Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

A simple model for calculating atomic charges in molecules

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Atomic charges in a.u.

Keywords:
File TZVPMol001.out
Molecule PMol001 fulvene
 SP Mol001 B3LYP/Def2TZVP VAC.
  0 16
Dipole 0.0000 0.0000 -0.6984 0.6984
Quadrupole -0.2265 0.8549 -0.6284 0.8224 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.7626	-1.4095	-0.1684	-0.2492	-0.0493	-0.1546	-0.1584	-0.0336	-0.3840	0.0341	-0.1480
6	0.0000	-0.7626	-1.4095	-0.1684	-0.2492	-0.0493	-0.1546	-0.1584	-0.0237	-0.3840	0.0342	-0.1480
6	-0.5190	-1.1076	-0.0154	-0.1640	-0.2106	-0.0503	-0.2317	-0.1541	-0.1079	-0.4362	0.0257	-0.1511
6	0.0000	0.0000	0.8704	0.0301	-0.1941	0.0089	0.1989	-0.0140	0.2467	0.0266	-0.0388	0.0469
6	0.5190	1.1076	-0.0154	-0.1640	-0.2106	-0.0503	-0.2317	-0.1541	-0.1242	-0.4362	0.0252	-0.1511
1	0.5920	1.1996	-2.2124	0.0944	0.1271	0.0289	0.0842	0.0833	0.0145	0.2044	-0.0078	0.0793
1	-1.0222	1.1306	-1.5298	0.0820	0.1334	0.0272	0.0841	0.0829	0.0339	0.1902	-0.0151	0.0741
1	1.0222	-1.1306	-1.5298	0.0820	0.1334	0.0272	0.0841	0.0829	0.0312	0.1902	-0.0151	0.0741
1	-0.5920	-1.1996	-2.2124	0.0944	0.1271	0.0289	0.0842	0.0833	0.0105	0.2044	-0.0078	0.0793
1	-1.6133	-1.0870	-0.0141	0.0918	0.1437	0.0324	0.0976	0.0882	0.0540	0.2084	0.0015	0.0768
1	-0.2318	-2.0988	0.3346	0.1031	0.1364	0.0337	0.0993	0.0888	0.0436	0.2155	0.0053	0.0808
1	0.2318	2.0988	0.3346	0.1031	0.1364	0.0337	0.0993	0.0888	0.0493	0.2155	0.0053	0.0808
1	1.6133	1.0870	-0.0141	0.0918	0.1437	0.0324	0.0976	0.0882	0.0583	0.2084	0.0015	0.0768
6	0.0000	0.0000	2.1976	-0.3119	-0.2063	-0.1124	-0.3808	-0.2121	-0.6693	-0.4030	-0.0846	-0.2230
1	0.3730	0.8416	2.7677	0.1020	0.1194	0.0291	0.1120	0.0824	0.2089	0.1899	0.0177	0.0762
1	-0.3730	-0.8416	2.7677	0.1020	0.1194	0.0291	0.1120	0.0824	0.2080	0.1899	0.0177	0.0762

Dipole mement (in D)	0.70 (DEN)	1.04	0.65	0.61	0.80	0.65	0.69	0.30	0.65	0.63		

File TZVPMol002.out
Molecule PMol002 propane
 SP Mol002 B3LYP/Def2TZVP VAC.
  0 11
Dipole 0.0000 0.0000 0.0904 0.0904
Quadrupole 0.4407 -0.4067 -0.0340 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	1.2624	-0.2572	-0.3206	-0.3136	-0.0850	-0.3238	-0.2368	-0.2849	-0.5865	0.0130	-0.2480
1	0.0000	2.1638	0.3545	0.1072	0.1153	0.0281	0.0959	0.0793	0.0525	0.2016	-0.0072	0.0814
1	-0.8769	1.3070	-0.9046	0.0986	0.1155	0.0266	0.0969	0.0783	0.0604	0.1937	-0.0102	0.0785
1	0.8769	1.3070	-0.9046	0.0986	0.1155	0.0266	0.0969	0.0783	0.0611	0.1937	-0.0102	0.0785
6	0.0000	0.0000	0.5840	-0.1336	-0.3226	-0.0439	-0.0907	-0.1587	0.3457	-0.3824	0.0636	-0.1318
1	-0.8696	0.0000	1.2458	0.0830	0.1286	0.0258	0.0795	0.0803	-0.0618	0.1887	-0.0173	0.0756
1	0.8696	0.0000	1.2458	0.0830	0.1286	0.0258	0.0795	0.0803	-0.0621	0.1887	-0.0173	0.0756
6	0.0000	-1.2624	-0.2572	-0.3206	-0.3136	-0.0850	-0.3238	-0.2368	-0.2849	-0.5865	0.0132	-0.2480
1	0.0000	-2.1638	0.3545	0.1072	0.1153	0.0281	0.0959	0.0793	0.0525	0.2016	-0.0072	0.0814
1	-0.8769	-1.3070	-0.9046	0.0986	0.1155	0.0266	0.0969	0.0783	0.0604	0.1937	-0.0102	0.0785
1	0.8769	-1.3070	-0.9046	0.0986	0.1155	0.0266	0.0969	0.0783	0.0611	0.1937	-0.0102	0.0785

Dipole mement (in D) 0.09 (DEN) 0.06 0.21 0.03 0.14 0.01 0.05 0.05 0.09 0.06

File TZVPMol003.out
Molecule PMol003 isobutane
SP Mol003 B3LYP/Def2TZVP VAC.
0 14
Dipole 0.1111 0.0723 0.0000 0.1326
Quadrupole 0.2387 -0.0236 -0.2150 0.2945 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.8673	1.1618	0.0000	-0.3269	-0.2869	-0.0860	-0.3587	-0.2359	-0.4843	-0.5845	0.0077	-0.2519
6	0.3147	0.2044	0.0000	0.0064	-0.3418	-0.0090	0.1035	-0.0856	0.5839	-0.2116	0.0896	-0.0217
1	1.2336	0.8012	0.0000	0.0581	0.1443	0.0255	0.0689	0.0835	-0.0728	0.1820	-0.0227	0.0718
1	-0.8671	1.8051	0.8802	0.1046	0.1174	0.0272	0.0998	0.0791	0.1015	0.2005	-0.0093	0.0793
1	-0.8671	1.8051	-0.8802	0.1046	0.1174	0.0272	0.0998	0.0791	0.1015	0.2005	-0.0093	0.0793
1	-1.8111	0.6117	0.0000	0.0962	0.1180	0.0260	0.1016	0.0784	0.1061	0.1933	-0.0113	0.0766
6	0.3147	-0.6581	-1.2529	-0.3268	-0.2869	-0.0859	-0.3586	-0.2358	-0.4560	-0.5844	0.0078	-0.2519
6	0.3147	-0.6581	1.2529	-0.3268	-0.2869	-0.0859	-0.3586	-0.2358	-0.4560	-0.5844	0.0077	-0.2519
1	1.1707	-1.3328	-1.2798	0.1046	0.1174	0.0272	0.0998	0.0791	0.0925	0.2005	-0.0093	0.0793
1	-0.5861	-1.2744	-1.2987	0.0962	0.1180	0.0260	0.1016	0.0784	0.1021	0.1933	-0.0113	0.0766
1	0.3407	-0.0541	-2.1601	0.1046	0.1174	0.0272	0.0998	0.0791	0.0934	0.2005	-0.0093	0.0793
1	-0.5861	-1.2744	1.2987	0.0962	0.1180	0.0260	0.1016	0.0784	0.1021	0.1933	-0.0113	0.0766
1	1.1707	-1.3328	1.2798	0.1046	0.1174	0.0272	0.0998	0.0791	0.0925	0.2005	-0.0093	0.0793
1	0.3407	-0.0541	2.1601	0.1046	0.1174	0.0272	0.0998	0.0791	0.0934	0.2005	-0.0093	0.0793

Dipole mement (in D) 0.13 (DEN) 0.00 0.36 0.04 0.16 0.00 0.11 0.12 0.12 0.09

File TZVPMol004.out
Molecule PMol004 cyclopropene
SP Mol004 B3LYP/Def2TZVP VAC.
0 7
Dipole 0.0000 0.0000 -0.4810 0.4810
Quadrupole -1.1348 1.5254 -0.3906 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6434	-0.4958	-0.1150	-0.1092	-0.0440	-0.1104	-0.1016	-0.1649	-0.1764	-0.1315	-0.0862
6	0.0000	-0.6434	-0.4958	-0.1150	-0.1092	-0.0440	-0.1104	-0.1016	-0.1649	-0.1764	-0.1313	-0.0862
6	0.0000	0.0000	0.8513	-0.2442	-0.2463	-0.0794	-0.2043	-0.1784	-0.0868	-0.4193	0.0621	-0.1802
1	-0.9092	0.0000	1.4514	0.0897	0.1088	0.0176	0.0706	0.0709	0.0506	0.1693	-0.0029	0.0628
1	0.9092	0.0000	1.4514	0.0897	0.1088	0.0176	0.0706	0.0709	0.0472	0.1693	-0.0029	0.0628
1	0.0000	1.5765	-1.0304	0.1473	0.1236	0.0662	0.1420	0.1198	0.1594	0.2167	0.1030	0.1135
1	0.0000	-1.5765	-1.0304	0.1473	0.1236	0.0662	0.1420	0.1198	0.1594	0.2167	0.1030	0.1135

Dipole mement (in D) 0.48 (DEN) 0.66 0.19 0.52 0.73 0.44 0.47 0.66 0.18 0.57

File TZVPMol005.out

Molecule PMol005 propene
 SP Mol005 B3LYP/Def2TZVP VAC.
  0 9
Dipole 0.4095 -0.0770 0.0000 0.4167
Quadrupole 0.7457 1.0481 -1.7939 -0.1460 0.0000 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2745	0.2181	-0.0000	-0.2655	-0.2235	-0.0956	-0.2999	-0.1984	-0.5656	-0.3968	-0.0766	-0.2001
1	-2.2319	-0.2851	-0.0000	0.1089	0.1184	0.0336	0.1068	0.0864	0.1900	0.1937	0.0262	0.0821
1	-1.2977	1.3021	0.0000	0.1018	0.1174	0.0320	0.1082	0.0851	0.2115	0.1825	0.0200	0.0794
6	-0.1302	-0.4516	0.0000	-0.0755	-0.2292	-0.0293	0.0295	-0.0957	0.0799	-0.1658	-0.0315	-0.0562
1	-0.1624	-1.5383	0.0000	0.0989	0.1360	0.0352	0.0835	0.0906	0.0809	0.1876	0.0165	0.0806
6	1.2237	0.1618	-0.0000	-0.2988	-0.2920	-0.0823	-0.3637	-0.2294	-0.2363	-0.6300	0.0177	-0.2442
1	1.1747	1.2496	-0.0000	0.1041	0.1228	0.0350	0.1136	0.0874	0.0895	0.2051	0.0073	0.0859
1	1.8018	-0.1491	0.8722	0.1131	0.1250	0.0356	0.1110	0.0870	0.0751	0.2118	0.0099	0.0862
1	1.8018	-0.1492	-0.8722	0.1131	0.1250	0.0356	0.1110	0.0870	0.0751	0.2118	0.0100	0.0863

Dipole mement (in D)	0.42 (DEN)	0.59	0.57	0.35	0.42	0.40	0.41	0.32	0.39	0.38	

File TZVPMol006.out
Molecule PMol006 propyne
 SP Mol006 B3LYP/Def2TZVP VAC.
  0 7
Dipole 0.0000 0.0000 -0.8251 0.8251
Quadrupole -1.8588 -1.8588 3.7176 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	1.4149	-0.1345	-0.1181	-0.1288	-0.3502	-0.1809	-0.5920	-0.2535	-0.1452	-0.1854
6	0.0000	0.0000	0.2144	-0.0727	-0.1462	-0.0463	0.1105	-0.0607	0.2113	-0.0014	-0.2187	-0.0230
6	0.0000	0.0000	-1.2293	-0.3961	-0.2771	-0.0594	-0.3734	-0.2028	-0.3536	-0.6704	0.0843	-0.2197
1	0.0000	1.0153	-1.6253	0.1406	0.1395	0.0512	0.1363	0.1032	0.1319	0.2319	0.0415	0.1005
1	-0.8793	-0.5077	-1.6253	0.1406	0.1395	0.0512	0.1363	0.1032	0.1326	0.2319	0.0415	0.1005
1	0.8793	-0.5077	-1.6253	0.1406	0.1395	0.0512	0.1363	0.1032	0.1329	0.2319	0.0415	0.1005
1	0.0000	0.0000	2.4762	0.1815	0.1230	0.0807	0.2042	0.1347	0.3369	0.2297	0.1552	0.1265

Dipole mement (in D)	0.83 (DEN)	0.21	1.12	0.81	0.82	0.91	0.81	0.46	0.84	0.84	

File TZVPMol007.out
Molecule PMol007 1,3-pentadiyne
 SP Mol007 B3LYP/Def2TZVP VAC.
  0 9
Dipole 0.0001 0.0000 -1.3443 1.3443
Quadrupole -4.2566 -4.2567 8.5134 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-1.0583	-0.0681	-0.0513	-0.0143	0.0928	-0.0262	0.1761	0.0944	-0.1412	-0.0026
6	0.0000	0.0000	0.1512	0.0294	-0.0736	-0.0576	-0.1204	-0.0584	-0.3172	-0.1106	-0.0539	-0.0560
6	0.0000	0.0000	1.5071	-0.0173	-0.1041	-0.0401	0.0631	-0.0427	0.2749	-0.0782	-0.0964	-0.0271
6	0.0000	0.0000	2.7151	-0.1820	-0.0552	-0.0838	-0.2770	-0.1351	-0.5030	-0.1744	-0.1132	-0.1426

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   1      0.0000    0.0000    3.7762    0.1839    0.1270    0.0883    0.2036    0.1423    0.3186    0.2321    0.1720    0.1344
   6      0.0000    0.0000   -2.4973   -0.3909   -0.2725   -0.0565   -0.3871   -0.1996   -0.3704   -0.6732    0.0877   -0.2174
   1     -1.0159    0.0000   -2.8944    0.1483    0.1432    0.0547    0.1416    0.1066    0.1401    0.2367    0.0483    0.1038
   1      0.5079    0.8798   -2.8944    0.1483    0.1432    0.0547    0.1416    0.1066    0.1404    0.2367    0.0483    0.1038
   1      0.5079   -0.8798   -2.8944    0.1483    0.1432    0.0547    0.1416    0.1066    0.1404    0.2367    0.0483    0.1038

 Dipole mement (in D)   1.34 (DEN)      0.29      1.67      1.35      1.29      1.45      1.33      0.99      1.44      1.37

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File TZVPMol008.out
Molecule PMol008    ammonia
 SP Mol008 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0001    1.7403    1.7403
Quadrupole      0.9757    0.9755   -1.9513    0.0000   -0.0001    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   7      0.0000   -0.0000   -0.1171   -0.6562   -0.3913   -0.2753   -0.9579   -0.8235   -0.9583   -1.0368   -1.0119   -0.6903
   1      0.8504   -0.3850    0.2733    0.2187    0.1304    0.0918    0.3193    0.2745    0.3199    0.3456    0.3373    0.2301
   1     -0.0918    0.9290    0.2733    0.2187    0.1304    0.0918    0.3193    0.2745    0.3179    0.3456    0.3373    0.2301
   1     -0.7587   -0.5439    0.2733    0.2187    0.1305    0.0918    0.3193    0.2745    0.3205    0.3456    0.3373    0.2301

 Dipole mement (in D)   1.74 (DEN)      1.23      0.73      0.52      1.80      1.54      1.80      1.94      1.90      1.29

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File TZVPMol009.out
Molecule PMol009    water
 SP Mol009 B3LYP/Def2TZVP VAC.
    0    3
Dipole          0.0000    0.0000   -2.0756    2.0756
Quadrupole     -1.4819    1.6966   -0.2147    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      0.0000    0.0000    0.1176   -0.6273   -0.3056   -0.3062   -0.8831   -0.6419   -0.7554   -0.9084   -1.1214   -0.5164
   1      0.0000    0.7567   -0.4702    0.3136    0.1528    0.1531    0.4415    0.3210    0.3777    0.4542    0.5607    0.2582
   1      0.0000   -0.7567   -0.4702    0.3136    0.1528    0.1531    0.4415    0.3210    0.3777    0.4542    0.5607    0.2582

 Dipole mement (in D)   2.08 (DEN)      1.77      0.86      0.86      2.49      1.81      2.13      2.56      3.17      1.46

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File TZVPMol010.out
Molecule PMol010    Z-diimine
 SP Mol010 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0000    2.9227    2.9227
Quadrupole      0.0281   -0.4131    0.3851    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   7      0.0000    0.6177   -0.1197   -0.1852   -0.1228   -0.0959   -0.2149   -0.2860   -0.3065   -0.2730   -0.3012   -0.2314
   7      0.0000   -0.6177   -0.1197   -0.1852   -0.1228   -0.0959   -0.2149   -0.2860   -0.3065   -0.2730   -0.3011   -0.2314
   1      0.0000    1.0264    0.8380    0.1852    0.1228    0.0959    0.2149    0.2860    0.3065    0.2730    0.3013    0.2314
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1	0.0000	-1.0264	0.8380	0.1852	0.1228	0.0959	0.2149	0.2860	0.3065	0.2730	0.3013	0.2314

Dipole mement (in D) 2.92 (DEN) 1.70 1.13 0.88 1.98 2.63 2.82 2.51 2.77 2.13

File TZVPMol011.out
Molecule PMol011 hydroxylamine
SP Mol011 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.1299 0.5763 0.0000 0.5908
Quadrupole 0.6911 -0.9173 0.2262 3.9011 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.0114	-0.7347	0.0000	-0.4152	-0.1693	-0.2138	-0.4739	-0.3822	-0.4487	-0.5761	-0.7651	-0.2913
7	-0.0114	0.7042	0.0000	-0.3497	-0.2543	-0.1423	-0.5076	-0.5521	-0.7330	-0.5251	-0.4956	-0.4372
1	0.5598	0.9437	0.8059	0.2225	0.1331	0.1015	0.2848	0.2968	0.3762	0.3238	0.3462	0.2304
1	0.5598	0.9437	-0.8059	0.2225	0.1331	0.1015	0.2848	0.2968	0.3762	0.3238	0.3462	0.2304
1	-0.9492	-0.9395	0.0000	0.3200	0.1575	0.1529	0.4120	0.3408	0.4292	0.4536	0.5681	0.2677

Dipole mement (in D) 0.59 (DEN) 0.88 0.23 0.52 0.74 0.64 0.59 1.18 1.73 0.43

File TZVPMol012.out
Molecule PMol012 nitrogen_monoxide
SP Mol012 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 0.1199 0.1199
Quadrupole -0.1596 0.9684 -0.8088 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	0.0000	-0.6126	0.0562	-0.1006	0.0307	0.0583	-0.0263	-0.0173	0.1845	0.4149	0.0551
8	0.0000	0.0000	0.5361	-0.0562	0.1006	-0.0307	-0.0583	0.0263	0.0173	-0.1845	-0.4149	-0.0551

Dipole mement (in D) 0.12 (DEN) 0.31 0.55 0.17 0.32 0.14 0.10 1.02 2.29 0.30

File TZVPMol013.out
Molecule PMol013 nitrogen_dioxide
SP Mol013 B3LYP/Def2TZVP VAC.
0 3
Dipole 0.0000 0.0000 0.3275 0.3275
Quadrupole 1.3100 -1.8584 0.5484 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	0.0000	0.3219	0.3568	-0.0981	0.2136	0.5112	0.1116	0.2406	0.4858	0.7230	0.2593
8	0.0000	1.0999	-0.1408	-0.1784	0.0491	-0.1068	-0.2556	-0.0558	-0.1203	-0.2429	-0.3615	-0.1297
8	0.0000	-1.0999	-0.1408	-0.1784	0.0491	-0.1068	-0.2556	-0.0558	-0.1203	-0.2429	-0.3615	-0.1297

Dipole mement (in D) 0.33 (DEN) 0.79 0.22 0.47 1.14 0.25 0.53 1.08 1.61 0.58

File TZVPMol014.out
Molecule PMol014 nitroxyl
 SP Mol014 B3LYP/Def2TZVP VAC.
    0   3
Dipole   -1.4132   0.8992   0.0000   1.6750
Quadrupole   0.0621   -0.7261   0.6640   -1.4088   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0632	0.5765	0.0000	-0.0096	-0.1286	0.0175	-0.0044	-0.1914	-0.1943	-0.0045	0.1335	-0.0844
8	0.0632	-0.6200	0.0000	-0.1737	0.0090	-0.1083	-0.1545	-0.0763	-0.0793	-0.2274	-0.4092	-0.1201
1	-0.9483	0.9249	0.0000	0.1834	0.1196	0.0908	0.1588	0.2677	0.2736	0.2319	0.2757	0.2045

 Dipole mement (in D)   1.68 (DEN)   1.58   0.60   0.89   1.39   1.57   1.61   2.04   3.12   1.43

File TZVPMol015.out
Molecule PMol015 methylamine
 SP Mol015 B3LYP/Def2TZVP VAC.
    0   7
Dipole   -1.3308   0.3270   0.0000   1.3704
Quadrupole   -1.0200   -0.3374   1.3575   2.2048   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0501	-0.7551	0.0000	-0.4957	-0.2082	-0.2157	-0.7472	-0.6744	-0.9315	-0.8113	-0.9904	-0.5889
1	-0.4452	-1.1075	0.8075	0.2027	0.1418	0.0929	0.2960	0.2807	0.3441	0.3413	0.3305	0.2268
1	-0.4452	-1.1075	-0.8075	0.2027	0.1418	0.0929	0.2960	0.2807	0.3441	0.3413	0.3305	0.2268
6	0.0501	0.6999	0.0000	-0.2219	-0.3810	-0.0465	-0.0878	-0.1421	0.3479	-0.3959	0.3437	-0.1209
1	-0.9383	1.1757	0.0000	0.0907	0.0889	0.0144	0.0570	0.0718	-0.0824	0.1547	-0.0241	0.0724
1	0.5886	1.0628	0.8743	0.1107	0.1084	0.0310	0.0930	0.0917	-0.0110	0.1849	0.0050	0.0920
1	0.5886	1.0628	-0.8743	0.1107	0.1084	0.0310	0.0930	0.0917	-0.0110	0.1849	0.0050	0.0920

 Dipole mement (in D)   1.37 (DEN)   0.98   0.68   0.35   1.31   1.24   1.34   1.59   1.83   1.16

File TZVPMol016.out
Molecule PMol016 dimethylamine
 SP Mol016 B3LYP/Def2TZVP VAC.
    0   10
Dipole   -0.9091   -0.3093   0.0000   0.9603
Quadrupole   -0.1495   -0.7114   0.8610   -2.1496   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0264	0.5827	0.0000	-0.3184	-0.0724	-0.1552	-0.4785	-0.5264	-0.6349	-0.5995	-0.9820	-0.4784
1	-0.7753	1.1974	0.0000	0.1813	0.1582	0.0958	0.2706	0.2887	0.3498	0.3422	0.3290	0.2247
6	0.0264	-0.2206	1.2042	-0.2373	-0.3552	-0.0459	-0.1334	-0.1373	-0.0009	-0.4000	0.3431	-0.1231
6	0.0264	-0.2206	-1.2042	-0.2373	-0.3552	-0.0459	-0.1334	-0.1373	-0.0009	-0.4000	0.3430	-0.1231
1	-0.7961	-0.9505	1.2619	0.0839	0.0914	0.0129	0.0558	0.0713	0.0223	0.1516	-0.0260	0.0680
1	-0.0261	0.4193	2.0834	0.1137	0.1100	0.0325	0.0917	0.0933	0.0460	0.1936	0.0064	0.0931
1	0.9594	-0.7833	1.2645	0.1083	0.1109	0.0301	0.0899	0.0916	0.0752	0.1834	0.0031	0.0888
1	-0.7961	-0.9505	-1.2619	0.0839	0.0914	0.0129	0.0558	0.0713	0.0223	0.1516	-0.0260	0.0680
1	-0.0261	0.4193	-2.0834	0.1137	0.1100	0.0325	0.0917	0.0933	0.0460	0.1936	0.0064	0.0931

1	0.9594	-0.7833	-1.2645	0.1083	0.1109	0.0301	0.0899	0.0916	0.0752	0.1834	0.0031	0.0888

