	1486.40	396.86941	YES	YES
63	a	1515.06	213.54415	YES	YES
64	a	1589.52	0.52817	YES	YES
65	a	1601.70	0.78501	YES	YES
66	a	1614.60	12.77237	YES	YES
67	a	1622.66	50.06897	YES	YES
68	a	3071.64	2.92299	YES	YES
69	a	3093.65	0.34226	YES	YES
70	a	3103.72	14.16686	YES	YES
71	a	3115.56	17.55188	YES	YES

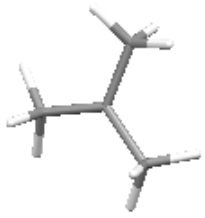
(RI-)MP2/def2-TZVPP level

SCF Energy = -838.2790139547 E_h
Symmetry = O_h

XYZ Coordinates:
7

Sb	0.00000	0.00000	0.00000
F	0.00000	1.88794	0.00000
F	0.00000	-1.88794	0.00000
F	0.00000	0.00000	1.88794
F	0.00000	0.00000	-1.88794
F	1.88794	0.00000	0.00000
F	-1.88794	0.00000	0.00000

35: $[C(CH_3)_3]^+$



(RI-)BP86/SV(P) level:

SCF Energy = -157.4126270447 E_h
Zero Point Energy = 0.1125788 E_h
Symmetry = C_1

XYZ Coordinates:
13

C	0.00088	0.00131	0.00465
C	-1.44473	-0.25018	-0.00958
H	-1.80288	0.00132	1.02870
H	-1.73346	-1.29804	-0.22782
H	-1.98867	0.48013	-0.65370
C	0.93948	-1.12809	0.00513
C	0.50487	1.37952	0.00593
H	0.60867	-1.91420	0.72768
H	1.34067	1.50561	0.73500
H	2.00082	-0.85395	0.16493
H	-0.27333	2.15865	0.12945
H	0.83421	-1.64365	-0.98815
H	1.00803	1.53359	-0.98912

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a	52.25	3.37204	YES YES
8		a	62.01	1.60483	YES YES
9		a	180.47	17.14319	YES YES
10		a	402.06	0.51145	YES YES
11		a	404.01	0.50696	YES YES
12		a	447.22	2.83071	YES YES
13		a	739.84	3.69086	YES YES
14		a	757.66	5.46120	YES YES
15		a	817.70	1.30369	YES YES
16		a	949.16	9.83394	YES YES
17		a	960.51	14.98237	YES YES
18		a	965.91	19.76635	YES YES
19		a	1068.40	43.33553	YES YES
20		a	1240.65	148.20902	YES YES
21		a	1243.50	116.67886	YES YES
22		a	1271.64	1.23740	YES YES
23		a	1300.94	86.08384	YES YES
24		a	1309.93	85.86253	YES YES
25		a	1346.87	3.06878	YES YES
26		a	1357.59	1.06744	YES YES
27		a	1379.25	53.29733	YES YES
28		a	1436.77	1.46522	YES YES
29		a	1453.20	37.25682	YES YES
30		a	1457.25	35.36943	YES YES
31		a	2868.91	117.74263	YES YES
32		a	2877.64	84.28624	YES YES
33		a	2893.34	29.20329	YES YES
34		a	2963.18	21.64613	YES YES
35		a	2973.98	22.67130	YES YES
36		a	2979.38	17.20698	YES YES
37		a	3081.87	6.77553	YES YES
38		a	3085.00	4.78460	YES YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -157.1658146287 E_h
Symmetry = C_1

XYZ Coordinates:
13

C	0.00340	0.00156	0.01580
C	-1.44569	-0.09036	-0.01389
H	-1.69128	-0.04080	1.06458

H	-1.82106	-1.04062	-0.38078
H	-1.92347	0.77343	-0.46868
C	0.80115	-1.21603	0.00842
C	0.64446	1.30715	0.00908
H	0.28471	-2.04808	0.48377
H	1.59997	1.32027	0.52508
H	1.81637	-1.08545	0.36525
H	-0.01730	2.11533	0.30553
H	0.84431	-1.48088	-1.06296
H	0.86823	1.45918	-1.06320

35-F:C(CH$_3$)$_3$F

(RI-)BP86/SV(P) level:

SCF Energy = -257.4901658364 E_h
Zero Point Energy = 0.1195764 E_h
Symmetry = C_{3V}