Dipole mement (in D) 0.96 (DEN) 0.65 0.46 0.22 0.79 1.02 0.94 1.29 1.70 0.96

File TZVPMol017.out
Molecule PMol017 trimethylamine
SP Mol017 B3LYP/Def2TZVP VAC.
0 13
Dipole 0.4219 -0.2667 0.0000 0.4991
Quadrupole -1.3026 0.1606 1.1420 1.5483 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.3177	0.2012	0.0000	-0.1698	0.0189	-0.0988	-0.1278	-0.3820	-0.0983	-0.4108	-0.9772	-0.3645
6	0.7888	1.1322	0.0000	-0.2475	-0.3281	-0.0445	-0.1985	-0.1329	-0.3646	-0.4006	0.3392	-0.1258
6	-0.3177	-0.6146	1.1939	-0.2473	-0.3281	-0.0444	-0.1984	-0.1329	-0.3926	-0.4005	0.3394	-0.1257
6	-0.3177	-0.6146	-1.1939	-0.2473	-0.3281	-0.0444	-0.1984	-0.1329	-0.3926	-0.4005	0.3393	-0.1257
1	1.7735	0.6331	0.0000	0.0803	0.0955	0.0131	0.0593	0.0724	0.1203	0.1517	-0.0248	0.0659
1	0.5821	-1.2477	1.2849	0.0803	0.0955	0.0131	0.0593	0.0724	0.1250	0.1517	-0.0248	0.0659
1	0.5821	-1.2477	-1.2849	0.0803	0.0955	0.0131	0.0593	0.0724	0.1250	0.1517	-0.0248	0.0659
1	0.7398	1.7704	0.8819	0.1119	0.1131	0.0322	0.0909	0.0940	0.1405	0.1929	0.0057	0.0907
1	-1.1875	-1.2712	1.1975	0.1119	0.1131	0.0321	0.0908	0.0940	0.1486	0.1928	0.0056	0.0907
1	-0.3691	0.0189	-2.0790	0.1118	0.1131	0.0322	0.0909	0.0940	0.1498	0.1928	0.0056	0.0907
1	0.7398	1.7704	-0.8819	0.1119	0.1131	0.0322	0.0909	0.0940	0.1405	0.1929	0.0057	0.0907
1	-0.3691	0.0189	2.0790	0.1118	0.1131	0.0322	0.0909	0.0940	0.1498	0.1928	0.0056	0.0907
1	-1.1875	-1.2712	-1.1975	0.1119	0.1131	0.0321	0.0908	0.0940	0.1486	0.1928	0.0056	0.0907

Dipole mement (in D) 0.50 (DEN) 0.39 0.22 0.06 0.20 0.91 0.55 1.14 1.59 0.81

File TZVPMol018.out
Molecule PMol018 ethylamine
SP Mol018 B3LYP/Def2TZVP VAC.
0 10
Dipole -1.0218 -0.8755 0.0000 1.3456
Quadrupole -3.2602 1.1746 2.0856 -2.3313 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	1.3313	-0.7911	0.8073	0.1939	0.1419	0.0906	0.2968	0.2786	0.3502	0.3393	0.3261	0.2224
7	1.2923	-0.1817	0.0000	-0.4745	-0.1721	-0.2151	-0.7778	-0.6713	-0.9926	-0.8067	-0.9910	-0.5926
6	0.0417	0.5686	-0.0000	-0.0659	-0.3732	-0.0086	0.0929	-0.0669	0.5242	-0.2088	0.3734	-0.0137
6	-1.2301	-0.2616	0.0000	-0.3198	-0.3279	-0.0941	-0.3618	-0.2417	-0.4181	-0.6090	-0.0004	-0.2503
1	0.0529	1.2299	0.8690	0.0948	0.1247	0.0287	0.0794	0.0931	-0.0337	0.1792	-0.0030	0.0862
1	0.0529	1.2298	-0.8690	0.0948	0.1247	0.0287	0.0794	0.0931	-0.0337	0.1792	-0.0030	0.0862
1	-2.1234	0.3639	-0.0000	0.0967	0.1166	0.0301	0.0994	0.0815	0.0749	0.2026	-0.0035	0.0832
1	-1.2803	-0.9058	0.8789	0.0931	0.1117	0.0245	0.0975	0.0776	0.0893	0.1924	-0.0123	0.0781
1	-1.2803	-0.9058	-0.8789	0.0931	0.1117	0.0245	0.0975	0.0776	0.0893	0.1924	-0.0123	0.0781
1	1.3313	-0.7911	-0.8073	0.1939	0.1419	0.0906	0.2968	0.2786	0.3502	0.3393	0.3261	0.2224

Dipole mement (in D) 1.35 (DEN) 0.76 0.84 0.31 1.21 1.25 1.32 1.70 1.80 1.20

File TZVPMol019.out
Molecule PMol019 propylamine
 SP Mol019 B3LYP/Def2TZVP VAC.
  0 13
Dipole -0.1781 1.4003 0.0000 1.4116
Quadrupole 1.9524 -4.5309 2.5785 -1.9269 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.4187	1.2843	0.0000	-0.3351	-0.3108	-0.0843	-0.3317	-0.2360	-0.2701	-0.5890	0.0097	-0.2477
6	0.0000	0.7486	0.0000	-0.1493	-0.3121	-0.0555	-0.1590	-0.1646	0.1029	-0.4014	0.0416	-0.1402
1	1.4469	2.3726	0.0000	0.1108	0.1167	0.0297	0.1011	0.0810	0.0844	0.2047	-0.0031	0.0832
1	1.9707	0.9442	0.8770	0.1020	0.1170	0.0279	0.0965	0.0797	0.0438	0.1962	-0.0079	0.0801
1	1.9707	0.9442	-0.8770	0.1020	0.1170	0.0279	0.0965	0.0797	0.0438	0.1962	-0.0078	0.0801
6	-0.0539	-0.7732	0.0000	-0.0778	-0.3478	-0.0110	0.0732	-0.0673	0.4093	-0.2000	0.3652	-0.0187
1	-0.5437	1.1251	0.8718	0.0728	0.1259	0.0222	0.0789	0.0787	-0.0347	0.1852	-0.0231	0.0722
1	-0.5437	1.1251	-0.8718	0.0728	0.1259	0.0222	0.0789	0.0787	-0.0347	0.1852	-0.0231	0.0722
1	0.4886	-1.1553	-0.8694	0.0909	0.1264	0.0273	0.0785	0.0921	-0.0259	0.1744	-0.0063	0.0832
1	0.4886	-1.1553	0.8694	0.0909	0.1264	0.0273	0.0785	0.0921	-0.0259	0.1744	-0.0063	0.0832
7	-1.3798	-1.3759	0.0000	-0.4678	-0.1690	-0.2146	-0.7809	-0.6712	-0.9506	-0.8059	-0.9939	-0.5922
1	-1.9039	-1.0639	0.8077	0.1940	0.1422	0.0906	0.2947	0.2785	0.3288	0.3401	0.3265	0.2223
1	-1.9039	-1.0639	-0.8077	0.1940	0.1422	0.0906	0.2947	0.2785	0.3288	0.3401	0.3265	0.2223

 Dipole mement (in D) 1.41 (DEN) 0.76 0.61 0.35 1.27 1.27 1.39 1.70 1.87 1.24

File TZVPMol020.out
Molecule PMol020 cyclopropylamine
 SP Mol020 B3LYP/Def2TZVP VAC.
  0 11
Dipole -0.7704 1.0426 0.0000 1.2964
Quadrupole -1.8165 1.5712 0.2453 0.6863 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.2613	0.9642	0.0000	0.0781	0.1215	0.0230	0.0524	0.0874	0.0170	0.1708	0.0017	0.0750
6	-0.3202	0.4169	0.0000	-0.0185	-0.3284	-0.0019	0.2040	-0.0121	0.2634	-0.0693	0.3216	0.0591
7	0.9060	1.1657	0.0000	-0.4867	-0.1379	-0.1989	-0.7870	-0.6495	-0.8254	-0.8126	-1.0048	-0.5839
1	0.9612	1.7664	0.8123	0.2054	0.1488	0.0950	0.3022	0.2831	0.3174	0.3495	0.3353	0.2264
1	0.9612	1.7664	-0.8123	0.2054	0.1488	0.0950	0.3022	0.2831	0.3174	0.3495	0.3353	0.2264
6	-0.3202	-0.8763	-0.7489	-0.1938	-0.2287	-0.0775	-0.2695	-0.1807	-0.3142	-0.4154	-0.0497	-0.1748
6	-0.3202	-0.8763	0.7489	-0.1938	-0.2287	-0.0775	-0.2695	-0.1807	-0.3142	-0.4154	-0.0495	-0.1748
1	-1.2201	-1.1735	-1.2673	0.1015	0.1233	0.0344	0.1058	0.0896	0.1192	0.2057	0.0186	0.0851
1	-1.2201	-1.1735	1.2673	0.1015	0.1233	0.0344	0.1058	0.0896	0.1192	0.2057	0.0186	0.0851
1	0.6008	-1.1476	-1.2439	0.1005	0.1291	0.0369	0.1269	0.0951	0.1501	0.2157	0.0365	0.0882
1	0.6008	-1.1476	1.2439	0.1005	0.1291	0.0369	0.1269	0.0951	0.1501	0.2157	0.0365	0.0882

 Dipole mement (in D) 1.30 (DEN) 0.82 0.94 0.47 1.41 1.21 1.25 1.40 1.72 1.11

File TZVPMol021.out
Molecule PMol021 isopropylamine
 SP Mol021 B3LYP/Def2TZVP VAC.
  0 13
Dipole 0.9705 0.8612 0.0000 1.2975
Quadrupole -2.8949 2.2797 0.6153 -0.5790 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	1.2155	0.8191	0.0000	0.0537	0.1251	0.0122	0.0334	0.0771	-0.1106	0.1462	-0.0353	0.0630
6	0.2927	0.2161	0.0000	0.1173	-0.3951	0.0230	0.2964	0.0025	0.6724	-0.0426	0.3788	0.0917
7	-0.9113	1.0505	0.0000	-0.5019	-0.1490	-0.2070	-0.8054	-0.6615	-0.9814	-0.8192	-0.9961	-0.5938
1	-0.9202	1.6577	0.8097	0.1959	0.1445	0.0901	0.2988	0.2784	0.3375	0.3460	0.3274	0.2216
1	-0.9202	1.6577	-0.8097	0.1959	0.1445	0.0901	0.2988	0.2784	0.3375	0.3460	0.3274	0.2216
6	0.2927	-0.6369	-1.2534	-0.3338	-0.2899	-0.0895	-0.3890	-0.2342	-0.4189	-0.5919	0.0111	-0.2461
6	0.2927	-0.6369	1.2534	-0.3338	-0.2899	-0.0895	-0.3890	-0.2342	-0.4189	-0.5919	0.0108	-0.2461
1	-0.5940	-1.2706	-1.2813	0.1087	0.1211	0.0291	0.1193	0.0841	0.1135	0.2051	0.0071	0.0812
1	1.1728	-1.2773	-1.2960	0.0972	0.1186	0.0293	0.1043	0.0818	0.0816	0.2017	-0.0060	0.0817
1	0.2889	-0.0233	-2.1550	0.0975	0.1152	0.0269	0.1046	0.0809	0.0960	0.1969	-0.0128	0.0812
1	-0.5940	-1.2706	1.2813	0.1087	0.1211	0.0291	0.1193	0.0841	0.1135	0.2051	0.0071	0.0812
1	1.1728	-1.2773	1.2960	0.0972	0.1186	0.0293	0.1043	0.0818	0.0816	0.2017	-0.0060	0.0817
1	0.2889	-0.0233	2.1550	0.0975	0.1152	0.0269	0.1046	0.0809	0.0960	0.1969	-0.0128	0.0812

Dipole mement (in D)	1.30 (DEN)	0.86	0.54	0.35	1.41	1.19	1.28	1.40	1.72	1.19

File TZVPMol022.out
Molecule PMol022 aziridine
 SP Mol022 B3LYP/Def2TZVP VAC.
  0 8
Dipole 0.0000 -0.8813 1.4732 1.7167
Quadrupole 0.5547 -1.3611 0.8064 0.0000 0.0000 2.5797

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-0.0000	1.3870	0.6903	0.1999	0.1568	0.0996	0.2779	0.2908	0.3517	0.3389	0.3414	0.2288
7	-0.0000	0.8532	-0.1710	-0.3637	-0.0365	-0.1838	-0.4913	-0.5178	-0.5358	-0.5720	-0.9009	-0.4856
6	-0.7337	-0.3957	0.0228	-0.1224	-0.2918	-0.0345	-0.0853	-0.0869	-0.1355	-0.2583	0.2273	-0.0614
6	0.7337	-0.3957	0.0228	-0.1224	-0.2918	-0.0345	-0.0853	-0.0869	-0.2273	-0.2583	0.2273	-0.0614
1	-1.2771	-0.7423	-0.8468	0.1037	0.1185	0.0396	0.1014	0.1021	0.1408	0.1910	0.0320	0.0963
1	-1.2442	-0.5632	0.9634	0.1006	0.1131	0.0370	0.0907	0.0984	0.1075	0.1839	0.0206	0.0936
1	1.2771	-0.7423	-0.8468	0.1037	0.1185	0.0396	0.1014	0.1021	0.1638	0.1910	0.0320	0.0963
1	1.2442	-0.5632	0.9634	0.1006	0.1131	0.0370	0.0907	0.0984	0.1348	0.1839	0.0206	0.0936

Dipole mement (in D)	1.72 (DEN)	1.41	0.79	0.66	1.69	1.83	1.71	2.23	3.21	1.88

File TZVPMol023.out
Molecule PMol023 piperidine_(NH_equatoria
 SP Mol023 B3LYP/Def2TZVP VAC.
  0 17
Dipole 0.2375 -0.0058 0.7929 0.8277

Quadrupole 1.6475 0.5514 -2.1989 -0.0260 1.4033 -0.0336

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	1.3711	-0.0327	-0.3155	-0.3172	-0.0144	-0.1527	-0.5448	-0.5164	-0.7444	-0.6092	-0.9884	-0.4900
6	-0.7402	-1.2347	-0.2279	-0.1423	-0.2640	-0.0530	-0.1921	-0.1579	-0.1275	-0.3946	0.0430	-0.1420
6	-0.6803	1.2686	-0.2280	-0.1420	-0.2640	-0.0529	-0.1920	-0.1579	-0.1315	-0.3945	0.0432	-0.1420
6	0.7725	1.1889	0.2051	-0.1079	-0.3099	-0.0129	0.0530	-0.0643	0.2116	-0.2109	0.3479	-0.0261
6	0.7148	-1.2244	0.2051	-0.1078	-0.3098	-0.0129	0.0530	-0.0643	0.2039	-0.2109	0.3478	-0.0261
6	-1.4425	0.0345	0.2344	-0.1526	-0.2652	-0.0499	-0.1480	-0.1583	0.1167	-0.3860	0.0387	-0.1445
1	-0.7823	-1.3023	-1.3182	0.0738	0.1347	0.0265	0.0884	0.0847	0.0605	0.1962	-0.0073	0.0744
1	-0.7190	1.3381	-1.3183	0.0737	0.1347	0.0265	0.0884	0.0847	0.0612	0.1962	-0.0073	0.0744
1	0.8174	1.2369	1.3087	0.0652	0.1120	0.0106	0.0365	0.0733	-0.0138	0.1437	-0.0362	0.0606
1	0.7576	-1.2747	1.3086	0.0652	0.1120	0.0106	0.0365	0.0733	-0.0123	0.1437	-0.0362	0.0606
1	-1.4972	0.0358	1.3287	0.0738	0.1321	0.0223	0.0721	0.0785	-0.0041	0.1862	-0.0226	0.0694
1	-1.2406	-2.1210	0.1657	0.0842	0.1313	0.0278	0.0784	0.0829	0.0105	0.2000	-0.0150	0.0777
1	-1.1379	2.1779	0.1656	0.0842	0.1313	0.0277	0.0784	0.0829	0.0109	0.2000	-0.0150	0.0777
1	1.3376	2.0424	-0.1722	0.0922	0.1250	0.0298	0.0713	0.0942	0.0178	0.1932	-0.0035	0.0872
1	1.2386	-2.1039	-0.1724	0.0922	0.1250	0.0298	0.0713	0.0942	0.0201	0.1932	-0.0035	0.0872
1	-2.4738	0.0591	-0.1217	0.0904	0.1306	0.0276	0.0806	0.0823	-0.0164	0.2018	-0.0138	0.0776
1	2.3570	-0.0563	-0.0978	0.1748	0.1588	0.0949	0.2688	0.2880	0.3368	0.3518	0.3288	0.2238
Dipole mement (in D)	0.83 (DEN)			0.69	0.56	0.19	0.88	0.99	0.87	1.17	1.59	0.96

File TZVPMol024.out
Molecule PMol024 piperidine_(NH_axial)
SP Mol024 B3LYP/Def2TZVP VAC.
0 17
Dipole 0.0000 1.0413 -0.5768 1.1904
Quadrupole 1.4922 -3.6383 2.1461 0.0000 0.0000 1.5740

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.0000	-1.4612	-0.1792	-0.2876	-0.0152	-0.1605	-0.5474	-0.5225	-0.7777	-0.5993	-0.9782	-0.4935
6	-1.2521	0.7052	-0.2305	-0.1598	-0.2735	-0.0574	-0.1974	-0.1632	-0.1208	-0.4066	0.0286	-0.1486
6	1.2521	0.7052	-0.2305	-0.1598	-0.2735	-0.0574	-0.1974	-0.1632	-0.1086	-0.4066	0.0286	-0.1486
6	1.2083	-0.7490	0.2239	-0.1393	-0.3130	-0.0126	0.0353	-0.0654	0.1347	-0.2143	0.3509	-0.0275
6	-1.2083	-0.7490	0.2239	-0.1393	-0.3130	-0.0126	0.0353	-0.0654	0.1751	-0.2143	0.3508	-0.0275
6	0.0000	1.4431	0.2235	-0.1415	-0.2664	-0.0508	-0.1501	-0.1595	0.0894	-0.3876	0.0383	-0.1456
1	-0.0000	-1.5714	-1.1865	0.1672	0.1592	0.0899	0.2655	0.2829	0.3613	0.3381	0.3190	0.2153
1	-1.3198	0.7376	-1.3235	0.0727	0.1294	0.0217	0.0761	0.0788	0.0402	0.1839	-0.0256	0.0698
1	1.3198	0.7376	-1.3235	0.0727	0.1294	0.0217	0.0761	0.0788	0.0418	0.1839	-0.0256	0.0698
1	1.2567	-0.7870	1.3180	0.0824	0.1291	0.0260	0.0709	0.0918	0.0606	0.1729	-0.0093	0.0796
1	-1.2567	-0.7870	1.3180	0.0824	0.1291	0.0260	0.0709	0.0918	0.0496	0.1729	-0.0093	0.0796
1	0.0000	1.5083	1.3172	0.0796	0.1337	0.0243	0.0757	0.0804	0.0007	0.1874	-0.0210	0.0715
1	-2.1523	1.1953	0.1476	0.0844	0.1312	0.0277	0.0796	0.0825	0.0072	0.2014	-0.0139	0.0775
1	2.1523	1.1952	0.1476	0.0844	0.1312	0.0277	0.0796	0.0825	0.0057	0.2014	-0.0139	0.0775
1	2.0749	-1.3026	-0.1407	0.1050	0.1260	0.0296	0.0735	0.0938	0.0293	0.1927	-0.0026	0.0867
1	-2.0749	-1.3026	-0.1407	0.1050	0.1260	0.0296	0.0735	0.0938	0.0203	0.1927	-0.0026	0.0867
1	0.0000	2.4718	-0.1411	0.0915	0.1301	0.0270	0.0804	0.0817	-0.0089	0.2013	-0.0139	0.0771

Dipole mement (in D) 1.19 (DEN) 0.94 0.51 0.25 0.78 1.11 1.14 1.47 1.85 1.16

File TZVPMol025.out
Molecule PMol025 1,2,3,6-Tetrahydropyridi
SP Mol025 B3LYP/Def2TZVP VAC.
0 15
Dipole -0.2334 -0.5240 0.7976 0.9825
Quadrupole 2.2709 1.6588 -3.9297 0.5332 -0.5267 -0.8862

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.5958	-1.1892	0.2992	-0.1072	-0.2992	-0.0109	0.0527	-0.0611	0.1992	-0.2069	0.3561	-0.0257
6	1.4734	-0.0260	-0.1277	-0.0694	-0.2516	-0.0532	-0.2144	-0.1530	-0.0544	-0.4345	0.0481	-0.1396
6	0.7155	1.2589	-0.0442	-0.1819	-0.1728	-0.0455	-0.0668	-0.1043	-0.0971	-0.1802	-0.0473	-0.0827
6	-0.6082	1.2964	0.0683	-0.1385	-0.1780	-0.0504	-0.1231	-0.1064	-0.2924	-0.1981	-0.0553	-0.0839
6	-1.4539	0.0680	0.0635	-0.0600	-0.2977	-0.0128	0.0338	-0.0588	0.3953	-0.2513	0.3532	-0.0234
7	-0.6886	-1.0872	-0.3785	-0.3209	-0.0073	-0.1512	-0.5401	-0.5120	-0.7094	-0.6030	-0.9849	-0.4906
1	1.2802	2.1845	-0.0648	0.0995	0.1365	0.0332	0.0816	0.0891	0.0957	0.1983	0.0167	0.0785
1	-1.1247	2.2443	0.1647	0.1009	0.1380	0.0350	0.0836	0.0911	0.1118	0.2006	0.0191	0.0806
1	1.8363	-0.1827	-1.1484	0.0825	0.1411	0.0322	0.0957	0.0892	0.0617	0.2102	0.0072	0.0774
1	2.3657	0.0212	0.5017	0.0826	0.1373	0.0317	0.0855	0.0870	0.0212	0.2051	-0.0052	0.0801
1	-2.3015	0.2062	-0.6137	0.0974	0.1334	0.0334	0.0795	0.0978	-0.0079	0.2000	0.0092	0.0881
1	-1.8948	-0.0638	1.0690	0.0751	0.1204	0.0174	0.0464	0.0792	-0.0438	0.1653	-0.0191	0.0664
1	0.4949	-1.1755	1.3981	0.0673	0.1151	0.0127	0.0405	0.0757	-0.0050	0.1480	-0.0292	0.0598
1	1.0554	-2.1417	0.0348	0.0964	0.1253	0.0314	0.0737	0.0960	0.0131	0.1935	-0.0017	0.0892
1	-1.2270	-1.9306	-0.2460	0.1761	0.1595	0.0968	0.2713	0.2903	0.3118	0.3530	0.3319	0.2258

Dipole mement (in D) 0.98 (DEN) 0.81 1.03 0.35 0.97 1.09 1.01 1.27 1.63 0.96

File TZVPMol026.out
Molecule PMol026 1,2,3,6-Tetrahydropyridi
SP Mol026 B3LYP/Def2TZVP VAC.
0 15
Dipole -0.5119 0.6955 -0.4815 0.9887
Quadrupole 1.9061 -2.6535 0.7474 1.9561 -0.2283 0.9171

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.7535	-1.1013	0.3143	-0.1219	-0.3008	-0.0102	0.0349	-0.0618	0.2550	-0.2107	0.3559	-0.0269
6	-1.4598	0.1795	-0.1157	-0.1390	-0.2630	-0.0579	-0.2223	-0.1588	-0.0458	-0.4502	0.0300	-0.1472
6	-0.5249	1.3458	-0.0549	-0.1339	-0.1779	-0.0497	-0.0747	-0.1090	-0.1347	-0.1881	-0.0572	-0.0874
6	0.7914	1.1967	0.0626	-0.1633	-0.1842	-0.0552	-0.1328	-0.1120	-0.2891	-0.2085	-0.0711	-0.0903
6	1.4498	-0.1481	0.0864	-0.0859	-0.3018	-0.0126	0.0169	-0.0604	0.3252	-0.2565	0.3541	-0.0253
7	0.5735	-1.2588	-0.2705	-0.3009	-0.0106	-0.1589	-0.5435	-0.5182	-0.8241	-0.5939	-0.9721	-0.4921
1	-0.9536	2.3412	-0.0954	0.1031	0.1362	0.0325	0.0824	0.0883	0.1068	0.1983	0.0167	0.0778
1	1.4331	2.0675	0.1495	0.0959	0.1367	0.0335	0.0832	0.0893	0.1097	0.1992	0.0174	0.0787
1	-2.3322	0.3642	0.5175	0.0871	0.1385	0.0327	0.0890	0.0877	0.0130	0.2083	-0.0021	0.0810
1	-1.8630	0.0718	-1.1297	0.0865	0.1363	0.0275	0.0846	0.0835	0.0411	0.1997	-0.0087	0.0739
1	1.8670	-0.3364	1.0843	0.0955	0.1347	0.0297	0.0760	0.0939	0.0300	0.1893	0.0053	0.0815
1	2.3107	-0.1602	-0.5860	0.1068	0.1340	0.0357	0.0834	0.1002	0.0058	0.2006	0.0087	0.0913

1	-1.3511	-1.9816	0.0746	0.1094	0.1261	0.0304	0.0753	0.0946	-0.0101	0.1929	-0.0002	0.0876
1	-0.6284	-1.0980	1.4010	0.0873	0.1328	0.0296	0.0773	0.0960	0.0431	0.1784	-0.0014	0.0808
1	0.4848	-1.2927	-1.2785	0.1734	0.1629	0.0926	0.2700	0.2863	0.3742	0.3413	0.3249	0.2162