XYZ Coordinates:
14

C	0.00000	0.00000	-0.08027
C	-0.73409	1.27149	-0.52010
C	-0.73409	-1.27149	-0.52010
C	1.46819	0.00000	-0.52010
H	-0.21463	2.17220	-0.12664
H	-1.77387	-1.27197	-0.12664
H	1.98849	-0.90023	-0.12664
H	-1.77387	1.27197	-0.12664
H	-0.21463	-2.17220	-0.12664
H	1.98849	0.90023	-0.12664
H	-0.77725	1.34623	-1.62872
H	-0.77725	-1.34623	-1.62872
H	1.55449	0.00000	-1.62872
F	0.00000	0.00000	1.33675

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	52.25	3.37204	YES YES
8	a	62.01	1.60483	YES YES
9	a	180.47	17.14319	YES YES
10	a	402.06	0.51145	YES YES
11	a	404.01	0.50696	YES YES
12	a	447.22	2.83071	YES YES
13	a	739.84	3.69086	YES YES
14	a	757.66	5.46120	YES YES
15	a	817.70	1.30369	YES YES
16	a	949.16	9.83394	YES YES
17	a	960.51	14.98237	YES YES
18	a	965.91	19.76635	YES YES
19	a	1068.40	43.33553	YES YES
20	a	1240.65	148.20902	YES YES
21	a	1243.50	116.67886	YES YES
22	a	1271.64	1.23740	YES YES
23	a	1300.94	86.08384	YES YES
24	a	1309.93	85.86253	YES YES
25	a	1346.87	3.06878	YES YES
26	a	1357.59	1.06744	YES YES
27	a	1379.25	53.29733	YES YES
28	a	1436.77	1.46522	YES YES
29	a	1453.20	37.25682	YES YES
30	a	1457.25	35.36943	YES YES
31	a	2868.91	117.74263	YES YES
32	a	2877.64	84.28624	YES YES
33	a	2893.34	29.20329	YES YES
34	a	2963.18	21.64613	YES YES
35	a	2973.98	22.67130	YES YES
36	a	2979.38	17.20698	YES YES
37	a	3081.87	6.77553	YES YES
38	a	3085.00	4.78460	YES YES

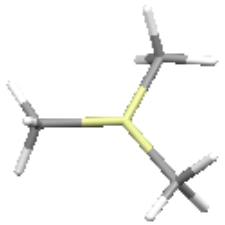
(RI-)MP2/def2-TZVPP level

SCF Energy = -257.2214767613 E_h
Symmetry = C_{3V}

XYZ Coordinates:
14

C	0.00000	0.00000	-0.07914
C	-0.72464	1.25511	-0.51734
C	-0.72464	-1.25511	-0.51734
C	1.44928	0.00000	-0.51734
H	-0.21199	2.13624	-0.13689
H	-1.74405	-1.25171	-0.13689
H	1.95603	-0.88453	-0.13689
H	-1.74405	1.25171	-0.13689
H	-0.21199	-2.13624	-0.13689
H	1.95603	0.88453	-0.13689
H	-0.75754	1.31211	-1.60419
H	-0.75754	-1.31211	-1.60419
H	1.51509	0.00000	-1.60419
F	0.00000	0.00000	1.33016

36: [Si(Me)$_3$]$^+$



(RI-)BP86/SV(P) level:
SCF Energy = -408.8074319901 E_h
Zero Point Energy = 0.1053006 E_h
Symmetry = C_3

XYZ Coordinates:
13

Si	0.00000	0.00000	-0.02283
C	-1.61259	-0.90014	0.00853
H	-2.08844	-0.74616	1.00948
H	-1.50661	-1.99203	-0.16439
H	-2.32324	-0.46845	-0.73474
C	1.58584	-0.94648	0.00853
C	0.02675	1.84662	0.00853
H	1.69041	-1.43557	1.00948
H	0.39803	2.18172	1.00948
H	2.47845	-0.30875	-0.16439
H	-0.97184	2.30077	-0.16439
H	1.56731	-1.77776	-0.73474
H	0.75592	2.24621	-0.73474

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	52.25	3.37204	YES YES
8	a	62.01	1.60483	YES YES
9	a	180.47	17.14319	YES YES
10	a	402.06	0.51145	YES YES
11	a	404.01	0.50696	YES YES
12	a	447.22	2.83071	YES YES
13	a	739.84	3.69086	YES YES
14	a	757.66	5.46120	YES YES
15	a	817.70	1.30369	YES YES
16	a	949.16	9.83394	YES YES
17	a	960.51	14.98237	YES YES
18	a	965.91	19.76635	YES YES
19	a	1068.40	43.33553	YES YES
20	a	1240.65	148.20902	YES YES
21	a	1243.50	116.67886	YES YES
22	a	1271.64	1.23740	YES YES
23	a	1300.94	86.08384	YES YES
24	a	1309.93	85.86253	YES YES
25	a	1346.87	3.06878	YES YES
26	a	1357.59	1.06744	YES YES
27	a	1379.25	53.29733	YES YES
28	a	1436.77	1.46522	YES YES
29	a	1453.20	37.25682	YES YES
30	a	1457.25	35.36943	YES YES
31	a	2868.91	117.74263	YES YES
32	a	2877.64	84.28624	YES YES
33	a	2893.34	29.20329	YES YES
34	a	2963.18	21.64613	YES YES
35	a	2973.98	22.67130	YES YES
36	a	2979.38	17.20698	YES YES
37	a	3081.87	6.77553	YES YES
38	a	3085.00	4.78460	YES YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -408.2381403124 E_h
Symmetry = C_3

XYZ Coordinates:
13

Si	0.00000	0.00000	-0.00048
C	-1.60871	-0.86009	0.00018
H	-2.18135	-0.54588	0.87701
H	-1.51242	-1.94219	-0.00277
H	-2.18576	-0.54102	-0.87189
C	1.54922	-0.96314	0.00018
C	0.05950	1.82323	0.00018
H	1.56342	-1.61617	0.87701
H	0.61793	2.16204	0.87701
H	2.43820	-0.33870	-0.00277
H	-0.92578	2.28089	-0.00277
H	1.56142	-1.62242	-0.87189
H	0.62434	2.16344	-0.87189

36-F:Si(Me)$_3$F

(RI-)BP86/SV(P) level:
SCF Energy = -508.9275499978 E_h
Zero Point Energy = 0.1099442 E_h
Symmetry = C_{3V}

XYZ Coordinates:
14

F	0.00000	0.00000	1.59619
Si	0.00000	0.00000	-0.05953
C	0.90154	-1.56152	-0.61158
C	0.90154	1.56152	-0.61158
C	-1.80308	0.00000	-0.61158
H	0.94170	-1.63108	-1.72225
H	0.39081	-2.47475	-0.23276
H	1.94779	-1.57582	-0.23276
H	0.94170	1.63108	-1.72225
H	1.94779	1.57582	-0.23276
H	0.39081	2.47475	-0.23276
H	-1.88340	0.00000	-1.72225
H	-2.33860	0.89892	-0.23276
H	-2.33860	-0.89892	-0.23276

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	52.25	3.37204	YES YES
8	a	62.01	1.60483	YES YES
9	a	180.47	17.14319	YES YES
10	a	402.06	0.51145	YES YES
11	a	404.01	0.50696	YES YES
12	a	447.22	2.83071	YES YES
13	a	739.84	3.69086	YES YES
14	a	757.66	5.46120	YES YES
15	a	817.70	1.30369	YES YES
16	a	949.16	9.83394	YES YES
17	a	960.51	14.98237	YES YES
18	a	965.91	19.76635	YES YES
19	a	1068.40	43.33553	YES YES
20	a	1240.65	148.20902	YES YES
21	a	1243.50	116.67886	YES YES
22	a	1271.64	1.23740	YES YES
23	a	1300.94	86.08384	YES YES
24	a	1309.93	85.86253	YES YES
25	a	1346.87	3.06878	YES YES
26	a	1357.59	1.06744	YES YES
27	a	1379.25	53.29733	YES YES
28	a	1436.77	1.46522	YES YES
29	a	1453.20	37.25682	YES YES
30	a	1457.25	35.36943	YES YES
31	a	2868.91	117.74263	YES YES

32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -508.3395592834 E_h
Symmetry = C_{3V}