Dipole mement (in D) 0.99 (DEN) 0.46 0.81 0.18 0.74 0.93 0.93 1.52 1.54 1.06

File TZVPMol027.out
Molecule PMol027 aniline
SP Mol027 B3LYP/Def2TZVP VAC.
0 14
Dipole -0.9489 1.3727 0.0000 1.6687
Quadrupole -7.0215 4.4643 2.5572 -3.0894 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0021	0.9333	0.0000	0.2967	-0.2424	0.0428	0.3908	0.0924	0.3853	0.1545	0.3786	0.1680
6	0.0019	0.2199	1.2019	-0.2214	-0.1383	-0.0666	-0.2348	-0.1153	-0.2654	-0.2612	-0.0346	-0.1101
6	0.0019	0.2199	-1.2019	-0.2214	-0.1383	-0.0666	-0.2348	-0.1153	-0.2654	-0.2612	-0.0345	-0.1101
6	0.0019	-1.1650	1.1961	-0.0933	-0.1438	-0.0412	-0.0515	-0.0969	-0.1273	-0.1825	-0.0219	-0.0833
6	0.0019	-1.1650	-1.1961	-0.0933	-0.1438	-0.0412	-0.0515	-0.0969	-0.1273	-0.1825	-0.0217	-0.0833
6	0.0022	-1.8710	0.0000	-0.1488	-0.1676	-0.0633	-0.1515	-0.1193	-0.1192	-0.2541	-0.0336	-0.1079
1	0.0060	0.7613	2.1411	0.0944	0.1392	0.0340	0.1058	0.0930	0.1491	0.2000	0.0151	0.0789
1	0.0060	0.7613	-2.1411	0.0944	0.1392	0.0340	0.1058	0.0930	0.1491	0.2000	0.0151	0.0789
1	0.0003	-1.6975	2.1392	0.1028	0.1418	0.0387	0.0920	0.0949	0.1218	0.2052	0.0251	0.0822
1	0.0003	-1.6975	-2.1392	0.1028	0.1418	0.0387	0.0920	0.0949	0.1218	0.2052	0.0251	0.0822
1	0.0010	-2.9525	0.0000	0.1013	0.1385	0.0348	0.0913	0.0909	0.1024	0.2068	0.0227	0.0781
7	0.0665	2.3216	0.0000	-0.4495	-0.0450	-0.1696	-0.8335	-0.6239	-0.7841	-0.7696	-1.0817	-0.5589
1	-0.2749	2.7703	-0.8328	0.2176	0.1593	0.1127	0.3399	0.3043	0.3296	0.3697	0.3731	0.2426
1	-0.2749	2.7703	0.8328	0.2176	0.1593	0.1127	0.3399	0.3043	0.3296	0.3697	0.3731	0.2426

Dipole mement (in D) 1.67 (DEN) 1.75 2.26 1.36 1.48 1.65 1.75 1.52 1.45 1.13

File TZVPMol028.out
Molecule PMol028 pyrrole
SP Mol028 B3LYP/Def2TZVP VAC.
0 10
Dipole -1.9141 0.0000 -0.0001 1.9141
Quadrupole 4.4845 1.1726 -5.6571 0.0001 0.0005 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-1.1156	-0.0000	-0.0001	-0.2188	0.1789	-0.0505	-0.3662	-0.4188	-0.1152	-0.4857	-1.1969	-0.3887
6	-0.3300	-1.1197	-0.0000	-0.0596	-0.2397	-0.0357	0.0177	-0.0228	-0.2080	-0.0808	0.3389	0.0091
6	0.9782	-0.7076	-0.0000	-0.1698	-0.2008	-0.0918	-0.2002	-0.1386	-0.1815	-0.2980	-0.0408	-0.1249
1	1.8396	-1.3540	-0.0000	0.1044	0.1329	0.0385	0.1091	0.0948	0.1461	0.2158	0.0396	0.0814
6	-0.3300	1.1197	0.0000	-0.0596	-0.2397	-0.0357	0.0177	-0.0228	-0.2080	-0.0808	0.3390	0.0091
6	0.9782	0.7077	0.0001	-0.1698	-0.2008	-0.0918	-0.2002	-0.1386	-0.1815	-0.2980	-0.0409	-0.1249
1	-0.7649	-2.1040	-0.0000	0.1278	0.1268	0.0438	0.0958	0.1079	0.1597	0.2052	0.0545	0.0950
1	1.8395	1.3541	0.0002	0.1044	0.1329	0.0385	0.1091	0.0948	0.1461	0.2158	0.0396	0.0814
1	-0.7650	2.1039	-0.0000	0.1278	0.1268	0.0438	0.0958	0.1079	0.1597	0.2052	0.0545	0.0950

1	-2.1183	-0.0001	-0.0001	0.2133	0.1826	0.1410	0.3213	0.3361	0.2827	0.4013	0.4125	0.2676

Dipole mement (in D) 1.91 (DEN) 1.50 2.53 1.55 2.02 1.52 1.90 1.72 1.06 1.10

File TZVPMol029.out
Molecule PMol029 pyridine
SP Mol029 B3LYP/Def2TZVP VAC.
0 11
Dipole 0.0000 0.0000 -2.2364 2.2364
Quadrupole -3.1522 5.0022 -1.8500 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-1.3768	-0.1022	-0.1222	-0.0207	-0.0287	-0.0744	0.2940	-0.1707	-0.0214	-0.0616
6	0.0000	1.1918	-0.6691	-0.0990	-0.1494	-0.0426	-0.1742	-0.0931	-0.5316	-0.2500	-0.0345	-0.0818
6	0.0000	-1.1918	-0.6691	-0.0990	-0.1494	-0.0426	-0.1742	-0.0931	-0.5316	-0.2500	-0.0346	-0.0818
6	0.0000	1.1369	0.7182	-0.0378	-0.2060	0.0216	0.1460	0.0457	0.5131	0.0322	0.5057	0.0812
6	0.0000	-1.1369	0.7182	-0.0378	-0.2060	0.0216	0.1460	0.0457	0.5131	0.0322	0.5059	0.0812
7	0.0000	0.0000	1.4120	-0.2132	0.1284	-0.1613	-0.3776	-0.3558	-0.6785	-0.4090	-1.1221	-0.3982
1	0.0000	2.1469	-1.1779	0.1140	0.1440	0.0459	0.1057	0.1023	0.1787	0.2138	0.0400	0.0908
1	0.0000	-2.1469	-1.1779	0.1140	0.1440	0.0459	0.1057	0.1023	0.1787	0.2138	0.0400	0.0908
1	0.0000	2.0527	1.3017	0.1192	0.1358	0.0419	0.0749	0.1079	0.0037	0.1880	0.0398	0.0930
1	0.0000	-2.0527	1.3017	0.1192	0.1358	0.0419	0.0749	0.1079	0.0037	0.1880	0.0398	0.0930
1	0.0000	0.0000	-2.4597	0.1228	0.1449	0.0485	0.1015	0.1045	0.0566	0.2115	0.0412	0.0936

Dipole mement (in D) 2.24 (DEN) 1.64 0.43 1.10 1.70 2.05 2.23 2.38 4.20 2.18

File TZVPMol030.out
Molecule PMol030 2-methylpyridine
SP Mol030 B3LYP/Def2TZVP VAC.
0 14
Dipole -0.6737 1.7281 0.0000 1.8548
Quadrupole 4.0444 -0.6742 -3.3701 1.7738 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.8743	0.0064	-0.0000	0.1838	-0.2394	0.0645	0.3773	0.1249	0.8969	0.2034	0.4971	0.1967
6	0.1583	1.2021	-0.0000	-0.1687	-0.1270	-0.0493	-0.2255	-0.0975	-0.6119	-0.2498	-0.0364	-0.0939
6	-1.2265	1.1640	-0.0000	-0.0877	-0.1219	-0.0228	-0.0175	-0.0764	0.2501	-0.1632	-0.0233	-0.0632
6	-1.8605	-0.0678	0.0000	-0.1065	-0.1564	-0.0498	-0.1899	-0.1002	-0.5107	-0.2627	-0.0372	-0.0889
6	-1.0678	-1.2067	0.0000	-0.0523	-0.2056	0.0202	0.1554	0.0449	0.4371	0.0425	0.5115	0.0805
7	0.2619	-1.1848	0.0000	-0.2303	0.1522	-0.1628	-0.4136	-0.3542	-0.7179	-0.4214	-1.1277	-0.4087
1	-1.8009	2.0823	-0.0000	0.1191	0.1446	0.0472	0.1006	0.1033	0.0706	0.2102	0.0387	0.0920
1	0.6864	2.1476	-0.0000	0.1071	0.1446	0.0411	0.1099	0.0983	0.1848	0.2095	0.0317	0.0850
1	-2.9393	-0.1483	0.0000	0.1115	0.1429	0.0440	0.1051	0.1004	0.1758	0.2135	0.0377	0.0887
1	-1.5266	-2.1915	0.0000	0.1141	0.1353	0.0403	0.0736	0.1064	0.0254	0.1867	0.0368	0.0911
6	2.3673	-0.0133	0.0000	-0.3346	-0.2533	-0.0868	-0.4567	-0.2260	-0.7488	-0.6205	0.0162	-0.2453
1	2.7432	-0.5467	0.8725	0.1205	0.1314	0.0404	0.1331	0.0949	0.1878	0.2243	0.0271	0.0906
1	2.7432	-0.5468	-0.8724	0.1205	0.1314	0.0404	0.1331	0.0949	0.1878	0.2243	0.0271	0.0906
1	2.7899	0.9888	-0.0000	0.1034	0.1214	0.0333	0.1150	0.0865	0.1731	0.2033	0.0007	0.0849

Dipole mement (in D) 1.85 (DEN) 1.11 0.73 0.82 1.51 1.68 1.84 1.99 3.68 1.86

File TZVPMol031.out
Molecule PMol031 4-methylpyridine
SP Mol031 B3LYP/Def2TZVP VAC.
0 14
Dipole 0.0508 2.7483 0.0000 2.7488
Quadrupole -2.1895 -3.0255 5.2150 0.0886 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.0067	-1.2142	1.1329	-0.0425	-0.2070	0.0191	0.1553	0.0432	0.5235	0.0383	0.5025	0.0791
6	-0.0067	0.1710	1.1850	-0.1292	-0.1272	-0.0498	-0.2328	-0.0980	-0.6868	-0.2520	-0.0424	-0.0945
6	-0.0041	0.9015	0.0000	0.1045	-0.1586	0.0229	0.2173	0.0071	0.7312	0.0179	-0.0029	0.0589
6	-0.0067	0.1710	-1.1850	-0.1292	-0.1272	-0.0498	-0.2328	-0.0980	-0.6868	-0.2520	-0.0424	-0.0945
6	-0.0067	-1.2142	-1.1329	-0.0425	-0.2070	0.0191	0.1553	0.0432	0.5235	0.0383	0.5024	0.0791
7	-0.0061	-1.9157	0.0000	-0.2149	0.1225	-0.1678	-0.3890	-0.3618	-0.6978	-0.4165	-1.1208	-0.4046
1	-0.0120	0.6787	-2.1425	0.1050	0.1452	0.0417	0.1106	0.0987	0.2024	0.2087	0.0311	0.0855
1	-0.0103	-1.7923	-2.0525	0.1158	0.1355	0.0406	0.0746	0.1066	0.0121	0.1869	0.0373	0.0914
1	-0.0103	-1.7923	2.0525	0.1158	0.1355	0.0406	0.0746	0.1066	0.0121	0.1869	0.0373	0.0914
6	0.0237	2.3947	0.0000	-0.3583	-0.2467	-0.0781	-0.4146	-0.2232	-0.5733	-0.6175	0.0143	-0.2473
1	-0.4609	2.8079	0.8826	0.1209	0.1281	0.0390	0.1221	0.0916	0.1455	0.2151	0.0148	0.0900
1	1.0514	2.7623	0.0000	0.1286	0.1335	0.0416	0.1266	0.0936	0.1464	0.2221	0.0226	0.0901
1	-0.4609	2.8079	-0.8826	0.1209	0.1281	0.0390	0.1221	0.0916	0.1455	0.2151	0.0148	0.0900
1	-0.0120	0.6787	2.1425	0.1050	0.1452	0.0417	0.1106	0.0987	0.2024	0.2087	0.0311	0.0855

Dipole mement (in D) 2.75 (DEN) 2.25 1.40 1.62 1.97 2.65 2.74 2.84 4.79 2.66

File TZVPMol032.out
Molecule PMol032 indole
SP Mol032 B3LYP/Def2TZVP VAC.
0 16
Dipole -0.9023 1.9937 0.0000 2.1884
Quadrupole 1.8228 6.6583 -8.4810 -2.1036 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.3595	1.0039	0.0000	-0.2140	-0.1348	-0.0615	-0.2141	-0.1103	-0.3200	-0.2350	-0.0206	-0.1054
6	2.2398	-0.0624	0.0000	-0.1036	-0.1527	-0.0520	-0.0892	-0.1076	-0.1279	-0.2114	-0.0259	-0.0958
6	1.7770	-1.3863	0.0000	-0.1081	-0.1590	-0.0577	-0.1263	-0.1135	-0.1323	-0.2307	-0.0300	-0.1022
6	0.4257	-1.6714	0.0000	-0.1963	-0.1121	-0.0450	-0.1174	-0.0975	-0.3485	-0.1820	-0.0215	-0.0934
6	-0.4920	-0.6156	0.0000	0.1383	-0.1233	-0.0279	0.0275	-0.0268	0.3588	-0.0960	-0.0092	-0.0009
6	0.0000	0.7124	0.0000	0.1486	-0.1632	0.0278	0.2444	0.0887	0.2742	0.1177	0.3706	0.1339
7	-1.0911	1.5465	0.0000	-0.2523	0.1957	-0.0587	-0.4615	-0.4182	-0.5021	-0.4973	-1.1896	-0.4025
6	-2.2412	0.7923	0.0000	0.0003	-0.2061	-0.0138	0.0731	-0.0016	0.0320	-0.0279	0.3454	0.0301
6	-1.9159	-0.5322	0.0000	-0.2536	-0.1571	-0.0892	-0.2715	-0.1341	-0.5559	-0.2905	-0.0369	-0.1315
1	1.7170	2.0263	0.0000	0.0949	0.1398	0.0367	0.1032	0.0944	0.1596	0.2060	0.0240	0.0799
1	3.3052	0.1280	0.0000	0.1023	0.1403	0.0358	0.0914	0.0920	0.1234	0.2057	0.0234	0.0791
1	2.4960	-2.1953	0.0000	0.0998	0.1397	0.0346	0.0900	0.0907	0.1237	0.2057	0.0213	0.0777

1	0.0787	-2.6975	0.0000	0.0967	0.1423	0.0385	0.0955	0.0949	0.1717	0.2061	0.0270	0.0796
1	-1.0567	2.5484	0.0000	0.2105	0.1831	0.1410	0.3352	0.3366	0.3733	0.4027	0.4151	0.2664
1	-3.2058	1.2715	0.0000	0.1317	0.1305	0.0497	0.1013	0.1138	0.1456	0.2072	0.0605	0.1015
1	-2.6148	-1.3516	0.0000	0.1049	0.1368	0.0417	0.1183	0.0982	0.2247	0.2196	0.0459	0.0837

Dipole mement (in D) 2.19 (DEN) 2.01 2.61 1.89 2.12 1.84 2.15 1.81 1.20 1.47

File TZVPMol033.out
Molecule PMol033 quinoline
SP Mol033 B3LYP/Def2TZVP VAC.
0 17
Dipole 0.1196 -2.0627 0.0000 2.0662
Quadrupole 7.0753 -0.7553 -6.3201 2.4507 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.7030	0.0000	0.1762	-0.1650	0.0456	0.2644	0.1125	0.6967	0.1374	0.4435	0.1604
6	1.2551	1.3476	0.0000	-0.2210	-0.0958	-0.0374	-0.1770	-0.0843	-0.3561	-0.1822	-0.0197	-0.0769
6	2.4121	0.6143	0.0000	-0.0638	-0.1333	-0.0346	-0.0769	-0.0901	-0.0757	-0.1978	-0.0249	-0.0794
6	2.3695	-0.7935	0.0000	-0.1020	-0.1375	-0.0384	-0.0952	-0.0942	-0.1743	-0.2017	-0.0239	-0.0832
6	1.1666	-1.4487	0.0000	-0.1780	-0.1024	-0.0383	-0.1254	-0.0913	-0.1525	-0.1787	-0.0265	-0.0885
6	-0.0434	-0.7224	0.0000	0.0875	-0.1018	-0.0058	0.0149	-0.0083	-0.1679	-0.0975	-0.0080	0.0169
6	-1.3130	-1.3340	0.0000	-0.1421	-0.0811	-0.0197	-0.0635	-0.0707	0.0689	-0.1370	-0.0229	-0.0663
6	-2.4345	-0.5513	0.0000	-0.1067	-0.1505	-0.0458	-0.1868	-0.0962	-0.4569	-0.2547	-0.0365	-0.0858
6	-2.2813	0.8495	0.0000	-0.0353	-0.2063	0.0258	0.1609	0.0544	0.4011	0.0513	0.5655	0.0880
7	-1.1244	1.4677	0.0000	-0.1900	0.1625	-0.1580	-0.4083	-0.3468	-0.6953	-0.3954	-1.1191	-0.4042
1	-3.1652	1.4825	0.0000	0.1140	0.1359	0.0415	0.0739	0.1077	0.0479	0.1860	0.0382	0.0926
1	-3.4255	-0.9852	0.0000	0.1147	0.1442	0.0455	0.1078	0.1019	0.1819	0.2145	0.0402	0.0904
1	-1.3814	-2.4162	0.0000	0.1141	0.1481	0.0474	0.1012	0.1041	0.1093	0.2088	0.0394	0.0903
1	1.1260	-2.5320	0.0000	0.1055	0.1456	0.0410	0.0959	0.0978	0.1335	0.2044	0.0304	0.0831
1	3.2943	-1.3561	0.0000	0.1119	0.1436	0.0426	0.0974	0.0987	0.1411	0.2102	0.0331	0.0869
1	3.3710	1.1168	0.0000	0.1122	0.1442	0.0435	0.0986	0.0996	0.1336	0.2105	0.0343	0.0878
1	1.2648	2.4298	0.0000	0.1029	0.1496	0.0450	0.1182	0.1050	0.1647	0.2220	0.0566	0.0879

Dipole mement (in D) 2.07 (DEN) 1.29 0.48 1.02 1.67 1.92 2.06 2.23 3.87 2.05

File TZVPMol034.out
Molecule PMol034 isoquinoline
SP Mol034 B3LYP/Def2TZVP VAC.
0 17
Dipole 2.3962 -0.9822 0.0000 2.5897
Quadrupole -1.3068 5.9393 -4.6325 4.3097 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6968	0.0000	0.1255	-0.1029	-0.0063	-0.0018	-0.0085	-0.2276	-0.1100	-0.0149	0.0161
6	1.2346	1.3775	0.0000	-0.1656	-0.0929	-0.0304	-0.1099	-0.0834	-0.1577	-0.1631	-0.0237	-0.0804
6	2.4106	0.6749	0.0000	-0.1018	-0.1358	-0.0375	-0.1007	-0.0934	-0.1345	-0.2087	-0.0222	-0.0830
6	2.3946	-0.7339	0.0000	-0.0867	-0.1279	-0.0308	-0.0724	-0.0866	-0.0695	-0.1868	-0.0219	-0.0756
6	1.2093	-1.4217	0.0000	-0.1952	-0.0969	-0.0359	-0.1424	-0.0891	-0.3852	-0.1840	-0.0243	-0.0870

6	-0.0182	-0.7251	0.0000	0.0997	-0.0899	0.0074	0.1105	0.0019	0.5948	-0.0408	-0.0021	0.0284
6	-1.2807	-1.3532	0.0000	-0.1303	-0.1132	-0.0451	-0.2170	-0.0927	-0.6245	-0.2200	-0.0354	-0.0897
6	-2.4145	-0.5869	0.0000	-0.0353	-0.2071	0.0103	0.1225	0.0300	0.3975	0.0112	0.4430	0.0663
6	-1.2449	1.3668	0.0000	-0.0807	-0.1681	0.0297	0.1377	0.0611	0.3630	0.0837	0.5687	0.0872
7	-2.4112	0.7688	0.0000	-0.2069	0.1276	-0.1638	-0.3822	-0.3572	-0.6268	-0.4091	-1.1244	-0.4008
1	-3.3947	-1.0512	0.0000	0.1168	0.1360	0.0411	0.0791	0.1069	0.0518	0.1911	0.0405	0.0919
1	-1.3458	-2.4347	0.0000	0.1045	0.1472	0.0441	0.1086	0.1012	0.1982	0.2113	0.0370	0.0868
1	-1.2502	2.4558	0.0000	0.1113	0.1394	0.0407	0.0702	0.1074	0.0467	0.1824	0.0364	0.0895
1	1.2351	2.4614	0.0000	0.1090	0.1484	0.0447	0.0975	0.1015	0.1366	0.2105	0.0372	0.0873
1	3.3584	1.1974	0.0000	0.1147	0.1443	0.0437	0.0991	0.0998	0.1311	0.2118	0.0356	0.0882
1	3.3324	-1.2750	0.0000	0.1148	0.1450	0.0447	0.0986	0.1008	0.1323	0.2111	0.0360	0.0893
1	1.1989	-2.5051	0.0000	0.1061	0.1470	0.0432	0.1024	0.1000	0.1737	0.2095	0.0345	0.0856

Dipole mement (in D)	2.59 (DEN)	1.60	0.85	1.49	2.05	2.43	2.57	2.73	4.67	2.54

File TZVPMol035.out
Molecule PMol035 imidazole
SP Mol035 B3LYP/Def2TZVP VAC.
0 9
Dipole 1.6521 3.3817 0.0001 3.7637
Quadrupole 5.0770 -1.3745 -3.7025 0.7333 0.0000 -0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.7573	0.7975	0.0000	-0.2294	0.1744	-0.0493	-0.4175	-0.4082	-0.1293	-0.5060	-1.2003	-0.3752
7	-0.1405	-1.2207	-0.0000	-0.2738	0.0854	-0.2074	-0.4353	-0.3894	-0.4848	-0.4465	-1.0774	-0.4312
6	-0.6026	0.9837	-0.0000	-0.0635	-0.2489	-0.0372	-0.0340	-0.0169	-0.2910	-0.1166	0.3182	0.0138
6	-1.1325	-0.2745	0.0000	-0.0954	-0.2646	-0.0384	0.0167	-0.0121	0.1073	-0.0960	0.3889	0.0261
6	0.9803	-0.5441	-0.0000	0.0566	-0.3156	0.0354	0.2414	0.1339	0.1452	0.1502	0.9504	0.1838
1	1.4540	1.5211	0.0001	0.2205	0.1855	0.1470	0.3357	0.3417	0.2697	0.4072	0.4220	0.2735
1	-2.1734	-0.5527	0.0001	0.1188	0.1284	0.0451	0.0970	0.1098	0.1039	0.2038	0.0557	0.0950
1	-1.0445	1.9642	-0.0001	0.1313	0.1294	0.0508	0.1093	0.1150	0.1800	0.2129	0.0696	0.1027
1	1.9746	-0.9611	-0.0000	0.1349	0.1259	0.0540	0.0867	0.1264	0.0990	0.1911	0.0728	0.1117

Dipole mement (in D)	3.76 (DEN)	2.63	2.52	2.36	3.33	3.32	3.76	3.73	3.52	3.04

File TZVPMol036.out
Molecule PMol036 pyridazine
SP Mol036 B3LYP/Def2TZVP VAC.
0 10
Dipole 0.0000 0.0000 4.2100 4.2100
Quadrupole -1.4334 4.8457 -3.4124 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	1.3165	-0.0659	-0.0604	-0.2187	0.0196	0.0709	0.0510	0.4184	-0.0040	0.4852	0.0860
6	0.0000	0.6882	1.1736	-0.0834	-0.1298	-0.0199	-0.1107	-0.0679	-0.2008	-0.2092	-0.0220	-0.0556
6	0.0000	-0.6882	1.1736	-0.0834	-0.1298	-0.0199	-0.1107	-0.0679	-0.2008	-0.2092	-0.0220	-0.0556
6	0.0000	-1.3165	-0.0659	-0.0604	-0.2187	0.0196	0.0709	0.0510	0.4184	-0.0040	0.4851	0.0860
7	0.0000	0.6657	-1.2268	-0.1079	0.0597	-0.1066	-0.1652	-0.2135	-0.3304	-0.2050	-0.5757	-0.2364

7	0.0000	-0.6657	-1.2268	-0.1079	0.0597	-0.1066	-0.1652	-0.2135	-0.3304	-0.2050	-0.5758	-0.2364
1	0.0000	-2.3974	-0.1488	0.1258	0.1406	0.0510	0.0897	0.1182	-0.0210	0.1990	0.0570	0.1039
1	0.0000	-1.2641	2.0901	0.1259	0.1482	0.0558	0.1153	0.1122	0.1338	0.2191	0.0557	0.1020
1	0.0000	1.2641	2.0901	0.1259	0.1482	0.0558	0.1153	0.1122	0.1338	0.2191	0.0557	0.1020
1	0.0000	2.3974	-0.1488	0.1258	0.1406	0.0510	0.0897	0.1182	-0.0210	0.1990	0.0570	0.1039

Dipole mement (in D) 4.21 (DEN) 2.72 0.75 2.07 2.84 3.80 4.08 4.18 7.27 4.01

File TZVPMol037.out
Molecule PMol037 pyrimidine
SP Mol037 B3LYP/Def2TZVP VAC.
0 10
Dipole 0.0000 0.0000 2.3432 2.3432
Quadrupole -1.1907 -2.5624 3.7531 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	1.1930	-0.7124	-0.2219	0.1201	-0.1614	-0.4307	-0.3505	-0.7896	-0.4344	-1.1138	-0.3901
7	0.0000	-1.1930	-0.7124	-0.2219	0.1201	-0.1614	-0.4307	-0.3505	-0.7896	-0.4344	-1.1138	-0.3901
6	0.0000	1.1781	0.6194	-0.0114	-0.1845	0.0416	0.1949	0.0684	0.6414	0.0657	0.5096	0.1033
6	0.0000	0.0000	1.3477	-0.1162	-0.1569	-0.0451	-0.2502	-0.0894	-0.7235	-0.2915	-0.0386	-0.0789
6	0.0000	-1.1781	0.6194	-0.0114	-0.1845	0.0416	0.1949	0.0684	0.6414	0.0657	0.5099	0.1033
6	0.0000	0.0000	-1.3028	0.0716	-0.2725	0.0829	0.3602	0.1871	0.8133	0.2449	1.0258	0.2421
1	0.0000	-2.1443	1.1158	0.1299	0.1395	0.0510	0.0862	0.1168	0.0076	0.1933	0.0534	0.1030
1	0.0000	0.0000	2.4291	0.1212	0.1465	0.0523	0.1226	0.1091	0.2168	0.2208	0.0529	0.0983
1	0.0000	2.1443	1.1158	0.1299	0.1395	0.0510	0.0862	0.1168	0.0076	0.1933	0.0534	0.1030
1	0.0000	0.0000	-2.3889	0.1300	0.1330	0.0476	0.0666	0.1239	-0.0253	0.1767	0.0611	0.1061

Dipole mement (in D) 2.34 (DEN) 1.57 0.45 1.15 1.82 2.16 2.35 2.56 4.48 2.29

File TZVPMol038.out
Molecule PMol038 2-methylpyrimidine
SP Mol038 B3LYP/Def2TZVP VAC.
0 13
Dipole 1.6491 -0.0591 0.0000 1.6502
Quadrupole 5.6989 -3.7422 -1.9567 0.0362 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.2207	1.1953	0.0000	-0.2349	0.1401	-0.1635	-0.4660	-0.3493	-0.8375	-0.4467	-1.1138	-0.4011
6	-0.8403	0.0098	0.0000	0.2136	-0.3092	0.1224	0.5927	0.2610	1.1261	0.4057	0.9854	0.3512
6	1.1106	1.1703	-0.0000	-0.0143	-0.1855	0.0381	0.2003	0.0652	0.5951	0.0732	0.5094	0.1006
7	-0.2342	-1.1857	0.0000	-0.2374	0.1429	-0.1641	-0.4660	-0.3501	-0.8379	-0.4452	-1.1174	-0.4015
6	1.8347	-0.0081	-0.0000	-0.1187	-0.1646	-0.0531	-0.2668	-0.0974	-0.7210	-0.3053	-0.0428	-0.0869
6	1.0938	-1.1791	-0.0000	-0.0219	-0.1863	0.0391	0.2029	0.0669	0.5971	0.0753	0.5203	0.1020
6	-2.3300	0.0064	-0.0000	-0.3144	-0.2528	-0.0890	-0.5038	-0.2227	-0.6737	-0.6342	0.0191	-0.2394
1	1.6105	2.1352	-0.0000	0.1252	0.1387	0.0488	0.0847	0.1147	0.0196	0.1916	0.0496	0.1005
1	2.9155	-0.0155	-0.0000	0.1184	0.1452	0.0500	0.1215	0.1068	0.2170	0.2201	0.0497	0.0957
1	1.5822	-2.1500	-0.0000	0.1247	0.1386	0.0488	0.0842	0.1147	0.0195	0.1911	0.0492	0.1005
1	-2.7211	1.0185	-0.0001	0.1236	0.1273	0.0375	0.1374	0.0947	0.1644	0.2229	0.0319	0.0910

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   1     -2.7077   -0.5259    0.8720    0.1181    0.1329    0.0426    0.1395    0.0979    0.1657    0.2258    0.0293    0.0937
   1     -2.7077   -0.5261   -0.8719    0.1181    0.1328    0.0426    0.1395    0.0979    0.1657    0.2258    0.0293    0.0937

 Dipole mement (in D)   1.65 (DEN)      0.82      0.62      0.65      1.62      1.52      1.66      1.77      3.60      1.70

-----------------------------------------
File TZVPMol039.out
Molecule PMol039    hydrogen_cyanide
 SP Mol039 B3LYP/Def2TZVP VAC.
    0    3
Dipole          0.0000    0.0000   -3.0304    3.0304
Quadrupole     -0.6611   -0.6611    1.3222    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1      0.0000    0.0000   -1.5660    0.1901    0.1243    0.1269    0.2104    0.1867    0.2160    0.2247    0.2143    0.1841
   6      0.0000    0.0000   -0.4989   -0.1741   -0.1723    0.0549    0.0771    0.1240    0.1252    0.0761    0.9354    0.1460
   7      0.0000    0.0000    0.6514   -0.0159    0.0480   -0.1818   -0.2874   -0.3107   -0.3412   -0.3008   -1.1497   -0.3302

 Dipole mement (in D)   3.03 (DEN)      1.06      0.37      1.65      2.67      2.67      2.99      2.81      7.45      2.77

-----------------------------------------
File TZVPMol040.out
Molecule PMol040    acetonitrile
 SP Mol040 B3LYP/Def2TZVP VAC.
    0    6
Dipole          0.0000   -4.0096    0.0000    4.0096
Quadrupole      1.0690   -2.1379    1.0689    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.2752    0.0000   -0.1966   -0.2314    0.0729    0.3793    0.1793    0.4522    0.2782    0.9117    0.2372
   6      0.0000   -1.1678    0.0000   -0.2579   -0.2660   -0.0410   -0.4371   -0.1817   -0.4726   -0.7040    0.0832   -0.2038
   1      1.0189   -1.5496    0.0000    0.1532    0.1490    0.0658    0.1603    0.1187    0.1718    0.2491    0.0674    0.1179
   1     -0.5094   -1.5496    0.8824    0.1532    0.1490    0.0658    0.1603    0.1187    0.1730    0.2491    0.0674    0.1179
   1     -0.5094   -1.5496   -0.8824    0.1532    0.1490    0.0658    0.1603    0.1187    0.1730    0.2491    0.0674    0.1179
   7     -0.0000    1.4292    0.0000   -0.0052    0.0505   -0.2292   -0.4231   -0.3538   -0.4974   -0.3214   -1.1969   -0.3872

 Dipole mement (in D)   4.01 (DEN)      2.27      1.79      2.72      3.53      3.82      4.02      3.45      8.98      3.84

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File TZVPMol041.out
Molecule PMol041    malonic_dinitrile
 SP Mol041 B3LYP/Def2TZVP VAC.
    0    7
Dipole          0.0002    3.8336    0.0000    3.8336
Quadrupole      5.3096    5.2938  -10.6034    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1     -0.8748    1.4769    0.0000    0.1778    0.1906    0.0900    0.1820    0.1475    0.1834    0.2855    0.1148    0.1370
   6      0.0000    0.8222    0.0000   -0.0200   -0.2050    0.0264   -0.3284   -0.0620   -0.3322   -0.5893    0.1765   -0.0614
   1      0.8750    1.4768    0.0000    0.1778    0.1906    0.0900    0.1820    0.1475    0.1840    0.2855    0.1148    0.1370
   6     -0.0000    0.0245    1.2160   -0.2007   -0.1792    0.0850    0.3426    0.1963    0.4218    0.2741    0.9355    0.2385
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6	-0.0000	0.0245	-1.2160	-0.2007	-0.1792	0.0850	0.3426	0.1963	0.4218	0.2741	0.9355	0.2385
7	-0.0000	-0.5844	2.1945	0.0329	0.0911	-0.1882	-0.3604	-0.3127	-0.4394	-0.2650	-1.1385	-0.3448
7	-0.0000	-0.5844	-2.1945	0.0329	0.0911	-0.1882	-0.3604	-0.3127	-0.4394	-0.2650	-1.1385	-0.3448

Dipole mement (in D) 3.83 (DEN) 2.21 1.34 2.46 3.39 3.65 3.86 3.28 8.94 3.69

File TZVPMol042.out
Molecule PMol042 propionitrile
SP Mol042 B3LYP/Def2TZVP VAC.
0 9
Dipole -2.3256 3.3919 0.0000 4.1126
Quadrupole -0.9849 -1.4310 2.4159 3.8480 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.7651	-0.4290	0.0000	-0.2164	-0.2051	0.0712	0.3542	0.1794	0.2718	0.2813	0.9007	0.2336
6	0.0000	0.8032	0.0000	-0.0919	-0.2637	-0.0118	-0.2217	-0.1137	0.1021	-0.4974	0.1166	-0.1001
7	1.3581	-1.4196	0.0000	-0.0029	0.0511	-0.2317	-0.4258	-0.3564	-0.4595	-0.3256	-1.2032	-0.3901
6	-1.5051	0.5655	0.0000	-0.3258	-0.2785	-0.0686	-0.3321	-0.2191	-0.1687	-0.5724	0.0283	-0.2382
1	0.3001	1.3879	0.8717	0.1327	0.1608	0.0587	0.1329	0.1148	0.0365	0.2406	0.0505	0.1074
1	0.3001	1.3879	-0.8717	0.1327	0.1608	0.0587	0.1329	0.1148	0.0365	0.2406	0.0505	0.1074
1	-2.0362	1.5143	0.0000	0.1225	0.1228	0.0406	0.1189	0.0923	0.0514	0.2096	0.0142	0.0952
1	-1.8152	0.0043	0.8784	0.1246	0.1259	0.0415	0.1203	0.0939	0.0649	0.2117	0.0213	0.0925
1	-1.8152	0.0043	-0.8784	0.1246	0.1259	0.0415	0.1203	0.0939	0.0649	0.2117	0.0213	0.0925

Dipole mement (in D) 4.11 (DEN) 2.38 1.90 2.85 3.63 3.96 4.09 3.53 9.20 3.94

File TZVPMol043.out
Molecule PMol043 butanenitrile(anti)
SP Mol043 B3LYP/Def2TZVP VAC.
0 12
Dipole 3.3353 2.3214 0.4854 4.0925
Quadrupole -5.3538 2.4997 2.8541 -3.5772 -0.8780 0.1059

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2838	0.0512	0.0468	-0.2337	-0.2049	0.0728	0.3606	0.1806	0.3544	0.2821	0.8980	0.2357
7	-2.1491	-0.6904	-0.1411	-0.0009	0.0497	-0.2316	-0.4281	-0.3570	-0.4797	-0.3295	-1.2059	-0.3886
6	-0.1753	0.9615	0.2638	-0.0942	-0.2404	-0.0153	-0.2593	-0.1157	-0.2053	-0.5004	0.1076	-0.1063
6	1.1233	0.4749	-0.3844	-0.1504	-0.2710	-0.0333	-0.1161	-0.1448	0.2398	-0.3661	0.0632	-0.1286
1	-0.4588	1.9432	-0.1193	0.1358	0.1615	0.0583	0.1310	0.1145	0.0890	0.2450	0.0498	0.1070
1	-0.0407	1.0799	1.3419	0.1303	0.1622	0.0565	0.1321	0.1131	0.1019	0.2378	0.0468	0.1041
6	1.5926	-0.8578	0.1627	-0.3527	-0.3009	-0.0823	-0.3486	-0.2333	-0.2882	-0.5973	0.0108	-0.2497
1	0.9773	0.4102	-1.4638	0.1055	0.1401	0.0372	0.0986	0.0929	-0.0133	0.2037	0.0078	0.0849
1	1.8822	1.2421	-0.2254	0.1030	0.1366	0.0366	0.0978	0.0915	-0.0250	0.2024	0.0017	0.0876
1	2.5192	-1.1767	-0.3100	0.1172	0.1208	0.0357	0.1115	0.0872	0.0686	0.2114	0.0059	0.0896
1	1.7728	-0.8059	1.2369	0.1034	0.1192	0.0310	0.1056	0.0830	0.0690	0.1977	-0.0041	0.0827
1	0.8512	-1.6388	-0.0059	0.1368	0.1270	0.0342	0.1149	0.0877	0.0887	0.2132	0.0179	0.0815

Dipole mement (in D) 4.09 (DEN) 2.35 1.81 2.81 3.66 3.93 4.06 3.49 9.15 3.92

File TZVPMol044.out
Molecule PMol044 butanenitrile(gauche)
 SP Mol044 B3LYP/Def2TZVP VAC.
  0 12
Dipole 4.2455 0.0200 0.0000 4.2455
Quadrupole -8.6090 4.4112 4.1977 1.0326 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.4442	0.5081	0.0000	-0.2192	-0.2034	0.0706	0.3522	0.1788	0.3164	0.2855	0.8994	0.2336
7	-2.5930	0.3918	0.0000	0.0052	0.0507	-0.2329	-0.4283	-0.3575	-0.4705	-0.3263	-1.2044	-0.3913
6	0.0000	0.6241	0.0000	-0.1087	-0.2392	-0.0156	-0.2580	-0.1157	-0.1470	-0.4991	0.1080	-0.1064
6	0.7131	-0.7289	0.0000	-0.1632	-0.2695	-0.0332	-0.1222	-0.1449	0.2387	-0.3671	0.0639	-0.1292
1	0.2992	1.2108	0.8723	0.1295	0.1617	0.0565	0.1324	0.1132	0.0872	0.2383	0.0470	0.1037
1	0.2992	1.2108	-0.8723	0.1295	0.1617	0.0565	0.1324	0.1132	0.0872	0.2383	0.0470	0.1037
6	2.2190	-0.5679	0.0000	-0.3295	-0.3032	-0.0791	-0.3309	-0.2309	-0.3283	-0.5899	0.0137	-0.2448
1	0.3893	-1.3013	0.8705	0.1081	0.1400	0.0378	0.0999	0.0936	-0.0138	0.2046	0.0094	0.0850
1	0.3893	-1.3013	-0.8705	0.1081	0.1400	0.0378	0.0999	0.0936	-0.0138	0.2046	0.0094	0.0850
1	2.7219	-1.5328	0.0000	0.1237	0.1226	0.0375	0.1124	0.0890	0.0869	0.2134	0.0098	0.0916
1	2.5626	-0.0205	-0.8783	0.1083	0.1193	0.0320	0.1052	0.0838	0.0785	0.1989	-0.0019	0.0846
1	2.5626	-0.0205	0.8783	0.1083	0.1193	0.0320	0.1052	0.0838	0.0785	0.1989	-0.0019	0.0846

Dipole mement (in D)	4.25 (DEN)	2.45	2.16	3.04	3.76	4.16	4.25	3.67	9.39	4.10

File TZVPMol045.out
Molecule PMol045 cyclopropane_carbonitril
 SP Mol045 B3LYP/Def2TZVP VAC.
  0 10
Dipole -4.2883 -0.0007 0.9101 4.3838
Quadrupole -6.2519 2.4803 3.7716 -0.0014 0.5777 -0.0003

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2546	0.7419	-0.2246	-0.1989	-0.1838	-0.0465	-0.2212	-0.1531	-0.2465	-0.3717	-0.0174	-0.1555
6	-0.2127	-0.0003	0.5766	0.0092	-0.2071	-0.0093	-0.1220	-0.0664	-0.1675	-0.3456	0.0466	-0.0369
6	-1.2549	-0.7415	-0.2251	-0.1989	-0.1838	-0.0465	-0.2212	-0.1531	-0.2458	-0.3717	-0.0172	-0.1555
1	-2.0137	1.2651	0.3372	0.1220	0.1337	0.0503	0.1273	0.1054	0.1402	0.2188	0.0454	0.1022
1	-0.3272	-0.0006	1.6519	0.1322	0.1653	0.0621	0.1333	0.1213	0.1645	0.2491	0.0716	0.1083
1	-2.0141	-1.2648	0.3365	0.1220	0.1337	0.0503	0.1272	0.1054	0.1402	0.2188	0.0453	0.1022
1	-0.9173	1.2546	-1.1127	0.1319	0.1391	0.0529	0.1323	0.1091	0.1581	0.2249	0.0561	0.1010
6	1.1422	-0.0005	0.1320	-0.2510	-0.1894	0.0673	0.3397	0.1792	0.3734	0.2776	0.9082	0.2258
1	-0.9178	-1.2538	-1.1135	0.1319	0.1391	0.0529	0.1323	0.1091	0.1575	0.2249	0.0561	0.1010
7	2.2386	0.0003	-0.2361	-0.0004	0.0532	-0.2335	-0.4277	-0.3570	-0.4742	-0.3252	-1.1951	-0.3925

Dipole mement (in D)	4.38 (DEN)	2.74	2.11	3.14	3.89	4.21	4.37	3.81	9.45	4.21

File TZVPMol046.out
Molecule PMol046 isobutyronitrile

SP Mol046 B3LYP/Def2TZVP VAC.
0 12
Dipole 1.1966 3.9593 0.0000 4.1362
Quadrupole 2.8197 -6.1359 3.3162 -1.8056 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	1.5291	0.2625	0.0000	0.1011	0.1732	0.0536	0.1108	0.1133	0.0036	0.2314	0.0383	0.0992
6	0.4354	0.3047	0.0000	0.0653	-0.2915	0.0165	0.0134	-0.0475	0.3642	-0.3162	0.1402	0.0048
6	-0.0249	-1.0784	0.0000	-0.2384	-0.1806	0.0710	0.3343	0.1812	0.2246	0.2854	0.8943	0.2318
7	-0.4047	-2.1692	0.0000	0.0040	0.0526	-0.2333	-0.4269	-0.3580	-0.4522	-0.3282	-1.2077	-0.3921
6	-0.0249	1.0240	1.2665	-0.3324	-0.2551	-0.0723	-0.3728	-0.2210	-0.3933	-0.5697	0.0205	-0.2440
6	-0.0249	1.0240	-1.2665	-0.3324	-0.2551	-0.0723	-0.3728	-0.2210	-0.3933	-0.5697	0.0202	-0.2440
1	-1.1117	1.0804	1.3063	0.1190	0.1270	0.0392	0.1200	0.0923	0.1155	0.2094	0.0168	0.0891
1	0.3648	2.0403	1.2782	0.1182	0.1241	0.0384	0.1186	0.0907	0.1030	0.2075	0.0099	0.0916
1	0.3169	0.5172	2.1659	0.1292	0.1271	0.0408	0.1183	0.0934	0.1048	0.2166	0.0203	0.0914
1	-1.1117	1.0804	-1.3063	0.1190	0.1270	0.0392	0.1200	0.0923	0.1155	0.2094	0.0168	0.0891
1	0.3648	2.0403	-1.2782	0.1182	0.1241	0.0384	0.1186	0.0907	0.1030	0.2075	0.0099	0.0916
1	0.3169	0.5172	-2.1659	0.1292	0.1271	0.0408	0.1183	0.0934	0.1048	0.2166	0.0203	0.0914

Dipole mement (in D) 4.14 (DEN) 2.40 2.06 2.90 3.58 4.04 4.13 3.60 9.28 3.97

File TZVPMol047.out
Molecule PMol047 cyclobutane_carbonitrile
SP Mol047 B3LYP/Def2TZVP VAC.
0 13
Dipole -3.0052 -3.1534 0.0000 4.3560
Quadrupole -0.3912 -3.5239 3.9151 -6.8190 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.7308	1.3613	0.0000	-0.2702	-0.1854	0.0659	0.3196	0.1774	0.2020	0.2863	0.8901	0.2246
7	1.6056	2.1166	0.0000	0.0113	0.0532	-0.2332	-0.4253	-0.3570	-0.4359	-0.3256	-1.2026	-0.3920
6	-0.3356	0.3896	0.0000	0.0468	-0.2182	0.0068	-0.0701	-0.0505	0.1521	-0.3283	0.1034	-0.0164
6	-0.3356	-0.7259	1.0700	-0.1859	-0.1893	-0.0368	-0.1778	-0.1429	-0.1355	-0.3564	0.0305	-0.1426
6	-0.3356	-0.7259	-1.0700	-0.1859	-0.1893	-0.0368	-0.1778	-0.1429	-0.1355	-0.3564	0.0304	-0.1426
1	0.6834	-0.9841	1.3533	0.1079	0.1410	0.0408	0.1039	0.0974	0.0861	0.2081	0.0202	0.0864
1	0.6834	-0.9841	-1.3533	0.1079	0.1410	0.0408	0.1039	0.0974	0.0861	0.2081	0.0202	0.0864
1	-0.9147	-0.5513	1.9742	0.1077	0.1249	0.0369	0.0944	0.0908	0.0427	0.2073	0.0130	0.0871
1	-0.9147	-0.5513	-1.9742	0.1077	0.1249	0.0369	0.0944	0.0908	0.0427	0.2073	0.0130	0.0871
1	-1.2933	0.9130	0.0000	0.1073	0.1725	0.0549	0.1137	0.1152	0.0577	0.2342	0.0448	0.0989
6	-0.8864	-1.6764	0.0000	-0.1512	-0.2323	-0.0451	-0.1649	-0.1535	-0.0408	-0.3898	0.0266	-0.1464
1	-1.9759	-1.6897	0.0000	0.0938	0.1336	0.0342	0.0932	0.0895	0.0456	0.1983	0.0022	0.0836
1	-0.5326	-2.7047	0.0000	0.1028	0.1233	0.0346	0.0927	0.0883	0.0327	0.2067	0.0079	0.0857