XYZ Coordinates:
14

F	0.00000	0.00000	1.56705
Si	0.00000	0.00000	-0.04833
C	0.88811	-1.53825	-0.60615
C	0.88811	1.53825	-0.60615
C	-1.77622	0.00000	-0.60615
H	0.91938	-1.59241	-1.69435
H	0.38662	-2.43298	-0.23960
H	1.91372	-1.55131	-0.23960
H	0.91938	1.59241	-1.69435
H	1.91372	1.55131	-0.23960
H	0.38662	2.43298	-0.23960
H	-1.83876	0.00000	-1.69435
H	-2.30033	0.88167	-0.23960
H	-2.30033	-0.88167	-0.23960

37: $[(CF_3)(CF_2)PF]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -1015.7175795720 E_h
Zero Point Energy = 0.0282816 E_h
Symmetry = C_1

XYZ Coordinates:
9

C	0.02991	-0.32500	-1.52595
P	0.80614	0.66738	-0.18119
F	-0.06984	1.99720	-0.33191
C	-0.12220	-0.26392	1.33748
F	0.43156	0.18110	2.44740
F	0.10207	-1.56539	1.17204
F	-1.41316	0.01705	1.30172
F	-0.63907	0.20453	-2.46915
F	0.33250	-1.55022	-1.70554

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	36.66	0.08842	YES YES
8	a	70.03	0.53354	YES YES
9	a	98.00	1.37631	YES YES
10	a	147.86	4.36349	YES YES
11	a	163.94	3.89136	YES YES
12	a	239.34	0.19383	YES YES
13	a	254.40	3.48884	YES YES
14	a	335.18	7.77233	YES YES
15	a	359.09	0.42108	YES YES
16	a	421.20	0.71656	YES YES
17	a	514.95	4.01052	YES YES
18	a	533.88	1.57125	YES YES
19	a	610.50	14.14997	YES YES
20	a	700.25	31.84341	YES YES
21	a	728.22	80.52606	YES YES
22	a	891.31	82.88785	YES YES
23	a	1014.63	512.47368	YES YES
24	a	1243.06	203.27620	YES YES
25	a	1270.01	272.23832	YES YES
26	a	1338.34	373.70894	YES YES

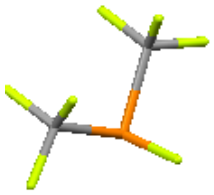
(RI-)MP2/def2-TZVPP level

SCF Energy = -1014.9832974974 E_h
Symmetry = C_1

XYZ Coordinates:
9

C	0.06714	-0.29428	-1.45290
P	0.83798	0.73946	-0.11376
F	-0.09641	1.97722	-0.26752
C	-0.11742	-0.27640	1.22121
F	0.10718	0.29154	2.38470
F	0.37765	-1.50740	1.19750
F	-1.42049	-0.30680	0.97941
F	-0.70302	0.18558	-2.31304
F	0.40067	-1.48492	-1.64910

37-F: $(CF_3)_2PF$



(RI-)BP86/SV(P) level:
SCF Energy = -1115.8515115770 E_h
Zero Point Energy = 0.0312480 E_h
Symmetry = C_1

XYZ Coordinates:
10

C	1.43464	-0.00516	0.24330
F	2.56614	0.10924	-0.48532
F	1.58374	0.70281	1.38457
F	1.27756	-1.30170	0.56083
P	0.00009	0.78742	-0.76377
C	-1.43846	-0.00506	0.24180
F	-1.48730	-1.34331	0.16756
F	-2.60710	0.48089	-0.22972
F	-1.32150	0.36114	1.53824
F	-0.00926	-0.28636	-1.99765

Vibrational Spectrum:

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -

6		0.00	0.00000	-	-
7	a	22.03	0.03297	YES	YES
8	a	54.03	0.12061	YES	YES
9	a	108.47	0.65451	YES	YES
10	a	143.10	1.87741	YES	YES
11	a	161.89	3.23946	YES	YES
12	a	220.77	0.84890	YES	YES
13	a	258.07	0.23833	YES	YES
14	a	261.93	0.25719	YES	YES
15	a	331.59	0.65752	YES	YES
16	a	431.69	25.51929	YES	YES
17	a	435.65	24.98526	YES	YES
18	a	505.39	1.25012	YES	YES
19	a	523.48	2.22561	YES	YES
20	a	528.83	0.84803	YES	YES
21	a	549.42	11.99635	YES	YES
22	a	726.13	1.43402	YES	YES
23	a	729.50	5.41704	YES	YES
24	a	820.34	66.34508	YES	YES
25	a	1102.54	231.73283	YES	YES
26	a	1125.45	315.13040	YES	YES
27	a	1148.81	88.79335	YES	YES
28	a	1154.27	19.36874	YES	YES
29	a	1170.73	346.92142	YES	YES