Dipole mement (in D) 4.36 (DEN) 2.87 2.13 3.16 3.88 4.24 4.32 3.72 9.65 4.22

File TZVPMol048.out
Molecule PMol048 t-butyl_cyanide
SP Mol048 B3LYP/Def2TZVP VAC.

```
    0   15
Dipole         -4.1313   -0.0001    0.0000    4.1313
Quadrupole     -7.3510    3.6757    3.6753   -0.0002    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      1.1904   -0.0000    0.0000   -0.2638   -0.1596    0.0718    0.3239    0.1842    0.2481    0.2912    0.8917    0.2313
   7      2.3456    0.0000    0.0000    0.0145    0.0541   -0.2349   -0.4203   -0.3598   -0.4708   -0.3305   -1.2120   -0.3940
   6     -0.2750    0.0000    0.0000    0.1691   -0.3462    0.0442    0.2187    0.0177    0.5295   -0.1563    0.1533    0.1107
   6     -0.7673    1.4507    0.0000   -0.3389   -0.2325   -0.0748   -0.4119   -0.2215   -0.4719   -0.5690    0.0158   -0.2487
   6     -0.7673   -0.7254    1.2564   -0.3389   -0.2325   -0.0748   -0.4118   -0.2214   -0.4664   -0.5690    0.0160   -0.2486
   6     -0.7673   -0.7254   -1.2564   -0.3389   -0.2325   -0.0748   -0.4118   -0.2214   -0.4664   -0.5690    0.0163   -0.2486
   1     -1.8570    1.4650    0.0000    0.1163    0.1262    0.0369    0.1244    0.0899    0.1225    0.2058    0.0071    0.0888
   1     -1.8570   -0.7324    1.2689    0.1164    0.1262    0.0369    0.1244    0.0899    0.1214    0.2058    0.0071    0.0888
   1     -1.8570   -0.7324   -1.2689    0.1164    0.1262    0.0369    0.1244    0.0899    0.1214    0.2058    0.0071    0.0888
   1     -0.4214    1.9885   -0.8810    0.1247    0.1284    0.0388    0.1234    0.0921    0.1231    0.2142    0.0163    0.0886
   1     -0.4215   -1.7572    1.2814    0.1246    0.1284    0.0388    0.1233    0.0921    0.1211    0.2142    0.0162    0.0886
   1     -0.4212   -0.2314   -2.1625    0.1246    0.1284    0.0388    0.1233    0.0921    0.1221    0.2142    0.0162    0.0886
   1     -0.4214    1.9885    0.8810    0.1247    0.1284    0.0388    0.1234    0.0921    0.1231    0.2142    0.0163    0.0886
   1     -0.4212   -0.2314    2.1625    0.1246    0.1284    0.0388    0.1233    0.0921    0.1221    0.2142    0.0162    0.0886
   1     -0.4215   -1.7572   -1.2814    0.1246    0.1284    0.0388    0.1233    0.0921    0.1211    0.2142    0.0162    0.0886

 Dipole mement (in D)   4.13 (DEN)      2.45      2.21      2.93      3.44      4.10      4.15      3.67      9.32      3.97

-----------------------------------------
File TZVPMol049.out
Molecule PMol049    pentanenitrile
 SP Mol049 B3LYP/Def2TZVP VAC.
    0   15
Dipole         -3.8938    1.9676    0.0000    4.3627
Quadrupole     -5.7247   -0.0355    5.7602    8.3456    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0250   -1.1191    0.0000   -0.0972   -0.2375   -0.0157   -0.2613   -0.1158   -0.3009   -0.4973    0.1078   -0.1063
   6      0.0000    0.4088    0.0000   -0.1976   -0.2447   -0.0360   -0.1543   -0.1459    0.1064   -0.3654    0.0552   -0.1348
   1     -0.5067   -1.5076    0.8723    0.1299    0.1620    0.0563    0.1303    0.1130    0.1154    0.2386    0.0468    0.1036
   1     -0.5067   -1.5076   -0.8723    0.1299    0.1620    0.0563    0.1303    0.1130    0.1154    0.2386    0.0468    0.1036
   6     -1.4158    0.9574    0.0000   -0.1407   -0.2906   -0.0422   -0.1194   -0.1551    0.1868   -0.3828    0.0536   -0.1349
   1      0.5461    0.7782    0.8709    0.1063    0.1415    0.0364    0.0998    0.0927    0.0074    0.2032    0.0063    0.0821
   1      0.5461    0.7782   -0.8709    0.1063    0.1415    0.0364    0.0998    0.0927    0.0074    0.2032    0.0063    0.0821
   6     -1.4550    2.4726    0.0000   -0.3299   -0.3049   -0.0810   -0.3311   -0.2329   -0.3288   -0.5841    0.0143   -0.2457
   1     -1.9533    0.5709   -0.8709    0.0877    0.1334    0.0290    0.0857    0.0841   -0.0269    0.1915   -0.0138    0.0779
   1     -1.9533    0.5709    0.8709    0.0877    0.1334    0.0290    0.0857    0.0841   -0.0269    0.1915   -0.0138    0.0779
   1     -2.4754    2.8517    0.0000    0.1174    0.1191    0.0330    0.1050    0.0844    0.0874    0.2073    0.0018    0.0868
   1     -0.9541    2.8826    0.8774    0.1075    0.1189    0.0308    0.1025    0.0826    0.0736    0.1985   -0.0030    0.0833
   1     -0.9541    2.8826   -0.8774    0.1075    0.1189    0.0308    0.1025    0.0826    0.0736    0.1985   -0.0030    0.0833
   6      1.3654   -1.6689    0.0000   -0.2214   -0.2032    0.0704    0.3542    0.1786    0.4066    0.2861    0.8998    0.2335
   7      2.4420   -2.0863    0.0000    0.0065    0.0500   -0.2337   -0.4296   -0.3584   -0.4965   -0.3273   -1.2054   -0.3922

 Dipole mement (in D)   4.36 (DEN)      2.56      2.18      3.14      3.91      4.25      4.37      3.72      9.52      4.21
```

File TZVPMol050.out
Molecule PMol050 benzonitrile
 SP Mol050 B3LYP/Def2TZVP VAC.
  0 13
Dipole 0.0000 0.0000 -4.7113 4.7113
Quadrupole -0.4279 8.7173 -8.2894 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.6083	0.2526	-0.1456	0.0126	0.0237	0.0087	0.1268	-0.1765	0.0747	0.0425
6	0.0000	1.2106	-0.0907	-0.2006	-0.0747	-0.0179	-0.1010	-0.0702	-0.1763	-0.1518	-0.0022	-0.0701
6	0.0000	-1.2106	-0.0907	-0.2006	-0.0747	-0.0179	-0.1010	-0.0702	-0.1763	-0.1518	-0.0022	-0.0701
6	0.0000	1.2038	-1.4750	-0.0881	-0.1258	-0.0284	-0.0915	-0.0843	-0.1011	-0.2016	-0.0130	-0.0744
6	0.0000	-1.2038	-1.4750	-0.0881	-0.1258	-0.0284	-0.0915	-0.0843	-0.1011	-0.2016	-0.0132	-0.0744
6	0.0000	0.0000	-2.1677	-0.1047	-0.1191	-0.0223	-0.0670	-0.0784	-0.0833	-0.1814	-0.0171	-0.0677
1	0.0000	2.1423	0.4585	0.1350	0.1550	0.0540	0.1124	0.1115	0.1505	0.2234	0.0596	0.0944
1	0.0000	-2.1423	0.4585	0.1350	0.1550	0.0540	0.1124	0.1115	0.1505	0.2234	0.0596	0.0944
1	0.0000	2.1412	-2.0153	0.1229	0.1479	0.0494	0.1060	0.1056	0.1243	0.2168	0.0449	0.0946
1	0.0000	-2.1412	-2.0153	0.1229	0.1479	0.0494	0.1060	0.1056	0.1243	0.2168	0.0449	0.0946
1	0.0000	0.0000	-3.2500	0.1231	0.1469	0.0490	0.1024	0.1051	0.1166	0.2143	0.0435	0.0942
6	0.0000	0.0000	2.0313	-0.2249	-0.1543	0.0659	0.2913	0.1815	0.2886	0.2722	0.8931	0.2197
7	0.0000	0.0000	3.1887	0.0155	0.0674	-0.2194	-0.4024	-0.3420	-0.4432	-0.3022	-1.1731	-0.3776

Dipole mement (in D)	4.71 (DEN)	2.41	2.28	3.51	4.33	4.56	4.71	4.17	9.96	4.58

File TZVPMol051.out
Molecule PMol051 2-methylaziridine(cis)
 SP Mol051 B3LYP/Def2TZVP VAC.
  0 11
Dipole -1.2535 -0.9942 -0.8508 1.8121
Quadrupole -1.1590 -0.8807 2.0396 -2.3691 -0.8431 -1.3827

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.9101	0.8125	-0.0290	-0.3537	-0.0146	-0.1881	-0.5207	-0.5186	-0.5995	-0.5703	-0.9036	-0.4935
1	-2.0865	0.8241	0.1049	0.1161	0.1220	0.0338	0.1101	0.0864	0.1319	0.2067	0.0053	0.0865
6	1.0094	-0.6450	-0.1501	-0.1414	-0.2703	-0.0379	-0.1140	-0.0893	-0.2172	-0.2558	0.2132	-0.0682
1	1.8005	-1.0983	0.4338	0.0991	0.1184	0.0382	0.1010	0.1006	0.1336	0.1923	0.0298	0.0946
1	0.8595	-1.0961	-1.1246	0.0958	0.1148	0.0349	0.0942	0.0969	0.1302	0.1819	0.0170	0.0901
6	-0.1570	-0.0384	0.5046	0.0252	-0.3138	0.0028	0.1296	-0.0117	0.1737	-0.0798	0.2546	0.0506
1	-0.1768	-0.0422	1.5898	0.0955	0.1365	0.0375	0.0832	0.1036	0.0992	0.1874	0.0234	0.0909
6	-1.5009	-0.0591	-0.1531	-0.3303	-0.2936	-0.0826	-0.3779	-0.2273	-0.4279	-0.6058	0.0227	-0.2436
1	-1.4037	-0.0879	-1.2397	0.0939	0.1204	0.0316	0.1066	0.0860	0.1253	0.1971	-0.0047	0.0847
1	-2.0808	-0.9321	0.1477	0.1089	0.1244	0.0355	0.1103	0.0874	0.1021	0.2112	0.0080	0.0870
1	0.6081	1.1998	-0.9176	0.1909	0.1559	0.0943	0.2776	0.2859	0.3486	0.3350	0.3345	0.2210

Dipole mement (in D)	1.81 (DEN)	1.40	1.13	0.81	1.73	2.02	1.81	2.44	3.39	2.04

File TZVPMol052.out

Molecule PMol052 2-methylaziridine(trans)
 SP Mol052 B3LYP/Def2TZVP VAC.
    0   11
Dipole   -0.1808   0.5850   1.5291   1.6471
Quadrupole   1.2243   -0.5023   -0.7220   -0.0122   -1.7470   -2.3415

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.8506	-0.7393	-0.3377	-0.3773	-0.0161	-0.1830	-0.5132	-0.5146	-0.5735	-0.5812	-0.9095	-0.4912
1	-1.4794	-1.2645	0.2587	0.1949	0.1569	0.0977	0.2756	0.2889	0.3351	0.3416	0.3394	0.2267
6	-0.9844	0.6911	-0.0527	-0.1323	-0.2695	-0.0381	-0.1181	-0.0894	-0.1686	-0.2556	0.2134	-0.0683
1	-1.7537	1.0191	0.6357	0.0977	0.1134	0.0358	0.0907	0.0971	0.0871	0.1858	0.0190	0.0921
1	-0.8520	1.3359	-0.9135	0.0948	0.1197	0.0375	0.1046	0.1005	0.1470	0.1886	0.0275	0.0930
6	0.1645	-0.0599	0.4732	0.0417	-0.3150	0.0026	0.1354	-0.0118	0.1306	-0.0828	0.2530	0.0501
1	0.1463	-0.2608	1.5404	0.0922	0.1299	0.0338	0.0692	0.0986	0.0786	0.1801	0.0102	0.0869
6	1.5273	0.0525	-0.1326	-0.3265	-0.2866	-0.0850	-0.3775	-0.2285	-0.3935	-0.5966	0.0307	-0.2434
1	1.4529	0.2441	-1.2020	0.1131	0.1263	0.0357	0.1219	0.0912	0.1425	0.2112	0.0148	0.0879
1	2.0966	0.8652	0.3192	0.0970	0.1199	0.0306	0.1022	0.0827	0.0879	0.2030	-0.0020	0.0817
1	2.0988	-0.8663	-0.0013	0.1046	0.1210	0.0325	0.1092	0.0853	0.1269	0.2060	0.0034	0.0845

Dipole mement (in D)	1.65 (DEN)	1.43	0.50	0.61	1.72	1.72	1.57	2.12	3.16	1.86

File TZVPMol053.out
Molecule PMol053 E-ethanimine
 SP Mol053 B3LYP/Def2TZVP VAC.
    0   8
Dipole   -0.8108   1.8870   0.0004   2.0538
Quadrupole   1.5952   -0.9336   -0.6617   2.4185   0.0005   0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	1.2023	-0.3527	-0.0000	-0.2892	-0.0608	-0.2227	-0.5877	-0.5164	-0.7116	-0.6066	-1.1250	-0.4937
6	0.1858	0.4047	-0.0001	-0.0706	-0.2968	0.0583	0.3187	0.0837	0.4234	0.1404	0.7099	0.1450
1	0.2573	1.5026	0.0002	0.0706	0.1099	0.0327	0.0424	0.0954	-0.0222	0.1354	0.0106	0.0850
1	2.0613	0.1942	0.0001	0.1960	0.1538	0.0919	0.2717	0.2786	0.3303	0.3279	0.3308	0.2221
6	-1.1952	-0.1414	0.0000	-0.2451	-0.2913	-0.0845	-0.4361	-0.2260	-0.3092	-0.6593	-0.0016	-0.2391
1	-1.1820	-1.2280	-0.0001	0.1127	0.1278	0.0419	0.1425	0.0979	0.1179	0.2252	0.0387	0.0947
1	-1.7478	0.2102	0.8726	0.1128	0.1287	0.0412	0.1242	0.0935	0.0857	0.2185	0.0182	0.0930
1	-1.7480	0.2104	-0.8723	0.1128	0.1287	0.0412	0.1242	0.0935	0.0857	0.2185	0.0182	0.0930

Dipole mement (in D)	2.05 (DEN)	1.14	0.24	1.02	2.03	1.95	2.04	2.42	4.65	2.07

File TZVPMol054.out
Molecule PMol054 Z-ethanimine
 SP Mol054 B3LYP/Def2TZVP VAC.
    0   8
Dipole   2.5170   -0.4994   0.0000   2.5661
Quadrupole   -3.3188   3.0253   0.2935   1.3455   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-1.3076	-0.1572	0.0000	-0.2997	-0.0604	-0.2276	-0.5899	-0.5200	-0.7557	-0.5903	-1.1152	-0.4952

6	-0.1890	0.4369	-0.0000	-0.0324	-0.3009	0.0571	0.3084	0.0822	0.4467	0.1413	0.7148	0.1437
1	-0.2195	1.5315	0.0000	0.1013	0.1283	0.0385	0.0640	0.1043	0.0228	0.1533	0.0261	0.0917
1	-1.1718	-1.1704	0.0000	0.1802	0.1503	0.0871	0.2705	0.2731	0.3591	0.3136	0.3189	0.2143
6	1.1758	-0.1618	0.0000	-0.2868	-0.2998	-0.0821	-0.4350	-0.2253	-0.4119	-0.6723	-0.0086	-0.2407
1	1.1416	-1.2500	0.0000	0.0971	0.1204	0.0384	0.1239	0.0928	0.1106	0.2064	0.0123	0.0932
1	1.7413	0.1693	-0.8722	0.1201	0.1311	0.0443	0.1291	0.0964	0.1142	0.2240	0.0259	0.0965
1	1.7413	0.1693	0.8722	0.1201	0.1311	0.0443	0.1291	0.0964	0.1142	0.2240	0.0259	0.0965

Dipole mement (in D) 2.57 (DEN) 1.73 1.13 1.34 2.22 2.43 2.54 2.74 5.04 2.44

File TZVPMol055.out
Molecule PMol055 Z-N-ethylidene_methanami
SP Mol055 B3LYP/Def2TZVP VAC.
0 11
Dipole -0.3577 1.4193 0.0000 1.4637
Quadrupole 2.5745 -1.9446 -0.6298 0.0529 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.4974	-0.4732	-0.0000	-0.1740	0.0747	-0.1550	-0.3155	-0.3661	-0.4912	-0.3980	-1.1497	-0.3845
6	-0.4633	0.3477	-0.0000	-0.0570	-0.2675	0.0491	0.2554	0.0802	0.4245	0.1260	0.7096	0.1298
1	-0.2830	1.4375	0.0000	0.0458	0.1095	0.0263	0.0381	0.0902	-0.0058	0.1248	0.0034	0.0752
6	1.8373	0.0546	0.0000	-0.1966	-0.3335	-0.0468	-0.1887	-0.1320	0.0276	-0.4194	0.3388	-0.1204
6	-1.8835	-0.0842	0.0000	-0.2609	-0.2904	-0.0851	-0.4359	-0.2264	-0.4537	-0.6459	0.0052	-0.2396
1	1.8834	1.1517	0.0000	0.0723	0.0961	0.0201	0.0659	0.0798	0.0012	0.1585	-0.0130	0.0750
1	2.3749	-0.3170	0.8731	0.1174	0.1146	0.0363	0.1016	0.0975	0.0638	0.1987	0.0194	0.0951
1	2.3749	-0.3169	-0.8731	0.1174	0.1146	0.0363	0.1016	0.0975	0.0638	0.1987	0.0194	0.0951
1	-1.9590	-1.1682	-0.0000	0.1125	0.1273	0.0401	0.1340	0.0960	0.1267	0.2245	0.0360	0.0925
1	-2.4080	0.3084	0.8726	0.1115	0.1273	0.0394	0.1217	0.0916	0.1216	0.2162	0.0154	0.0909
1	-2.4080	0.3085	-0.8725	0.1115	0.1273	0.0394	0.1217	0.0916	0.1216	0.2162	0.0154	0.0909

Dipole mement (in D) 1.46 (DEN) 0.41 0.35 0.69 1.22 1.57 1.47 1.83 4.02 1.59

File TZVPMol056.out
Molecule PMol056 N-methylformaldimine
SP Mol056 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.0172 1.4844 0.0000 1.4845
Quadrupole 2.6589 -1.9999 -0.6589 0.5565 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.1375	-0.5329	-0.0000	-0.1657	0.0563	-0.1427	-0.2497	-0.3577	-0.4573	-0.3743	-1.1326	-0.3626
6	1.1755	0.1800	-0.0000	-0.1460	-0.2592	0.0106	0.0294	0.0052	0.1732	-0.0586	0.7007	0.0225
1	1.1605	1.2806	0.0000	0.0723	0.0921	0.0307	0.0598	0.0914	0.0394	0.1280	0.0160	0.0835
6	-1.1398	0.1342	0.0000	-0.1996	-0.3311	-0.0435	-0.2045	-0.1291	0.1105	-0.4286	0.3327	-0.1185
1	2.1543	-0.2965	0.0000	0.1194	0.1101	0.0422	0.0800	0.1050	0.0406	0.1677	0.0406	0.0988
1	-1.0711	1.2295	0.0000	0.0756	0.0973	0.0228	0.0715	0.0825	-0.0017	0.1596	-0.0088	0.0779
1	-1.7101	-0.1843	-0.8728	0.1220	0.1172	0.0400	0.1068	0.1014	0.0477	0.2031	0.0258	0.0992
1	-1.7101	-0.1843	0.8728	0.1220	0.1172	0.0400	0.1068	0.1014	0.0477	0.2031	0.0258	0.0992

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 Dipole mement (in D)   1.48 (DEN)      0.90      0.43      0.54      1.03      1.56      1.48      1.76      3.96      1.53

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File TZVPMol057.out
Molecule PMol057    diazomethane
 SP Mol057 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000   -1.6683    1.6683
Quadrupole     -1.3353    2.3417   -1.0064    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   7      0.0000    0.0000    1.2899   -0.1891   -0.0102   -0.0987   -0.2032   -0.1060   -0.3725   -0.0276    0.0550   -0.1177
   7      0.0000    0.0000    0.1524    0.1936    0.1441    0.1092    0.3549   -0.0053    0.6962    0.0485   -0.6030    0.0149
   6      0.0000    0.0000   -1.1364   -0.2960   -0.3846   -0.1158   -0.4819   -0.1248   -1.0072   -0.4747    0.3487   -0.1166
   1      0.0000    0.9511   -1.6387    0.1458    0.1253    0.0527    0.1651    0.1181    0.3418    0.2269    0.0997    0.1097
   1      0.0000   -0.9511   -1.6387    0.1458    0.1253    0.0527    0.1651    0.1181    0.3418    0.2269    0.0997    0.1097

 Dipole mement (in D)   1.67 (DEN)      1.71      0.17      0.73      0.97      1.84      1.68      1.12      3.57      1.81

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File TZVPMol058.out
Molecule PMol058    methyl_azide
 SP Mol058 B3LYP/Def2TZVP VAC.
    0    7
Dipole          2.1743    0.9331    0.0000    2.3661
Quadrupole     -0.4303   -0.3900    0.8203    1.8539    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   7     -1.7935    0.2663   -0.0000   -0.2223   -0.0341   -0.1222   -0.2762   -0.1235   -0.3917   -0.0826    0.0603   -0.1366
   7     -0.7140   -0.0925    0.0000    0.3513    0.0653    0.1593    0.4722    0.1447    0.6637    0.2213   -0.1386    0.1679
   7      0.3900   -0.6228    0.0000   -0.2910   -0.0508   -0.1334   -0.3291   -0.2253   -0.4850   -0.3150   -0.3575   -0.2383
   6      1.5440    0.2779    0.0000   -0.2187   -0.3230   -0.0311   -0.1953   -0.1121    0.0059   -0.4161    0.3334   -0.1027
   1      2.4294   -0.3478    0.0000    0.1345    0.1212    0.0494    0.1246    0.1126    0.1030    0.2106    0.0458    0.1125
   1      1.5644    0.9117    0.8879    0.1231    0.1107    0.0390    0.1019    0.1018    0.0520    0.1909    0.0284    0.0986
   1      1.5644    0.9117   -0.8879    0.1231    0.1107    0.0390    0.1019    0.1018    0.0520    0.1909    0.0284    0.0986

 Dipole mement (in D)   2.37 (DEN)      2.20      0.78      1.25      1.88      2.38      2.41      2.20      3.28      2.41

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File TZVPMol059.out
Molecule PMol059    E-2-butenenitrile
 SP Mol059 B3LYP/Def2TZVP VAC.
    0   10
Dipole          4.7898    0.5594    0.0003    4.8224
Quadrupole     -6.1563    4.6830    1.4733   -1.9743   -0.0005   -0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   6     -1.4905    0.0901   -0.0001   -0.2024   -0.1963    0.0612    0.3276    0.1737    0.4570    0.2496    0.8910    0.2203
   7     -2.6090   -0.2106   -0.0002   -0.0041    0.0607   -0.2238   -0.4096   -0.3463   -0.4852   -0.3072   -1.1756   -0.3819
   6     -0.1318    0.4842   -0.0000   -0.0703   -0.1678   -0.0283   -0.2245   -0.0787   -0.4447   -0.3389    0.0521   -0.0665
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   6      0.8841   -0.3840    0.0001   -0.0536   -0.1285    0.0134    0.0667   -0.0492    0.1231   -0.0659    0.0098   -0.0233
   6      2.3133   -0.0037    0.0001   -0.3138   -0.2762   -0.0723   -0.3872   -0.2195   -0.2748   -0.6365    0.0209   -0.2379
   1      0.0539    1.5534    0.0000    0.1355    0.1601    0.0587    0.1361    0.1162    0.2282    0.2296    0.0688    0.1011
   1      0.6542   -1.4452    0.0000    0.1318    0.1512    0.0540    0.1046    0.1109    0.0976    0.2051    0.0542    0.0962
   1      2.4517    1.0755    0.0001    0.1164    0.1278    0.0428    0.1252    0.0954    0.0990    0.2122    0.0193    0.0947
   1      2.8262   -0.4148    0.8714    0.1303    0.1345    0.0472    0.1305    0.0988    0.0999    0.2261    0.0300    0.0987
   1      2.8263   -0.4148   -0.8709    0.1303    0.1345    0.0472    0.1305    0.0988    0.0999    0.2261    0.0300    0.0987

 Dipole mement (in D)   4.82 (DEN)      3.19      2.81      3.62      4.30      4.71      4.84      4.27      9.99      4.66

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File TZVPMol060.out
Molecule PMol060    Z-2-butenenitrile
 SP Mol060 B3LYP/Def2TZVP VAC.
    0   10
Dipole         -4.1464    1.1772    0.0000    4.3103
Quadrupole     -4.2758    3.8987    0.3772    2.5940    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -1.2065    0.4070    0.0000   -0.0569   -0.1340    0.0125    0.0734   -0.0502    0.1756   -0.0635    0.0081   -0.0232
   6      0.0000    0.9846    0.0000   -0.0841   -0.1731   -0.0305   -0.2345   -0.0812   -0.5509   -0.3428    0.0502   -0.0687
   6      1.2106    0.2500    0.0000   -0.1920   -0.1970    0.0648    0.3417    0.1768    0.5575    0.2444    0.8867    0.2240
   6     -1.4706   -1.0482    0.0000   -0.3243   -0.2714   -0.0744   -0.4045   -0.2207   -0.3138   -0.6485    0.0148   -0.2419
   1     -2.0694    1.0648    0.0000    0.1254    0.1474    0.0512    0.1000    0.1071    0.0815    0.2016    0.0447    0.0985
   1      0.0985    2.0629    0.0000    0.1433    0.1613    0.0602    0.1344    0.1173    0.2285    0.2383    0.0743    0.1037
   1     -0.5541   -1.6344    0.0000    0.1418    0.1359    0.0437    0.1332    0.0986    0.1266    0.2271    0.0400    0.0892
   1     -2.0623   -1.3340    0.8713    0.1268    0.1351    0.0470    0.1323    0.0987    0.1052    0.2267    0.0292    0.0981
   1     -2.0623   -1.3340   -0.8713    0.1268    0.1351    0.0470    0.1323    0.0987    0.1052    0.2267    0.0292    0.0981
   7      2.2070   -0.3408    0.0000   -0.0068    0.0606   -0.2216   -0.4082   -0.3450   -0.5155   -0.3099   -1.1775   -0.3779

 Dipole mement (in D)   4.31 (DEN)      2.65      2.29      3.11      4.01      4.15      4.31      4.03      9.24      4.18

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File TZVPMol061.out
Molecule PMol061    cyanoacetylene
 SP Mol061 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000   -3.8804    3.8804
Quadrupole     -0.5547   -0.5547    1.1094    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.0000   -1.8315   -0.0900    0.0170   -0.0154   -0.1514   -0.0663   -0.2377   -0.0740   -0.0623   -0.0748
   6      0.0000    0.0000   -0.6285    0.0393   -0.0896   -0.0121   -0.0444   -0.0107   -0.0934   -0.1398   -0.0398    0.0005
   1      0.0000    0.0000   -2.8942    0.2193    0.1373    0.1103    0.2175    0.1642    0.2897    0.2419    0.2021    0.1600
   6      0.0000    0.0000    0.7332   -0.2012   -0.1775    0.0875    0.3154    0.2040    0.4686    0.2038    0.9844    0.2395
   7      0.0000    0.0000    1.8936    0.0326    0.1128   -0.1703   -0.3370   -0.2912   -0.4272   -0.2319   -1.0844   -0.3252

 Dipole mement (in D)   3.88 (DEN)      2.79      1.39      2.60      3.51      3.60      3.89      3.68      8.54      3.68

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File TZVPMol062.out
Molecule PMol062 acrylonitrile
 SP Mol062 B3LYP/Def2TZVP VAC.
    0   7
Dipole   3.9419   0.7372   0.0000   4.0102
Quadrupole   -2.8472   3.2406   -0.3934   -1.2411   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.5795	0.4990	0.0000	-0.0332	-0.1859	-0.0098	-0.1382	-0.0625	-0.2128	-0.3171	0.0635	-0.0414
6	-0.7772	0.0887	-0.0000	-0.1830	-0.1895	0.0678	0.3227	0.1806	0.4291	0.2415	0.8964	0.2255
7	-1.8919	-0.2231	-0.0000	0.0014	0.0716	-0.2112	-0.3921	-0.3338	-0.4673	-0.2918	-1.1616	-0.3685
1	0.7449	1.5705	0.0000	0.1465	0.1620	0.0657	0.1366	0.1226	0.1763	0.2361	0.0809	0.1098
6	1.6018	-0.3528	0.0000	-0.2112	-0.1219	-0.0277	-0.1919	-0.1289	-0.2748	-0.2767	-0.0123	-0.1380
1	2.6215	0.0046	0.0000	0.1366	0.1300	0.0567	0.1300	0.1097	0.1683	0.2031	0.0629	0.1078
1	1.4519	-1.4237	0.0000	0.1430	0.1336	0.0585	0.1329	0.1123	0.1813	0.2048	0.0703	0.1048

Dipole mement (in D)	4.01 (DEN)	2.22	1.75	2.81	3.61	3.85	4.02	3.61	9.07	3.88

File TZVPMol063.out
Molecule PMol063 methacrylonitrile
 SP Mol063 B3LYP/Def2TZVP VAC.
    0   10
Dipole   -0.9656   3.9257   0.0000   4.0427
Quadrupole   4.0172   -4.6111   0.5939   2.2095   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.3053	-0.9842	0.0000	-0.1973	-0.1589	0.0672	0.2945	0.1818	0.3291	0.2556	0.8886	0.2227
7	0.5173	-2.1223	0.0000	0.0044	0.0687	-0.2170	-0.3931	-0.3398	-0.4565	-0.3002	-1.1719	-0.3749
6	0.0000	0.4103	0.0000	0.0968	-0.2272	0.0269	0.1261	0.0121	0.1926	-0.1275	0.0766	0.0729
6	-1.4536	0.7640	0.0000	-0.3212	-0.2325	-0.0704	-0.4095	-0.2146	-0.3085	-0.6042	0.0288	-0.2415
6	0.9932	1.3015	0.0000	-0.2308	-0.1137	-0.0480	-0.2756	-0.1468	-0.5036	-0.2944	-0.0264	-0.1638
1	0.7829	2.3626	0.0000	0.1241	0.1290	0.0497	0.1306	0.1034	0.2145	0.1974	0.0505	0.0993
1	2.0305	0.9994	0.0000	0.1392	0.1340	0.0532	0.1314	0.1075	0.2060	0.2091	0.0646	0.0986
1	-1.5893	1.8424	0.0000	0.1161	0.1296	0.0442	0.1308	0.0972	0.1064	0.2154	0.0223	0.0963
1	-1.9572	0.3512	0.8740	0.1343	0.1355	0.0470	0.1324	0.0996	0.1100	0.2244	0.0336	0.0952
1	-1.9572	0.3512	-0.8740	0.1343	0.1355	0.0470	0.1324	0.0996	0.1100	0.2244	0.0336	0.0952

Dipole mement (in D)	4.04 (DEN)	2.14	1.90	2.85	3.43	3.93	4.05	3.51	9.23	3.88

File TZVPMol064.out
Molecule PMol064 2-cyanopyridine
 SP Mol064 B3LYP/Def2TZVP VAC.
    0   12
Dipole   1.7261   -5.5816   0.0000   5.8424
Quadrupole   5.0680   -5.6404   0.5724   1.0664   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.1279	-1.5280	0.0000	-0.0828	-0.1061	-0.0094	-0.0259	-0.0630	0.1786	-0.1650	-0.0076	-0.0523
6	-0.1177	-2.1344	0.0000	-0.0813	-0.1282	-0.0261	-0.1498	-0.0764	-0.4216	-0.2270	-0.0232	-0.0665

6	1.1964	-0.1453	0.0000	-0.1629	-0.0817	-0.0212	-0.1811	-0.0680	-0.4782	-0.1934	-0.0058	-0.0684
6	-1.2497	-1.3279	0.0000	-0.0510	-0.1874	0.0352	0.1474	0.0602	0.3806	0.0404	0.5273	0.0921
6	0.0000	0.5710	0.0000	0.2500	-0.2189	0.0699	0.2389	0.1444	0.5864	0.0614	0.5815	0.1995
7	-1.2105	-0.0006	0.0000	-0.2121	0.1855	-0.1377	-0.3690	-0.3240	-0.5982	-0.3631	-1.0713	-0.3852
1	-0.2161	-3.2115	0.0000	0.1285	0.1491	0.0544	0.1155	0.1109	0.1812	0.2210	0.0551	0.1006
1	2.1426	0.3781	0.0000	0.1385	0.1571	0.0590	0.1269	0.1168	0.2016	0.2297	0.0704	0.1002
1	-2.2400	-1.7715	0.0000	0.1301	0.1419	0.0514	0.0886	0.1177	0.0588	0.1977	0.0567	0.1038
6	0.0391	2.0031	0.0000	-0.2201	-0.1434	0.0690	0.2620	0.1920	0.2113	0.2591	0.9135	0.2315
1	2.0337	-2.1200	0.0000	0.1355	0.1509	0.0573	0.1145	0.1135	0.1042	0.2207	0.0573	0.1035
7	0.1110	3.1568	0.0000	0.0276	0.0812	-0.2019	-0.3682	-0.3241	-0.4048	-0.2815	-1.1532	-0.3587
Dipole mement (in D)	5.84 (DEN)			3.63	2.22	3.94	5.15	5.66	5.84	5.51	12.37	5.71

File TZVPMol065.out
Molecule PMol065 3-cyanopyridine
SP Mol065 B3LYP/Def2TZVP VAC.
0 12
Dipole -3.4885 1.9825 0.0003 4.0125
Quadrupole -8.0191 6.0869 1.9322 -4.4902 0.0008 0.0004

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.1289	1.2169	0.0000	-0.1537	-0.0566	0.0004	-0.0392	-0.0498	0.2535	-0.1176	0.0045	-0.0486
6	-1.5090	1.1510	0.0001	-0.0930	-0.1333	-0.0308	-0.1718	-0.0811	-0.5418	-0.2434	-0.0185	-0.0719
6	0.5929	0.0221	-0.0000	0.1922	-0.1538	0.0094	-0.0512	0.0113	-0.2914	-0.2136	0.0665	0.0444
6	-2.1169	-0.0976	0.0002	-0.0213	-0.1817	0.0395	0.1586	0.0635	0.5557	0.0542	0.5132	0.0968
6	-0.1185	-1.1836	0.0000	-0.0734	-0.1406	0.0451	0.1385	0.0742	0.4696	0.0881	0.5522	0.0968
7	-1.4424	-1.2472	0.0001	-0.1986	0.1448	-0.1461	-0.3577	-0.3412	-0.6665	-0.3964	-1.1124	-0.3824
1	-2.1075	2.0516	0.0002	0.1281	0.1504	0.0552	0.1200	0.1118	0.1930	0.2236	0.0569	0.1013
6	2.0133	0.0182	-0.0002	-0.2323	-0.1553	0.0672	0.2892	0.1831	0.3284	0.2655	0.8966	0.2200
1	-3.1990	-0.1801	0.0003	0.1337	0.1413	0.0513	0.0867	0.1174	0.0050	0.1963	0.0564	0.1037
1	0.4204	-2.1255	-0.0000	0.1454	0.1494	0.0558	0.0932	0.1231	0.0349	0.2034	0.0707	0.1030
1	0.3915	2.1654	-0.0000	0.1485	0.1578	0.0618	0.1202	0.1192	0.0862	0.2272	0.0717	0.1034
7	3.1705	0.0082	-0.0003	0.0245	0.0777	-0.2088	-0.3864	-0.3314	-0.4264	-0.2872	-1.1577	-0.3664
Dipole mement (in D)	4.01 (DEN)			2.21	1.97	2.99	3.64	3.88	3.99	3.57	8.52	3.91

File TZVPMol066.out
Molecule PMol066 4-cyanopyridine
SP Mol066 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -2.0901 2.0901
Quadrupole 2.4614 12.0391 -14.5005 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.5989	0.1833	-0.1363	0.0285	0.0793	0.0269	0.5169	-0.1397	0.0768	0.0623
6	0.0000	1.1994	-0.1127	-0.1382	-0.0833	-0.0217	-0.1845	-0.0685	-0.6013	-0.1965	-0.0086	-0.0689
6	0.0000	-1.1994	-0.1127	-0.1382	-0.0833	-0.0217	-0.1845	-0.0685	-0.6013	-0.1965	-0.0084	-0.0689
6	0.0000	1.1382	-1.4969	-0.0299	-0.1896	0.0334	0.1453	0.0577	0.5275	0.0386	0.5193	0.0906

6	0.0000	-1.1382	-1.4969	-0.0299	-0.1896	0.0334	0.1453	0.0577	0.5275	0.0386	0.5191	0.0906
7	0.0000	0.0000	-2.1887	-0.1969	0.1451	-0.1444	-0.3452	-0.3388	-0.6636	-0.3866	-1.1014	-0.3801
1	0.0000	2.1483	0.4053	0.1393	0.1567	0.0592	0.1268	0.1169	0.2196	0.2293	0.0704	0.1006
1	0.0000	-2.1483	0.4053	0.1393	0.1567	0.0592	0.1268	0.1169	0.2196	0.2293	0.0704	0.1006
1	0.0000	2.0537	-2.0794	0.1317	0.1420	0.0512	0.0887	0.1173	0.0198	0.1977	0.0564	0.1033
1	0.0000	-2.0537	-2.0794	0.1317	0.1420	0.0512	0.0887	0.1173	0.0198	0.1977	0.0564	0.1033
6	0.0000	0.0000	2.0226	-0.2225	-0.1445	0.0730	0.2863	0.1889	0.2259	0.2651	0.9001	0.2248
7	0.0000	0.0000	3.1793	0.0304	0.0842	-0.2012	-0.3730	-0.3239	-0.4103	-0.2773	-1.1506	-0.3583

Dipole mement (in D) 2.09 (DEN) 0.61 1.44 2.01 2.23 2.12 2.08 1.40 5.34 2.01

File TZVPMol067.out
Molecule PMol067 cyanimide
SP Mol067 B3LYP/Def2TZVP VAC.
0 5
Dipole -1.0065 -4.5486 0.0000 4.6586
Quadrupole -1.0412 -1.2482 2.2894 1.9498 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.2170	0.0000	-0.0477	-0.3518	0.0926	0.5701	0.2747	0.5298	0.3920	1.4309	0.3572
7	0.0849	-1.1156	0.0000	-0.4208	-0.0333	-0.1239	-0.8224	-0.5684	-0.7283	-0.8210	-1.0946	-0.4911
1	-0.2505	-1.5643	0.8382	0.2610	0.1859	0.1457	0.3809	0.3364	0.3648	0.4006	0.4187	0.2744
1	-0.2505	-1.5643	-0.8382	0.2610	0.1859	0.1457	0.3809	0.3364	0.3648	0.4006	0.4187	0.2744
7	-0.0133	1.3765	0.0000	-0.0535	0.0132	-0.2600	-0.5096	-0.3792	-0.5310	-0.3722	-1.1737	-0.4150

Dipole mement (in D) 4.66 (DEN) 2.22 2.93 3.17 4.27 4.35 4.68 3.89 6.84 3.95

File TZVPMol068.out
Molecule PMol068 cyanoallene
SP Mol068 B3LYP/Def2TZVP VAC.
0 8
Dipole 4.3917 0.7928 0.0000 4.4627
Quadrupole -4.6414 3.1853 1.4562 -3.8859 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.0768	0.0042	0.0000	0.0741	-0.0317	0.0365	0.2204	0.0243	0.2521	0.1685	-0.2584	0.0526
6	2.1475	-0.7178	0.0000	-0.2470	-0.1616	-0.0649	-0.3703	-0.1622	-0.5167	-0.4486	0.0654	-0.1725
6	0.0000	0.7504	0.0000	-0.1249	-0.1576	-0.0291	-0.2948	-0.0742	-0.4311	-0.4060	0.1525	-0.0666
1	2.6138	-1.0362	0.9247	0.1520	0.1466	0.0667	0.1669	0.1197	0.2326	0.2347	0.0905	0.1132
1	2.6138	-1.0362	-0.9247	0.1520	0.1466	0.0667	0.1669	0.1197	0.2326	0.2347	0.0905	0.1132
1	0.0893	1.8326	0.0000	0.1589	0.1744	0.0725	0.1629	0.1295	0.2191	0.2570	0.1030	0.1123
6	-1.3128	0.2183	0.0000	-0.1611	-0.1853	0.0667	0.3469	0.1806	0.5080	0.2568	0.9183	0.2211
7	-2.3980	-0.1843	0.0000	-0.0041	0.0686	-0.2152	-0.3988	-0.3375	-0.4966	-0.2971	-1.1620	-0.3734

Dipole mement (in D) 4.46 (DEN) 2.79 2.31 3.30 4.05 4.32 4.50 4.09 9.53 4.36

File TZVPMol069.out

Molecule PMol069 cyclopentadiene-1-carbon
 SP Mol069 B3LYP/Def2TZVP VAC.
    0   12
Dipole   0.4780   -4.6733   0.0000   4.6977
Quadrupole   7.4121   -8.5704   1.1583   2.9944   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0688	-0.6687	0.0000	-0.0976	-0.1708	-0.0386	-0.2846	-0.1358	0.0855	-0.4569	0.0191	-0.1397
1	-1.7273	-0.5800	0.8692	0.1294	0.1667	0.0599	0.1417	0.1154	0.0618	0.2531	0.0588	0.1017
1	-1.7273	-0.5800	-0.8692	0.1294	0.1667	0.0599	0.1417	0.1154	0.0618	0.2531	0.0588	0.1017
6	-0.2955	-1.9371	0.0000	-0.1849	-0.1192	-0.0229	-0.0386	-0.0823	-0.2023	-0.1409	-0.0473	-0.0672
6	0.0000	0.3818	0.0000	0.0809	-0.1546	0.0051	0.0256	-0.0017	0.0133	-0.1457	0.0560	0.0356
6	1.2103	-0.2289	0.0000	-0.1549	-0.0630	-0.0125	-0.0759	-0.0648	-0.1417	-0.1354	-0.0078	-0.0639
6	1.0220	-1.6615	0.0000	-0.0782	-0.1367	-0.0408	-0.1252	-0.0964	-0.1566	-0.2357	-0.0305	-0.0867
1	-0.7513	-2.9154	0.0000	0.1301	0.1377	0.0505	0.1078	0.1058	0.1367	0.2151	0.0572	0.0973
6	-0.2563	1.7630	0.0000	-0.2263	-0.1746	0.0568	0.2862	0.1719	0.2686	0.2580	0.8849	0.2107
1	2.1650	0.2766	0.0000	0.1371	0.1466	0.0585	0.1172	0.1146	0.1606	0.2236	0.0686	0.1004
1	1.8265	-2.3821	0.0000	0.1264	0.1398	0.0509	0.1131	0.1064	0.1549	0.2201	0.0538	0.0961
7	-0.4937	2.8985	0.0000	0.0088	0.0614	-0.2270	-0.4091	-0.3486	-0.4425	-0.3085	-1.1715	-0.3859

Dipole mement (in D)	4.70 (DEN)	2.65	2.39	3.55	4.34	4.57	4.69	4.22	9.85	4.61

File TZVPMol070.out
Molecule PMol070 methylaminonitrile
 SP Mol070 B3LYP/Def2TZVP VAC.
    0   8
Dipole   1.6239   2.1081   0.0000   2.6610
Quadrupole   -0.4852   -3.7947   4.2799   -7.0137   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	1.4488	0.7128	0.0000	-0.4595	-0.1351	-0.1919	-0.7545	-0.6447	-0.9441	-0.7787	-0.9676	-0.5695
1	1.7629	0.1950	0.8101	0.2165	0.1543	0.1073	0.3161	0.2961	0.3689	0.3553	0.3540	0.2365
1	1.7629	0.1950	-0.8101	0.2165	0.1543	0.1073	0.3161	0.2961	0.3689	0.3553	0.3540	0.2365
6	0.0000	0.8201	0.0000	-0.0141	-0.3208	0.0237	-0.0254	-0.0209	0.4486	-0.3173	0.4456	0.0187
6	-0.7218	-0.4520	0.0000	-0.2392	-0.2162	0.0588	0.3050	0.1716	0.1416	0.2467	0.8838	0.2282
1	-0.3180	1.3966	0.8700	0.1454	0.1556	0.0607	0.1282	0.1262	0.0167	0.2301	0.0620	0.1167
1	-0.3180	1.3966	-0.8700	0.1454	0.1556	0.0607	0.1282	0.1262	0.0167	0.2301	0.0620	0.1167
7	-1.2430	-1.4830	0.0000	-0.0110	0.0524	-0.2267	-0.4138	-0.3506	-0.4174	-0.3216	-1.1942	-0.3837

Dipole mement (in D)	2.66 (DEN)	1.61	1.80	2.42	2.22	2.65	2.67	1.86	7.24	2.65

File TZVPMol071.out
Molecule PMol071 methanol
 SP Mol071 B3LYP/Def2TZVP VAC.
    0   6
Dipole   1.4185   0.9083   0.0000   1.6844
Quadrupole   1.1874   -0.3550   -0.8323   -2.1511   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP

8	-0.0461	-0.7527	0.0000	-0.4633	-0.0723	-0.2379	-0.6039	-0.4607	-0.6092	-0.6898	-1.0812	-0.3990
6	-0.0461	0.6574	0.0000	-0.1419	-0.3839	-0.0083	-0.0156	-0.1344	0.1571	-0.2404	0.5084	-0.1047
1	0.8622	-1.0568	0.0000	0.2986	0.1645	0.1556	0.4102	0.3294	0.3978	0.4502	0.5555	0.2591
1	-1.0859	0.9759	0.0000	0.1145	0.1078	0.0396	0.0916	0.0999	0.0631	0.1771	0.0242	0.0892
1	0.4349	1.0792	0.8879	0.0960	0.0919	0.0255	0.0588	0.0829	-0.0044	0.1515	-0.0035	0.0777
1	0.4349	1.0792	-0.8879	0.0960	0.0919	0.0255	0.0588	0.0829	-0.0044	0.1515	-0.0035	0.0777

Dipole mement (in D) 1.68 (DEN) 1.71 0.69 0.78 1.94 1.60 1.68 2.57 3.59 1.46

File TZVPMol072.out
Molecule PMol072 ethanol
SP Mol072 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0268 1.5853 0.0000 1.5855
Quadrupole 1.6370 -0.7710 -0.8660 -2.3913 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.9425	0.3738	0.0000	0.2935	0.1635	0.1537	0.4078	0.3276	0.3848	0.4548	0.5544	0.2577
8	-1.1910	-0.2203	0.0000	-0.4558	-0.0472	-0.2348	-0.6243	-0.4536	-0.6456	-0.7014	-1.0824	-0.3995
6	0.0000	0.5515	0.0000	-0.0052	-0.3811	0.0236	0.1809	-0.0646	0.3750	-0.0552	0.5129	0.0024
6	1.1660	-0.3988	0.0000	-0.2935	-0.3108	-0.0866	-0.3844	-0.2356	-0.2186	-0.6069	0.0229	-0.2507
1	0.0405	1.2039	0.8815	0.0758	0.1085	0.0222	0.0414	0.0831	-0.0423	0.1470	-0.0131	0.0708
1	0.0405	1.2039	-0.8815	0.0758	0.1085	0.0222	0.0414	0.0831	-0.0423	0.1470	-0.0131	0.0708
1	2.1095	0.1438	0.0000	0.0957	0.1193	0.0329	0.1046	0.0848	0.0347	0.2031	-0.0013	0.0863
1	1.1421	-1.0395	-0.8798	0.1068	0.1196	0.0334	0.1162	0.0875	0.0772	0.2059	0.0100	0.0811
1	1.1421	-1.0395	0.8798	0.1068	0.1196	0.0334	0.1162	0.0875	0.0772	0.2059	0.0100	0.0811

Dipole mement (in D) 1.59 (DEN) 1.49 0.44 0.71 2.00 1.50 1.55 2.47 3.43 1.47

File TZVPMol073.out
Molecule PMol073 ethylene_glycol
SP Mol073 B3LYP/Def2TZVP VAC.
0 10
Dipole -1.3894 1.2195 1.4853 2.3714
Quadrupole -4.3311 2.1384 2.1927 0.1062 -1.8285 -1.1586

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.6776	0.5994	-0.2819	-0.0332	-0.3594	0.0189	0.0667	-0.0670	0.0727	-0.0954	0.4891	-0.0089
8	-1.3754	-0.5951	0.0513	-0.4687	-0.0466	-0.2222	-0.6184	-0.4440	-0.5841	-0.7043	-1.0830	-0.3861
1	-1.5973	-0.5659	0.9848	0.2999	0.1677	0.1557	0.4091	0.3300	0.3929	0.4544	0.5565	0.2619
1	-0.6460	0.6218	-1.3714	0.1023	0.1279	0.0403	0.0888	0.1065	0.0965	0.1810	0.0302	0.0840
1	-1.2169	1.4906	0.0562	0.0876	0.1159	0.0319	0.0559	0.0930	0.0106	0.1602	0.0010	0.0815
6	0.7237	0.5699	0.2781	0.0071	-0.3721	0.0145	0.0892	-0.0694	0.1622	-0.0870	0.5249	-0.0086
8	1.4264	-0.5690	-0.1598	-0.4550	-0.0374	-0.2382	-0.6215	-0.4544	-0.5809	-0.6912	-1.0908	-0.4034
1	0.6827	0.6092	1.3779	0.0662	0.1089	0.0189	0.0392	0.0815	0.0051	0.1399	-0.0183	0.0637
1	1.2851	1.4462	-0.0503	0.0889	0.1267	0.0404	0.0776	0.1040	0.0490	0.1786	0.0194	0.0864
1	0.8084	-1.3056	-0.1066	0.3049	0.1683	0.1398	0.4134	0.3197	0.3761	0.4638	0.5711	0.2297

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 Dipole mement (in D)   2.37 (DEN)      2.28      1.27      1.30      2.82      2.38      2.36      3.69      5.26      2.42

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File TZVPMol074.out
Molecule PMol074    propargyl_alcohol
 SP Mol074 B3LYP/Def2TZVP VAC.
    0    8
Dipole          0.9147    0.0702    1.0476    1.3925
Quadrupole     -0.2442    1.2204   -0.9762   -1.8452   -1.6058   -1.6377
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      1.9082   -0.2166   -0.0126   -0.1239   -0.0935   -0.1065   -0.3029   -0.1583   -0.4206   -0.2219   -0.1545   -0.1625
   6      0.7682    0.1605   -0.0055   -0.1361   -0.1259   -0.0512    0.0061   -0.0613   -0.0731   -0.0496   -0.2004   -0.0328
   1      2.9173   -0.5468   -0.0296    0.1887    0.1261    0.0868    0.2055    0.1408    0.3020    0.2321    0.1645    0.1339
   6     -0.6201    0.5832    0.0349   -0.0293   -0.3326    0.0424    0.1137   -0.0360    0.3547   -0.1396    0.5944    0.0200
   1     -0.8283    1.2616   -0.7940    0.1228    0.1458    0.0553    0.1030    0.1196    0.0665    0.2069    0.0573    0.0967
   1     -0.7969    1.1551    0.9550    0.1153    0.1340    0.0418    0.0727    0.1034   -0.0101    0.1841    0.0329    0.0851
   8     -1.5418   -0.4830   -0.0952   -0.4377   -0.0253   -0.2248   -0.6125   -0.4389   -0.6235   -0.6701   -1.0586   -0.3909
   1     -1.2949   -1.1687    0.5293    0.3002    0.1714    0.1562    0.4144    0.3308    0.4042    0.4581    0.5646    0.2505

 Dipole mement (in D)   1.39 (DEN)      1.84      0.88      0.57      1.68      1.28      1.41      2.56      3.23      1.25