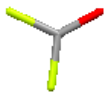
(RI-)MP2/def2-TZVPP level

SCF Energy = -1115.0955817761 E_h
Symmetry = C_1

XYZ Coordinates:
10

C	1.41607	-0.00349	0.23821
F	2.55596	0.24002	-0.42752
F	1.49140	0.60535	1.42867
F	1.34131	-1.31735	0.43902
P	0.00001	0.75814	-0.75594
C	-1.41768	-0.00315	0.23725
F	-1.40789	-1.33159	0.31399
F	-2.57042	0.35919	-0.34766
F	-1.40763	0.49799	1.47937
F	-0.00174	-0.28543	-1.95402

$[COF_2]^+$



(RI-)BP86/SV(P) level:
SCF Energy = -312.8030187593 E_h
Zero Point Energy = 0.0137944 E_h
Symmetry = C_{2V}

XYZ Coordinates:
4

C	0.00000	0.00000	0.16395
F	1.07247	0.00000	-0.61974
F	-1.07247	0.00000	-0.61974
O	0.00000	0.00000	1.34874

Vibrational Spectrum:

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm**(-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7	a		52.25	3.37204	YES YES
8	a		62.01	1.60483	YES YES
9	a		180.47	17.14319	YES YES
10	a		402.06	0.51145	YES YES
11	a		404.01	0.50696	YES YES
12	a		447.22	2.83071	YES YES
13	a		739.84	3.69086	YES YES
14	a		757.66	5.46120	YES YES
15	a		817.70	1.30369	YES YES
16	a		949.16	9.83394	YES YES
17	a		960.51	14.98237	YES YES
18	a		965.91	19.76635	YES YES
19	a		1068.40	43.33553	YES YES
20	a		1240.65	148.20902	YES YES
21	a		1243.50	116.67886	YES YES
22	a		1271.64	1.23740	YES YES
23	a		1300.94	86.08384	YES YES
24	a		1309.93	85.86253	YES YES
25	a		1346.87	3.06878	YES YES
26	a		1357.59	1.06744	YES YES
27	a		1379.25	53.29733	YES YES
28	a		1436.77	1.46522	YES YES
29	a		1453.20	37.25682	YES YES
30	a		1457.25	35.36943	YES YES
31	a		2868.91	117.74263	YES YES
32	a		2877.64	84.28624	YES YES
33	a		2893.34	29.20329	YES YES
34	a		2963.18	21.64613	YES YES
35	a		2973.98	22.67130	YES YES
36	a		2979.38	17.20698	YES YES
37	a		3081.87	6.77553	YES YES
38	a		3085.00	4.78460	YES YES

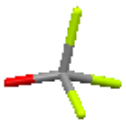
(RI-)MP2/def2-TZVPP level

SCF Energy = -312.6254592807 E_h
Symmetry = C_{2V}

XYZ Coordinates:
4

C	0.00000	0.00000	0.16208
F	1.06123	0.00000	-0.61476
F	-1.06123	0.00000	-0.61476
O	0.00000	0.00000	1.33831

COF_3



(RI-)BP86/SV(P) level:
SCF Energy = -412.6372750843 E_h
Zero Point Energy = 0.0154251 E_h
Symmetry = C_{3V}

XYZ Coordinates:

5

C	0.00000	0.00000	0.21333
F	1.28535	0.00000	-0.44824
F	-0.64267	1.11314	-0.44824
F	-0.64267	-1.11314	-0.44824
O	0.00000	0.00000	1.43663