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File TZVPMol075.out
Molecule PMol075    2-propanol
 SP Mol075 B3LYP/Def2TZVP VAC.
    0   12
Dipole         -0.0089   -1.6388    0.0000    1.6388
Quadrupole      3.2071   -3.0743   -0.1328   -1.3586    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -0.2865   -0.6064    1.2583   -0.3293   -0.2949   -0.0923   -0.4279   -0.2401   -0.5386   -0.6142    0.0026   -0.2592
   1     -0.2795    0.0192    2.1483    0.1211    0.1211    0.0326    0.1188    0.0866    0.1274    0.2130    0.0109    0.0816
   1      0.5963   -1.2489    1.2917    0.0883    0.1155    0.0261    0.1056    0.0798    0.1259    0.1902   -0.0140    0.0772
   1     -1.1612   -1.2548    1.3030    0.0998    0.1213    0.0327    0.1142    0.0850    0.1247    0.2048   -0.0003    0.0851
   6     -0.2865    0.2382    0.0000    0.1362   -0.4082    0.0573    0.3402    0.0054    0.5872    0.0951    0.5234    0.1101
   1     -1.1720    0.8799    0.0000    0.0716    0.1402    0.0350    0.0677    0.1025    0.0219    0.1670    0.0096    0.0775
   6     -0.2865   -0.6064   -1.2583   -0.3293   -0.2949   -0.0923   -0.4279   -0.2401   -0.5386   -0.6142    0.0028   -0.2592
   1     -0.2795    0.0192   -2.1483    0.1211    0.1211    0.0326    0.1188    0.0866    0.1274    0.2130    0.0109    0.0816
   1      0.5963   -1.2489   -1.2917    0.0883    0.1155    0.0261    0.1056    0.0798    0.1259    0.1902   -0.0140    0.0772
   1     -1.1612   -1.2548   -1.3030    0.0998    0.1213    0.0327    0.1142    0.0850    0.1247    0.2048   -0.0003    0.0851
   8      0.8001    1.1601    0.0000   -0.4524   -0.0216   -0.2363   -0.6373   -0.4512   -0.6812   -0.6956   -1.0772   -0.4040
   1      1.6171    0.6552    0.0000    0.2847    0.1636    0.1458    0.4078    0.3207    0.3930    0.4458    0.5454    0.2470

 Dipole mement (in D)   1.64 (DEN)      1.50      0.96      0.81      1.72      1.64      1.65      2.81      3.58      1.47

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File TZVPMol076.out
Molecule PMol076    1-propanol(trans)
 SP Mol076 B3LYP/Def2TZVP VAC.
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```
    0   12
Dipole         -1.1196   -0.9632    0.0000    1.4769
Quadrupole     -3.5967    4.1736   -0.5769   -0.9792    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -1.4375    1.2207    0.0000   -0.3435   -0.3092   -0.0829   -0.3276   -0.2346   -0.4260   -0.5886    0.0112   -0.2469
   6      0.0000    0.7392    0.0000   -0.1186   -0.2949   -0.0490   -0.1863   -0.1592    0.2403   -0.4040    0.0614   -0.1408
   6      0.0964   -0.7666    0.0000   -0.0158   -0.3561    0.0215    0.1635   -0.0648    0.2282   -0.0485    0.5084   -0.0021
   1      0.5335    1.1232    0.8718    0.0881    0.1339    0.0309    0.0984    0.0886   -0.0102    0.1991    0.0002    0.0747
   1      0.5335    1.1232   -0.8718    0.0881    0.1339    0.0309    0.0984    0.0886   -0.0102    0.1991    0.0002    0.0747
   8      1.4670   -1.1269    0.0000   -0.4503   -0.0422   -0.2336   -0.6328   -0.4526   -0.6830   -0.6989   -1.0858   -0.3981
   1      1.5347   -2.0824    0.0000    0.2935    0.1635    0.1539    0.4093    0.3278    0.4167    0.4550    0.5552    0.2580
   1     -1.4981    2.3071    0.0000    0.1148    0.1184    0.0318    0.1048    0.0832    0.1003    0.2072    0.0002    0.0855
   1     -1.9789    0.8656    0.8776    0.1011    0.1163    0.0273    0.0954    0.0791    0.0923    0.1950   -0.0090    0.0795
   1     -1.9789    0.8656   -0.8776    0.1011    0.1163    0.0273    0.0954    0.0791    0.0923    0.1950   -0.0090    0.0795
   1     -0.4179   -1.1735   -0.8817    0.0708    0.1101    0.0209    0.0408    0.0824   -0.0203    0.1448   -0.0158    0.0680
   1     -0.4179   -1.1735    0.8817    0.0708    0.1101    0.0209    0.0408    0.0824   -0.0203    0.1448   -0.0158    0.0680

 Dipole mement (in D)   1.48 (DEN)      1.37      0.48      0.69      1.86      1.49      1.49      2.51      3.37      1.41

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File TZVPMol077.out
Molecule PMol077    1-propanol(gauche)
 SP Mol077 B3LYP/Def2TZVP VAC.
    0   12
Dipole         -0.7311    0.9225    0.9498    1.5125
Quadrupole      2.7889   -1.5746   -1.2144    0.2392   -1.9554   -0.5647
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      1.5258   -0.5125    0.1273   -0.3319   -0.3100   -0.0867   -0.3293   -0.2375   -0.1655   -0.5916    0.0139   -0.2514
   6      0.6306    0.6396   -0.2866   -0.1228   -0.2992   -0.0480   -0.1766   -0.1581    0.1876   -0.4033    0.0605   -0.1389
   6     -0.7617    0.5441    0.2895   -0.0243   -0.3559    0.0223    0.1588   -0.0643    0.1621   -0.0527    0.5023   -0.0016
   1      0.5528    0.6838   -1.3755    0.0847    0.1351    0.0307    0.0958    0.0882   -0.0022    0.1991   -0.0009    0.0752
   1      1.0641    1.5920    0.0266    0.0795    0.1340    0.0299    0.0831    0.0850   -0.0538    0.1958   -0.0131    0.0797
   8     -1.3696   -0.6352   -0.2154   -0.4563   -0.0420   -0.2279   -0.6262   -0.4479   -0.6299   -0.7061   -1.0859   -0.3928
   1     -2.2411   -0.7226    0.1721    0.2935    0.1641    0.1543    0.4092    0.3284    0.4016    0.4565    0.5559    0.2605
   1      2.5228   -0.4208   -0.3005    0.1067    0.1154    0.0277    0.0979    0.0792    0.0270    0.2006   -0.0082    0.0810
   1      1.1106   -1.4652   -0.1960    0.1241    0.1217    0.0290    0.1154    0.0839    0.0539    0.2129    0.0181    0.0721
   1      1.6372   -0.5569    1.2118    0.0901    0.1149    0.0251    0.0934    0.0773    0.0340    0.1915   -0.0137    0.0764
   1     -0.7111    0.5138    1.3868    0.0743    0.1110    0.0212    0.0405    0.0827   -0.0022    0.1451   -0.0157    0.0689
   1     -1.3464    1.4310    0.0162    0.0824    0.1110    0.0223    0.0382    0.0834   -0.0128    0.1521   -0.0130    0.0709

 Dipole mement (in D)   1.51 (DEN)      1.41      0.65      0.73      1.97      1.51      1.50      2.41      3.28      1.55