Vibrational Spectrum:
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	52.25	3.37204	YES	YES
8	a	62.01	1.60483	YES	YES
9	a	180.47	17.14319	YES	YES
10	a	402.06	0.51145	YES	YES
11	a	404.01	0.50696	YES	YES
12	a	447.22	2.83071	YES	YES
13	a	739.84	3.69086	YES	YES
14	a	757.66	5.46120	YES	YES
15	a	817.70	1.30369	YES	YES
16	a	949.16	9.83394	YES	YES
17	a	960.51	14.98237	YES	YES
18	a	965.91	19.76635	YES	YES
19	a	1068.40	43.33553	YES	YES
20	a	1240.65	148.20902	YES	YES
21	a	1243.50	116.67886	YES	YES
22	a	1271.64	1.23740	YES	YES
23	a	1300.94	86.08384	YES	YES
24	a	1309.93	85.86253	YES	YES
25	a	1346.87	3.06878	YES	YES
26	a	1357.59	1.06744	YES	YES
27	a	1379.25	53.29733	YES	YES
28	a	1436.77	1.46522	YES	YES
29	a	1453.20	37.25682	YES	YES
30	a	1457.25	35.36943	YES	YES
31	a	2868.91	117.74263	YES	YES
32	a	2877.64	84.28624	YES	YES
33	a	2893.34	29.20329	YES	YES
34	a	2963.18	21.64613	YES	YES
35	a	2973.98	22.67130	YES	YES
36	a	2979.38	17.20698	YES	YES
37	a	3081.87	6.77553	YES	YES
38	a	3085.00	4.78460	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -412.4365159328 E_h
Symmetry = C_{3V}

XYZ Coordinates:
5

C	0.00000	0.00000	0.20666
F	0.63363	-1.09748	-0.44317
F	0.63363	1.09748	-0.44317
F	-1.26726	0.00000	-0.44317
O	0.00000	0.00000	1.42356

$[AsF_5]^+$

(RI-)BP86/SV(P) level:
SCF Energy = -2734.7773957770 E_h
Zero Point Energy = 0.0125995 E_h
Symmetry = D_{3h}

6

As	0.00000	0.00000	0.00000
F	0.00000	0.00000	1.73686
F	0.00000	0.00000	-1.73686
F	0.86033	-1.49013	0.00000
F	0.86033	1.49013	0.00000
F	-1.72065	0.00000	0.00000

$vibrational spectrum
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e'	114.74	0.70052	YES	YES
8	e'	114.74	0.70052	YES	YES
9	e'	338.11	38.32414	YES	YES
10	e'	338.11	38.32414	YES	YES
11	e"	351.13	0.00000	NO	YES
12	e"	351.13	0.00000	NO	YES
13	a2"	371.51	47.63066	YES	NO
14	a1'	622.65	0.00000	NO	YES
15	a1'	666.88	0.00000	NO	YES
16	a2"	748.96	131.37321	YES	NO
17	e'	756.28	103.10726	YES	YES
18	e'	756.28	103.10726	YES	YES

(RI-)MP2/def2-TZVPP level

SCF Energy = -2733.2170817481 E_h
Symmetry = D_{3h}

6

As	0.00000	0.00000	0.00000
F	0.00000	0.00000	1.69929
F	0.00000	0.00000	-1.69929
F	0.83800	-1.45146	0.00000
F	0.83800	1.45146	0.00000
F	-1.67600	0.00000	0.00000

AsF_6

(RI-)BP86/SV(P) level:
SCF Energy = -2834.6943201650 E_h
Zero Point Energy = 0.0149517 E_h
Symmetry = O_h

7

As	0.00000	0.00000	0.00000
F	0.00000	1.77423	0.00000
F	0.00000	-1.77423	0.00000
F	0.00000	0.00000	1.77423
F	0.00000	0.00000	-1.77423
F	1.77423	0.00000	0.00000
F	-1.77423	0.00000	0.00000

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	t2u	214.13	0.00000	NO NO
8	t2u	214.13	0.00000	NO NO
9	t2u	214.13	0.00000	NO NO
10	t2g	331.95	0.00000	NO YES
11	t2g	331.95	0.00000	NO YES
12	t2g	331.95	0.00000	NO YES
13	t1u	373.80	48.80967	YES NO
14	t1u	373.80	48.80967	YES NO
15	t1u	373.80	48.80967	YES NO
16	eg	563.53	0.00000	NO YES
17	eg	563.53	0.00000	NO YES
18	a1g	623.92	0.00000	NO YES
19	t1u	684.14	174.15408	YES NO
20	t1u	684.14	174.15408	YES NO
21	t1u	684.14	174.15408	YES NO

(RI-)MP2/def2-TZVPP level

SCF Energy = -2833.1171319602 E_h
Symmetry = O_h

7

As	0.00000	0.00000	0.00000
F	0.00000	1.73422	0.00000
F	0.00000	-1.73422	0.00000
F	0.00000	0.00000	1.73422
F	0.00000	0.00000	-1.73422
F	1.73422	0.00000	0.00000
F	-1.73422	0.00000	0.00000