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File TZVPMol078.out
Molecule PMol078    1,2-propanediol(CH3-gauc
 SP Mol078 B3LYP/Def2TZVP VAC.
    0   13
Dipole         -0.8136    1.0382    1.7774    2.2134
```

Quadrupole -4.4895 3.1280 1.3616 2.6897 -0.0745 0.4543

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.5452	0.0965	0.4818	0.0581	-0.3905	0.0496	0.2661	0.0011	0.3591	0.0660	0.4817	0.0986
8	-0.7228	1.2717	-0.3203	-0.4654	-0.0242	-0.2200	-0.6368	-0.4377	-0.6312	-0.7170	-1.0814	-0.3878
1	-0.4565	2.0356	0.1964	0.2977	0.1670	0.1534	0.4064	0.3280	0.3863	0.4585	0.5547	0.2603
1	-0.9994	0.2477	1.4696	0.0646	0.1320	0.0287	0.0404	0.0936	-0.0388	0.1584	-0.0076	0.0753
6	-1.2470	-1.0266	-0.2391	-0.2952	-0.2816	-0.0894	-0.4261	-0.2358	-0.2750	-0.6102	0.0191	-0.2584
6	0.9441	-0.1494	0.6622	0.0105	-0.3465	0.0139	0.0656	-0.0683	0.0924	-0.0800	0.5215	-0.0121
1	-2.2994	-0.7945	-0.3849	0.1134	0.1221	0.0335	0.1213	0.0882	0.0874	0.2122	0.0119	0.0811
8	1.6068	-0.2575	-0.5755	-0.4543	-0.0331	-0.2337	-0.6101	-0.4508	-0.5671	-0.6938	-1.0912	-0.3998
1	-0.7943	-1.1946	-1.2148	0.1119	0.1247	0.0337	0.1292	0.0911	0.0976	0.2160	0.0243	0.0767
1	1.1169	-1.0811	1.2042	0.0821	0.1279	0.0386	0.0821	0.1028	0.0698	0.1772	0.0166	0.0840
1	-1.1732	-1.9527	0.3287	0.0976	0.1235	0.0345	0.1113	0.0875	0.0558	0.2056	0.0010	0.0867
1	1.3743	0.6609	1.2702	0.0751	0.1106	0.0182	0.0390	0.0812	-0.0084	0.1436	-0.0205	0.0635
1	1.2491	0.4424	-1.1329	0.3038	0.1682	0.1389	0.4118	0.3191	0.3721	0.4635	0.5697	0.2319

Dipole mement (in D)	2.21 (DEN)	2.01	1.12	1.21	2.80	2.24	2.19	3.51	4.98	2.41

File TZVPMol079.out
Molecule PMol079 1,2-propanediol(CH3-anti
SP Mol079 B3LYP/Def2TZVP VAC.
0 13
Dipole 2.1867 -0.4368 1.2052 2.5348
Quadrupole -3.4245 0.6780 2.7465 -2.2205 0.0047 2.3041

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.4404	0.0272	-0.3523	0.0833	-0.3895	0.0493	0.2485	0.0002	0.2426	0.0629	0.4884	0.0969
8	0.3466	1.3971	0.0539	-0.4693	-0.0246	-0.2206	-0.6361	-0.4390	-0.6169	-0.7081	-1.0797	-0.3876
1	0.6189	1.4525	0.9744	0.2940	0.1675	0.1502	0.4091	0.3253	0.3958	0.4524	0.5511	0.2553
1	0.3316	0.0680	-1.4390	0.0791	0.1436	0.0384	0.0779	0.1083	0.0928	0.1762	0.0239	0.0788
6	1.7684	-0.5842	0.0223	-0.3475	-0.2905	-0.0875	-0.4373	-0.2355	-0.4917	-0.6208	-0.0016	-0.2552
6	-0.7387	-0.7344	0.2224	0.0329	-0.3484	0.0125	0.0708	-0.0693	0.1000	-0.0770	0.5267	-0.0128
1	2.5950	-0.0154	-0.3979	0.1288	0.1242	0.0369	0.1254	0.0908	0.1530	0.2175	0.0174	0.0872
8	-1.9602	-0.1212	-0.1036	-0.4545	-0.0345	-0.2396	-0.6201	-0.4556	-0.5912	-0.6917	-1.0961	-0.4048
1	1.8931	-0.6107	1.1073	0.0967	0.1183	0.0294	0.1045	0.0831	0.1197	0.1940	-0.0090	0.0813
1	-0.6114	-0.8180	1.3147	0.0556	0.1109	0.0172	0.0453	0.0805	0.0228	0.1385	-0.0208	0.0604
1	1.8456	-1.6099	-0.3377	0.1108	0.1271	0.0390	0.1193	0.0915	0.1157	0.2139	0.0110	0.0918
1	-0.7675	-1.7519	-0.1724	0.0863	0.1274	0.0377	0.0809	0.1020	0.0781	0.1762	0.0150	0.0825
1	-1.8161	0.8265	-0.0055	0.3038	0.1686	0.1369	0.4117	0.3177	0.3793	0.4661	0.5730	0.2262

Dipole mement (in D)	2.53 (DEN)	2.40	1.29	1.53	2.71	2.64	2.55	4.09	5.60	2.63

File TZVPMol080.out
Molecule PMol080 1-butanol
SP Mol080 B3LYP/Def2TZVP VAC.
0 15
Dipole 0.2468 -1.5231 0.0000 1.5430

Quadrupole 2.9157 -2.4076 -0.5081 -3.5170 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.3416	-0.3469	0.0000	-0.0190	-0.3539	0.0214	0.1630	-0.0649	0.1664	-0.0462	0.5074	-0.0022
6	0.0000	0.3415	0.0000	-0.1305	-0.2698	-0.0510	-0.2224	-0.1594	0.0752	-0.4023	0.0510	-0.1458
1	1.4287	-0.9966	0.8818	0.0716	0.1104	0.0208	0.0383	0.0823	-0.0073	0.1452	-0.0159	0.0680
1	1.4287	-0.9966	-0.8818	0.0716	0.1104	0.0208	0.0383	0.0823	-0.0073	0.1452	-0.0159	0.0680
6	-1.1625	-0.6361	0.0000	-0.1607	-0.2922	-0.0442	-0.1160	-0.1570	0.0653	-0.3811	0.0515	-0.1357
1	-0.0600	0.9981	0.8722	0.0846	0.1359	0.0301	0.0992	0.0882	0.0195	0.1978	-0.0024	0.0724
1	-0.0600	0.9981	-0.8722	0.0846	0.1359	0.0301	0.0992	0.0882	0.0195	0.1978	-0.0024	0.0724
6	-2.5124	0.0543	0.0000	-0.3245	-0.3092	-0.0834	-0.3248	-0.2352	-0.1744	-0.5822	0.0161	-0.2469
1	-1.0846	-1.2943	-0.8705	0.0806	0.1307	0.0253	0.0767	0.0805	-0.0161	0.1883	-0.0193	0.0738
1	-1.0846	-1.2943	0.8705	0.0806	0.1307	0.0253	0.0767	0.0805	-0.0161	0.1883	-0.0193	0.0738
1	-3.3360	-0.6582	0.0000	0.1098	0.1158	0.0286	0.0974	0.0799	0.0510	0.2019	-0.0061	0.0820
1	-2.6315	0.6915	0.8770	0.1028	0.1170	0.0280	0.0983	0.0798	0.0323	0.1956	-0.0074	0.0802
1	-2.6315	0.6915	-0.8770	0.1028	0.1170	0.0280	0.0983	0.0798	0.0323	0.1956	-0.0074	0.0802
8	2.3529	0.6461	0.0000	-0.4474	-0.0419	-0.2336	-0.6310	-0.4526	-0.6558	-0.6989	-1.0850	-0.3980
1	3.2079	0.2141	0.0000	0.2932	0.1633	0.1536	0.4087	0.3275	0.4157	0.4549	0.5548	0.2576

Dipole mement (in D) 1.54 (DEN) 1.41 0.39 0.70 1.97 1.48 1.51 2.46 3.43 1.46

File TZVPMol081.out
Molecule PMol081 cyclopropanol(gauche)
SP Mol081 B3LYP/Def2TZVP VAC.
0 10
Dipole 0.3634 1.2946 0.7095 1.5203
Quadrupole -0.3326 0.0926 0.2400 -3.2106 -0.0913 -0.1340

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.8870	0.7653	-0.1382	-0.2302	-0.2347	-0.0823	-0.3093	-0.1879	-0.4083	-0.4433	-0.0637	-0.1879
6	0.9015	-0.7387	-0.1310	-0.1889	-0.2218	-0.0727	-0.2849	-0.1779	-0.1804	-0.4226	-0.0401	-0.1783
6	-0.2353	-0.0088	0.4771	0.0594	-0.3509	0.0311	0.2564	-0.0122	0.2051	0.0731	0.4861	0.0753
1	1.5688	1.3006	0.5072	0.0989	0.1240	0.0362	0.1136	0.0911	0.1430	0.2082	0.0235	0.0869
1	1.5952	-1.2555	0.5156	0.1058	0.1259	0.0391	0.1151	0.0942	0.0906	0.2091	0.0257	0.0899
1	-0.3128	-0.0098	1.5606	0.0785	0.1231	0.0328	0.0548	0.0969	0.0518	0.1660	0.0224	0.0781
1	0.6853	1.2488	-1.0832	0.1086	0.1287	0.0381	0.1248	0.0953	0.1597	0.2139	0.0335	0.0854
1	0.7016	-1.2367	-1.0684	0.1087	0.1336	0.0438	0.1355	0.1019	0.1303	0.2210	0.0461	0.0873
8	-1.4532	-0.1087	-0.1994	-0.4390	0.0004	-0.2224	-0.6185	-0.4321	-0.5690	-0.6828	-1.0914	-0.3939
1	-1.9310	0.7155	-0.0835	0.2983	0.1718	0.1564	0.4125	0.3306	0.3772	0.4573	0.5579	0.2572

Dipole mement (in D) 1.52 (DEN) 1.39 0.87 0.68 1.88 1.46 1.49 2.43 3.61 1.40

File TZVPMol082.out
Molecule PMol082 cyclobutanol
SP Mol082 B3LYP/Def2TZVP VAC.
0 13
Dipole -0.3173 1.0404 1.0474 1.5100
Quadrupole -0.0968 -0.2102 0.3070 3.1192 2.2703 0.3141

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.8144	-0.0859	-0.1991	-0.4389	-0.0127	-0.2325	-0.6474	-0.4436	-0.6584	-0.6923	-1.0990	-0.4015
1	2.3831	0.5759	0.1983	0.2927	0.1667	0.1542	0.4123	0.3284	0.3863	0.4562	0.5556	0.2556
6	0.5334	0.0045	0.3762	0.0546	-0.3476	0.0493	0.3080	0.0056	0.3546	0.1038	0.5250	0.0948
6	-0.4486	-1.0628	-0.0880	-0.1369	-0.2181	-0.0554	-0.2467	-0.1602	-0.1549	-0.4035	0.0168	-0.1578
6	-0.4567	1.0707	-0.1176	-0.1461	-0.2291	-0.0634	-0.2648	-0.1687	-0.1811	-0.4195	-0.0038	-0.1655
1	-0.2372	-1.3199	-1.1261	0.0854	0.1382	0.0354	0.1131	0.0942	0.1022	0.2055	0.0144	0.0766
1	-0.2509	1.3047	-1.1621	0.0783	0.1342	0.0313	0.1059	0.0892	0.0801	0.2026	0.0086	0.0747
1	-0.5373	-1.9812	0.4900	0.0900	0.1186	0.0283	0.0880	0.0825	0.0362	0.1989	-0.0033	0.0771
1	-0.5563	2.0010	0.4413	0.0885	0.1153	0.0235	0.0817	0.0773	0.0305	0.1945	-0.0114	0.0731
1	0.5945	0.0197	1.4717	0.0534	0.1277	0.0248	0.0353	0.0901	-0.0032	0.1468	-0.0097	0.0685
6	-1.5530	0.0017	0.0029	-0.2004	-0.2408	-0.0514	-0.1559	-0.1598	-0.0703	-0.3877	0.0159	-0.1509
1	-2.0225	0.0135	0.9861	0.0864	0.1288	0.0279	0.0850	0.0832	0.0441	0.1931	-0.0073	0.0768
1	-2.3394	-0.0116	-0.7485	0.0931	0.1188	0.0281	0.0856	0.0818	0.0339	0.2014	-0.0017	0.0784

Dipole mement (in D)	1.51 (DEN)	1.40	0.64	0.67	1.82	1.42	1.48	2.36	3.48	1.39

File TZVPMol083.out
Molecule PMol083 phenol
SP Mol083 B3LYP/Def2TZVP VAC.
0 13
Dipole 0.0711 1.3171 0.0001 1.3190
Quadrupole 1.8728 3.5282 -5.4011 4.3356 0.0003 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.9354	-0.0246	0.0000	0.2742	-0.2753	0.0729	0.4240	0.0842	0.4683	0.2889	0.5044	0.1795
6	0.2198	-1.2177	0.0000	-0.1860	-0.1216	-0.0565	-0.2506	-0.1073	-0.2722	-0.2608	-0.0161	-0.1083
6	-1.1646	-1.1834	-0.0000	-0.0851	-0.1367	-0.0360	-0.0450	-0.0916	-0.0674	-0.1828	-0.0188	-0.0791
6	-1.8467	0.0278	-0.0000	-0.1332	-0.1600	-0.0564	-0.1401	-0.1125	-0.1948	-0.2431	-0.0282	-0.1014
6	-1.1252	1.2127	-0.0000	-0.1171	-0.1404	-0.0384	-0.0413	-0.0942	-0.0369	-0.1838	-0.0192	-0.0812
6	0.2624	1.1927	-0.0000	-0.1970	-0.1481	-0.0682	-0.2859	-0.1204	-0.3576	-0.2915	-0.0354	-0.1194
1	0.7620	-2.1537	0.0000	0.1121	0.1474	0.0445	0.1260	0.1039	0.1613	0.2190	0.0477	0.0802
1	-1.7168	-2.1147	-0.0000	0.1085	0.1434	0.0418	0.0961	0.0980	0.1106	0.2080	0.0307	0.0857
1	-2.9280	0.0467	-0.0000	0.1063	0.1405	0.0379	0.0940	0.0940	0.1207	0.2089	0.0274	0.0817
1	-1.6417	2.1642	-0.0000	0.1098	0.1429	0.0413	0.0962	0.0974	0.1109	0.2079	0.0304	0.0852
1	0.8256	2.1197	-0.0000	0.0969	0.1395	0.0363	0.1048	0.0945	0.1421	0.2009	0.0156	0.0796
8	2.2934	-0.1103	0.0000	-0.3965	0.0852	-0.1883	-0.6112	-0.3905	-0.5955	-0.6423	-1.1127	-0.3695
1	2.6653	0.7749	0.0001	0.3071	0.1832	0.1691	0.4332	0.3446	0.4105	0.4706	0.5746	0.2668

Dipole mement (in D)	1.32 (DEN)	0.97	1.54	0.62	1.53	1.30	1.31	1.95	3.64	1.12

File TZVPMol084.out
Molecule PMol084 methyl_propyl_ether
SP Mol084 B3LYP/Def2TZVP VAC.
0 15
Dipole 0.2510 1.0215 0.0000 1.0519
Quadrupole 1.2477 -0.9444 -0.3033 -2.1322 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-1.2653	-0.2961	0.0000	-0.3074	0.1448	-0.1645	-0.2996	-0.2728	-0.3878	-0.4911	-1.0644	-0.2757
6	-2.3100	0.6367	0.0000	-0.1654	-0.3622	-0.0075	-0.0693	-0.1290	0.0349	-0.2430	0.5136	-0.1022
1	-3.2482	0.0868	0.0000	0.1198	0.1090	0.0394	0.0879	0.0999	0.0730	0.1855	0.0239	0.0883
1	-2.2802	1.2820	0.8872	0.0936	0.0966	0.0243	0.0568	0.0829	0.0256	0.1525	-0.0044	0.0745
1	-2.2802	1.2820	-0.8872	0.0936	0.0966	0.0243	0.0568	0.0829	0.0256	0.1525	-0.0044	0.0745
6	0.0000	0.3215	0.0000	-0.0031	-0.3343	0.0240	0.1193	-0.0577	0.1750	-0.0544	0.5103	0.0014
6	1.0724	-0.7390	0.0000	-0.1139	-0.2908	-0.0488	-0.1941	-0.1587	0.1663	-0.4010	0.0606	-0.1412
1	0.1019	0.9753	0.8813	0.0656	0.1141	0.0210	0.0408	0.0836	0.0071	0.1442	-0.0156	0.0663
1	0.1019	0.9753	-0.8813	0.0656	0.1141	0.0210	0.0408	0.0836	0.0071	0.1442	-0.0156	0.0663
6	2.4653	-0.1408	0.0000	-0.3450	-0.3083	-0.0826	-0.3256	-0.2343	-0.2696	-0.5874	0.0117	-0.2466
1	0.9308	-1.3807	0.8720	0.0884	0.1342	0.0311	0.0945	0.0886	-0.0164	0.1995	-0.0001	0.0745
1	0.9308	-1.3807	-0.8720	0.0884	0.1342	0.0311	0.0945	0.0886	-0.0164	0.1995	-0.0001	0.0745
1	3.2337	-0.9113	0.0000	0.1154	0.1184	0.0318	0.1049	0.0833	0.0736	0.2073	0.0002	0.0855
1	2.6329	0.4847	-0.8777	0.1023	0.1168	0.0277	0.0962	0.0795	0.0510	0.1958	-0.0081	0.0799
1	2.6329	0.4847	0.8777	0.1023	0.1168	0.0277	0.0962	0.0795	0.0510	0.1958	-0.0081	0.0799

Dipole mement (in D)	1.05 (DEN)	1.23	0.28	0.60	1.16	1.34	1.09	2.41	3.50	1.35

File TZVPMol085.out
Molecule PMol085 dimethyl_ether
SP Mol085 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0000 0.0000 -1.2401 1.2401
Quadrupole -0.5995 2.2269 -1.6274 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	0.5914	-0.3142	0.1182	-0.1687	-0.2771	-0.2806	-0.3107	-0.4844	-1.0600	-0.2761
6	0.0000	1.1612	-0.1945	-0.1487	-0.3614	-0.0064	-0.0688	-0.1280	-0.0053	-0.2477	0.5112	-0.1017
6	0.0000	-1.1612	-0.1945	-0.1487	-0.3614	-0.0064	-0.0688	-0.1280	-0.0053	-0.2477	0.5112	-0.1017
1	0.8874	1.2167	-0.8375	0.0929	0.0965	0.0252	0.0593	0.0838	0.0470	0.1520	-0.0033	0.0754
1	0.0000	2.0169	0.4764	0.1200	0.1093	0.0404	0.0886	0.1008	0.0694	0.1860	0.0254	0.0890
1	-0.8874	1.2167	-0.8375	0.0929	0.0965	0.0252	0.0593	0.0838	0.0443	0.1520	-0.0033	0.0754
1	0.8874	-1.2167	-0.8375	0.0929	0.0965	0.0252	0.0593	0.0838	0.0470	0.1520	-0.0033	0.0754
1	-0.8874	-1.2167	-0.8375	0.0929	0.0965	0.0252	0.0593	0.0838	0.0443	0.1520	-0.0033	0.0754
1	0.0000	-2.0169	0.4764	0.1200	0.1093	0.0404	0.0886	0.1008	0.0694	0.1860	0.0254	0.0890

Dipole mement (in D)	1.24 (DEN)	1.56	0.04	0.69	1.21	1.44	1.29	2.51	3.80	1.40

File TZVPMol086.out
Molecule PMol086 diethylether
SP Mol086 B3LYP/Def2TZVP VAC.
0 15
Dipole 0.0000 0.0000 -1.2992 1.2992
Quadrupole -0.5964 2.4937 -1.8972 -0.0294 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	0.8667	-0.3235	0.1550	-0.1724	-0.3261	-0.2754	-0.4861	-0.5034	-1.0538	-0.2848

6	0.0000	1.1885	0.0984	0.0007	-0.3533	0.0260	0.1248	-0.0589	0.3466	-0.0662	0.5170	0.0008
6	1.3765	1.5557	-0.4096	-0.3116	-0.3144	-0.0908	-0.4014	-0.2403	-0.2940	-0.6194	0.0078	-0.2561
1	-0.3817	1.9672	0.7605	0.0992	0.1243	0.0343	0.0685	0.0982	0.0048	0.1798	0.0126	0.0793
1	-0.7105	1.1115	-0.7349	0.0659	0.1138	0.0239	0.0500	0.0868	-0.0316	0.1492	-0.0112	0.0716
1	1.3458	2.4918	-0.9665	0.1009	0.1196	0.0327	0.1080	0.0844	0.0567	0.2055	-0.0002	0.0859
1	2.0733	1.6763	0.4182	0.1081	0.1190	0.0323	0.1123	0.0860	0.0818	0.2061	0.0077	0.0806
1	1.7789	0.7939	-1.0768	0.0985	0.1136	0.0279	0.1009	0.0816	0.0816	0.1966	-0.0066	0.0805
6	0.0000	-1.1885	0.0984	0.0007	-0.3533	0.0260	0.1248	-0.0589	0.3327	-0.0662	0.5170	0.0008
6	-1.3765	-1.5557	-0.4096	-0.3116	-0.3144	-0.0908	-0.4014	-0.2403	-0.3091	-0.6194	0.0077	-0.2561
1	0.3817	-1.9672	0.7605	0.0992	0.1243	0.0343	0.0685	0.0982	0.0093	0.1798	0.0127	0.0793
1	0.7105	-1.1115	-0.7349	0.0659	0.1138	0.0239	0.0500	0.0868	-0.0280	0.1492	-0.0112	0.0716
1	-1.3458	-2.4918	-0.9665	0.1009	0.1196	0.0327	0.1080	0.0844	0.0629	0.2055	-0.0002	0.0859
1	-2.0733	-1.6763	0.4182	0.1081	0.1190	0.0323	0.1123	0.0860	0.0857	0.2061	0.0077	0.0806
1	-1.7789	-0.7939	-1.0768	0.0985	0.1136	0.0279	0.1009	0.0816	0.0866	0.1966	-0.0066	0.0805

Dipole mement (in D)	1.30 (DEN)	1.38	0.15	0.72	1.11	1.43	1.34	2.57	3.65	1.41	

File TZVPMol087.out
Molecule PMol087 vinyl_methyl_ether
SP Mol087 B3LYP/Def2TZVP VAC.
0 10
Dipole -0.4429 0.8121 0.0000 0.9250
Quadrupole 1.9072 0.3496 -2.2568 -2.2965 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.6043	-0.7171	-0.0000	-0.2642	0.2187	-0.1283	-0.2451	-0.2271	-0.2858	-0.4550	-1.0953	-0.2461
6	-1.3596	0.4756	-0.0000	-0.1890	-0.3264	0.0031	-0.0941	-0.1194	0.0211	-0.2560	0.4809	-0.1008
6	0.7349	-0.5660	-0.0000	0.0853	-0.3122	0.0360	0.2092	0.0033	0.2022	0.1412	0.5031	0.0826
1	-1.1467	1.0770	-0.8877	0.1194	0.1071	0.0351	0.0852	0.0949	0.0587	0.1711	0.0214	0.0828
1	-1.1467	1.0770	0.8877	0.1194	0.1071	0.0351	0.0852	0.0949	0.0587	0.1711	0.0214	0.0828
1	-2.4053	0.1845	-0.0000	0.1296	0.1119	0.0453	0.0983	0.1063	0.0680	0.1908	0.0346	0.0948
6	1.4303	0.5682	0.0000	-0.3488	-0.2834	-0.1389	-0.4759	-0.2406	-0.6130	-0.5533	-0.0876	-0.2460
1	1.2159	-1.5366	-0.0000	0.1171	0.1341	0.0479	0.0804	0.1133	0.0890	0.1826	0.0542	0.0876
1	0.9758	1.5474	0.0000	0.1199	0.1187	0.0301	0.1247	0.0859	0.2101	0.1966	0.0291	0.0796
1	2.5075	0.5206	0.0000	0.1112	0.1244	0.0346	0.1320	0.0884	0.1911	0.2109	0.0380	0.0827

Dipole mement (in D)	0.93 (DEN)	1.00	1.19	0.64	0.75	1.00	0.96	1.67	3.74	0.83	

File TZVPMol088.out
Molecule PMol088 tetrahydrofuran
SP Mol088 B3LYP/Def2TZVP VAC.
0 13
Dipole -0.0001 1.4754 0.6070 1.5954
Quadrupole 2.4446 -2.8396 0.3950 0.0002 0.0001 -0.8191

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.7694	1.0062	-0.0506	-0.1735	-0.2565	-0.0532	-0.2144	-0.1601	0.0046	-0.4232	0.0248	-0.1540
1	1.1580	1.3656	-1.0017	0.0907	0.1306	0.0305	0.0883	0.0867	0.0133	0.2028	-0.0025	0.0800

1	1.1919	1.6405	0.7265	0.0871	0.1291	0.0304	0.0869	0.0855	-0.0113	0.2044	-0.0035	0.0812
6	-0.7695	1.0062	-0.0505	-0.1734	-0.2565	-0.0532	-0.2144	-0.1601	0.0227	-0.4233	0.0246	-0.1540
1	-1.1582	1.3657	-1.0015	0.0907	0.1305	0.0305	0.0883	0.0867	0.0055	0.2028	-0.0025	0.0800
1	-1.1919	1.6403	0.7267	0.0871	0.1291	0.0304	0.0869	0.0855	-0.0166	0.2044	-0.0035	0.0812
6	-1.1231	-0.4649	0.1588	-0.0040	-0.3151	0.0221	0.0925	-0.0588	0.1853	-0.0751	0.4928	-0.0091
1	-1.9946	-0.8031	-0.3990	0.0970	0.1215	0.0377	0.0706	0.1008	0.0183	0.1873	0.0187	0.0829
6	1.1231	-0.4648	0.1588	-0.0040	-0.3151	0.0221	0.0925	-0.0588	0.1635	-0.0751	0.4927	-0.0091
1	1.9947	-0.8031	-0.3988	0.0970	0.1215	0.0377	0.0706	0.1008	0.0251	0.1873	0.0187	0.0829
1	1.2987	-0.6763	1.2236	0.0653	0.1132	0.0215	0.0411	0.0836	0.0061	0.1478	-0.0132	0.0659
1	-1.2988	-0.6765	1.2235	0.0653	0.1132	0.0215	0.0411	0.0836	-0.0015	0.1478	-0.0132	0.0659
8	0.0001	-1.1937	-0.2998	-0.3252	0.1543	-0.1780	-0.3301	-0.2754	-0.4148	-0.4878	-1.0338	-0.2936

Dipole mement (in D)	1.60 (DEN)	1.73	0.13	0.92	1.32	1.64	1.58	2.83	4.31	1.67	

File TZVPMol089.out
Molecule PMol089 anisole
SP Mol089 B3LYP/Def2TZVP VAC.
0 16
Dipole 0.7850 1.0104 0.0000 1.2795
Quadrupole 4.5845 0.9110 -5.4955 2.8069 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.4527	-0.2781	0.0000	0.3218	-0.2505	0.0731	0.3649	0.0890	0.4731	0.2824	0.5050	0.1782
6	0.0417	1.0522	0.0000	-0.2415	-0.1457	-0.0674	-0.2846	-0.1200	-0.2725	-0.3028	-0.0402	-0.1199
6	-0.4974	-1.2999	0.0000	-0.1921	-0.1175	-0.0565	-0.2525	-0.1070	-0.3581	-0.2473	-0.0181	-0.1085
6	-1.3176	1.3470	0.0000	-0.1161	-0.1411	-0.0401	-0.0424	-0.0960	-0.1132	-0.1843	-0.0194	-0.0828
6	-1.8438	-0.9887	-0.0000	-0.0771	-0.1392	-0.0382	-0.0472	-0.0938	-0.0235	-0.1871	-0.0202	-0.0811
6	-2.2655	0.3376	0.0000	-0.1363	-0.1600	-0.0567	-0.1382	-0.1128	-0.2455	-0.2414	-0.0294	-0.1014
1	0.7643	1.8556	0.0000	0.1129	0.1450	0.0355	0.1062	0.0953	0.1385	0.2119	0.0287	0.0807
1	-0.1541	-2.3259	0.0000	0.1065	0.1469	0.0428	0.1186	0.1026	0.1624	0.2182	0.0461	0.0773
1	-1.6299	2.3839	0.0000	0.1083	0.1424	0.0397	0.0937	0.0959	0.1370	0.2063	0.0275	0.0834
1	-2.5728	-1.7893	-0.0000	0.1068	0.1429	0.0409	0.0950	0.0971	0.1191	0.2075	0.0291	0.0847
1	-3.3204	0.5765	-0.0000	0.1046	0.1400	0.0373	0.0929	0.0934	0.1465	0.2081	0.0260	0.0810
8	1.7507	-0.6766	0.0000	-0.2733	0.2430	-0.1294	-0.2762	-0.2206	-0.3436	-0.4515	-1.0964	-0.2525
6	2.7401	0.3263	0.0000	-0.1917	-0.3311	0.0032	-0.0915	-0.1190	-0.0023	-0.2487	0.4922	-0.1006
1	3.6975	-0.1861	0.0000	0.1326	0.1132	0.0460	0.1005	0.1071	0.0890	0.1926	0.0360	0.0956
1	2.6738	0.9601	0.8885	0.1173	0.1059	0.0347	0.0802	0.0943	0.0465	0.1680	0.0169	0.0829
1	2.6738	0.9601	-0.8885	0.1173	0.1059	0.0347	0.0802	0.0943	0.0465	0.1680	0.0169	0.0829

Dipole mement (in D)	1.28 (DEN)	1.40	1.31	0.97	1.19	1.39	1.30	2.04	3.59	1.31	

File TZVPMol090.out
Molecule PMol090 tetrahydropyran
SP Mol090 B3LYP/Def2TZVP VAC.
0 16
Dipole 0.9722 1.0905 0.0000 1.4609
Quadrupole -0.7411 -1.9790 2.7201 -1.6510 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.6285	1.3107	0.0000	-0.1662	-0.2649	-0.0493	-0.1474	-0.1588	0.0528	-0.3869	0.0371	-0.1460
6	-0.0218	-0.7879	1.1705	-0.0387	-0.3211	0.0226	0.1022	-0.0591	0.1249	-0.0663	0.5022	-0.0067
6	-0.0218	-0.7879	-1.1705	-0.0387	-0.3211	0.0226	0.1022	-0.0591	0.1249	-0.0663	0.5020	-0.0067
6	-0.0218	0.7267	-1.2461	-0.1441	-0.2680	-0.0552	-0.2332	-0.1631	-0.0878	-0.4169	0.0351	-0.1531
6	-0.0218	0.7267	1.2461	-0.1441	-0.2680	-0.0552	-0.2332	-0.1631	-0.0878	-0.4169	0.0350	-0.1531
8	-0.6641	-1.2562	0.0000	-0.3204	0.1575	-0.1742	-0.3321	-0.2748	-0.3990	-0.4976	-1.0505	-0.2887
1	1.6951	1.0615	0.0000	0.0802	0.1335	0.0244	0.0766	0.0805	0.0106	0.1881	-0.0198	0.0716
1	1.0144	-1.1623	1.1956	0.0693	0.1159	0.0207	0.0403	0.0835	0.0209	0.1432	-0.0156	0.0651
1	1.0144	-1.1623	-1.1956	0.0693	0.1159	0.0207	0.0403	0.0835	0.0209	0.1432	-0.0156	0.0651
1	-1.0543	1.0767	-1.3261	0.0795	0.1353	0.0290	0.0915	0.0866	0.0521	0.1963	-0.0069	0.0738
1	-1.0543	1.0767	1.3261	0.0795	0.1353	0.0290	0.0915	0.0866	0.0521	0.1963	-0.0069	0.0738
1	0.5693	2.3998	0.0000	0.0952	0.1313	0.0294	0.0862	0.0841	-0.0043	0.2038	-0.0098	0.0796
1	-0.5529	-1.2373	2.0094	0.1020	0.1250	0.0363	0.0687	0.1001	0.0469	0.1859	0.0150	0.0811
1	-0.5529	-1.2373	-2.0094	0.1020	0.1250	0.0363	0.0687	0.1001	0.0469	0.1859	0.0150	0.0811
1	0.4936	1.0520	-2.1516	0.0876	0.1342	0.0314	0.0889	0.0865	0.0130	0.2040	-0.0087	0.0814
1	0.4936	1.0520	2.1516	0.0876	0.1342	0.0314	0.0889	0.0865	0.0130	0.2040	-0.0087	0.0814
Dipole mement (in D)	1.46 (DEN)			1.85	0.11	0.82	1.21	1.52	1.45	2.65	3.96	1.52

File TZVPMol091.out
Molecule PMol091 1,3-dioxane
SP Mol091 B3LYP/Def2TZVP VAC.
0 14
Dipole 1.5812 0.0000 1.2915 2.0416
Quadrupole 2.5334 -2.2433 -0.2901 0.0001 -1.0288 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.7102	-1.1662	-0.2767	-0.3055	0.1645	-0.1723	-0.3665	-0.2696	-0.4060	-0.4974	-1.0512	-0.2900
8	-0.7103	1.1661	-0.2767	-0.3055	0.1645	-0.1723	-0.3665	-0.2696	-0.4060	-0.4974	-1.0510	-0.2900
6	1.3981	0.0000	-0.2193	-0.1335	-0.2725	-0.0603	-0.3101	-0.1655	-0.0165	-0.4486	0.0318	-0.1601
6	0.6225	-1.2314	0.2067	-0.0314	-0.3163	0.0242	0.1000	-0.0570	0.1984	-0.0737	0.4895	-0.0069
6	-1.3365	-0.0000	0.1738	0.0848	-0.4091	0.0882	0.3167	0.0372	0.2561	0.2055	1.0044	0.1315
6	0.6225	1.2314	0.2067	-0.0314	-0.3163	0.0242	0.1000	-0.0570	0.1984	-0.0737	0.4895	-0.0069
1	1.5177	0.0000	-1.3034	0.0867	0.1381	0.0352	0.1070	0.0945	0.0482	0.2072	0.0107	0.0769
1	0.6084	-1.3076	1.3051	0.0760	0.1175	0.0234	0.0438	0.0867	0.0004	0.1519	-0.0083	0.0684
1	-1.3589	-0.0000	1.2802	0.0683	0.1009	0.0196	0.0086	0.0907	0.0138	0.1091	-0.0039	0.0617
1	0.6084	1.3076	1.3051	0.0760	0.1175	0.0234	0.0438	0.0867	0.0004	0.1519	-0.0083	0.0684
1	2.3943	0.0000	0.2252	0.0851	0.1376	0.0373	0.1015	0.0927	-0.0227	0.2079	0.0005	0.0876
1	1.0521	-2.1519	-0.1851	0.1087	0.1265	0.0411	0.0796	0.1049	0.0266	0.1909	0.0241	0.0868
1	-2.3494	-0.0000	-0.2232	0.1131	0.1205	0.0470	0.0623	0.1203	0.0823	0.1753	0.0473	0.0857
1	1.0520	2.1519	-0.1851	0.1087	0.1265	0.0411	0.0796	0.1049	0.0266	0.1909	0.0241	0.0868
Dipole mement (in D)	2.04 (DEN)			2.45	0.33	1.20	2.02	2.24	2.04	3.85	5.62	2.22

File TZVPMol092.out
Molecule PMol092 3,4-dihydro-2,4-pyran

SP Mol092 B3LYP/Def2TZVP VAC.
0 14
Dipole -1.1727 -0.6059 0.2493 1.3433
Quadrupole -1.4310 2.6575 -1.2265 0.7984 0.1569 -0.5438

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.4446	0.2759	0.1275	-0.1345	-0.2567	-0.0505	-0.1477	-0.1551	0.3457	-0.4196	0.0495	-0.1444
6	0.5391	-1.2083	0.2896	-0.0017	-0.2838	0.0318	0.0916	-0.0501	0.3211	-0.0676	0.4728	-0.0053
6	0.8879	1.0739	-0.0832	0.0217	-0.2778	0.0223	0.1511	-0.0073	0.0862	0.1234	0.4721	0.0577
6	-0.4075	1.3504	0.0632	-0.2115	-0.2224	-0.0874	-0.2628	-0.1463	-0.4783	-0.3196	-0.0526	-0.1306
6	-0.8337	-1.0445	-0.3236	-0.1761	-0.2577	-0.0512	-0.2319	-0.1583	-0.1709	-0.4159	0.0410	-0.1507
8	1.4325	-0.1674	-0.1097	-0.2826	0.2218	-0.1428	-0.2876	-0.2332	-0.3582	-0.4688	-1.0853	-0.2625
1	-1.8521	0.1827	1.1400	0.0909	0.1368	0.0280	0.0855	0.0831	-0.0352	0.1998	-0.0058	0.0738
1	0.4711	-1.1969	1.3840	0.0801	0.1257	0.0313	0.0618	0.0950	-0.0046	0.1638	0.0080	0.0722
1	-0.7364	-1.0582	-1.4112	0.0955	0.1404	0.0325	0.0974	0.0906	0.0723	0.2022	0.0027	0.0747
1	-2.2977	0.5347	-0.5037	0.0967	0.1389	0.0330	0.0944	0.0880	-0.0408	0.2097	0.0005	0.0815
1	1.0219	-2.1369	-0.0091	0.1091	0.1264	0.0404	0.0743	0.1043	-0.0052	0.1880	0.0227	0.0861
1	1.6485	1.8346	-0.2027	0.1137	0.1325	0.0447	0.0771	0.1097	0.1182	0.1854	0.0508	0.0842
1	-0.7032	2.3896	0.0910	0.1034	0.1393	0.0325	0.1017	0.0890	0.1497	0.2109	0.0251	0.0775
1	-1.4600	-1.8943	-0.0512	0.0953	0.1365	0.0353	0.0950	0.0905	0.0001	0.2083	-0.0018	0.0859

Dipole mement (in D)	1.34 (DEN)	1.63	1.19	0.78	0.94	1.30	1.31	1.98	4.28	1.23

File TZVPMol093.out
Molecule PMol093 oxetane
SP Mol093 B3LYP/Def2TZVP VAC.
0 10
Dipole 0.0000 -1.9436 0.0000 1.9436
Quadrupole 0.8570 -2.7823 1.9252 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.0000	1.0653	0.0000	-0.3437	0.1142	-0.1978	-0.3511	-0.2855	-0.5184	-0.4950	-0.9895	-0.3065
6	0.0000	-1.0650	0.0000	-0.2570	-0.2502	-0.0560	-0.2781	-0.1599	-0.4473	-0.4471	0.0080	-0.1567
6	0.0000	0.0611	1.0274	0.0503	-0.2797	0.0302	0.1084	-0.0506	0.4542	-0.0565	0.4689	-0.0069
6	0.0000	0.0611	-1.0274	0.0503	-0.2797	0.0302	0.1084	-0.0506	0.4542	-0.0565	0.4688	-0.0069
1	0.8866	0.1331	1.6641	0.0735	0.1111	0.0309	0.0550	0.0915	-0.0394	0.1623	0.0074	0.0761
1	0.8866	0.1331	-1.6641	0.0735	0.1111	0.0309	0.0550	0.0915	-0.0394	0.1623	0.0074	0.0761
1	-0.8866	0.1331	1.6641	0.0735	0.1111	0.0309	0.0550	0.0915	-0.0403	0.1623	0.0074	0.0761
1	-0.8866	0.1331	-1.6641	0.0735	0.1111	0.0309	0.0550	0.0915	-0.0403	0.1623	0.0074	0.0761
1	0.8828	-1.6988	0.0000	0.1030	0.1255	0.0350	0.0962	0.0903	0.1084	0.2031	0.0072	0.0863
1	-0.8828	-1.6988	0.0000	0.1030	0.1255	0.0350	0.0962	0.0903	0.1082	0.2031	0.0072	0.0863

Dipole mement (in D)	1.94 (DEN)	1.91	0.06	1.20	1.74	1.91	1.97	3.18	4.93	1.99

File TZVPMol094.out
Molecule PMol094 3-methyleneoxetane
SP Mol094 B3LYP/Def2TZVP VAC.
0 11

Dipole 0.0000 0.0000 -1.5556 1.5556
Quadrupole -0.5601 3.8810 -3.3209 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	1.4942	-0.3544	0.1219	-0.1941	-0.3406	-0.2784	-0.5181	-0.4868	-0.9724	-0.3028
6	0.0000	0.0000	-0.5953	-0.0869	-0.2067	-0.0024	0.0781	-0.0180	-0.1065	-0.0338	-0.0477	0.0351
6	0.0000	1.0312	0.4886	0.0579	-0.2318	0.0285	0.0420	-0.0469	0.4156	-0.0978	0.4502	-0.0118
6	0.0000	-1.0312	0.4886	0.0579	-0.2318	0.0285	0.0420	-0.0469	0.4156	-0.0978	0.4499	-0.0118
1	-0.8884	1.6687	0.5513	0.0883	0.1224	0.0392	0.0723	0.0999	-0.0209	0.1774	0.0262	0.0813
1	-0.8884	-1.6687	0.5513	0.0883	0.1224	0.0392	0.0723	0.0999	-0.0209	0.1774	0.0262	0.0813
1	0.8884	1.6687	0.5513	0.0883	0.1224	0.0392	0.0723	0.0999	-0.0189	0.1774	0.0262	0.0813
1	0.8884	-1.6687	0.5513	0.0883	0.1224	0.0392	0.0723	0.0999	-0.0189	0.1774	0.0262	0.0813
6	0.0000	0.0000	-1.9144	-0.2588	-0.1922	-0.0961	-0.3537	-0.1947	-0.5089	-0.3919	-0.0584	-0.2072
1	0.0000	-0.9213	-2.4818	0.1154	0.1255	0.0394	0.1216	0.0927	0.1910	0.1991	0.0364	0.0867
1	0.0000	0.9213	-2.4818	0.1154	0.1255	0.0394	0.1216	0.0927	0.1910	0.1991	0.0364	0.0867

Dipole mement (in D) 1.56 (DEN) 1.46 0.45 0.89 1.35 1.53 1.55 3.12 4.78 1.63

File TZVPMol095.out
Molecule PMol095 formaldehyde
SP Mol095 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 -2.3077 2.3077
Quadrupole 0.2227 0.1725 -0.3952 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	0.6720	-0.2315	0.1099	-0.2153	-0.3832	-0.2774	-0.4044	-0.4767	-1.1037	-0.3258
6	0.0000	0.0000	-0.5227	0.0696	-0.2820	0.1321	0.3251	0.0794	0.4088	0.2807	1.0421	0.1587
1	0.0000	0.9370	-1.1200	0.0809	0.0860	0.0416	0.0291	0.0990	-0.0022	0.0980	0.0308	0.0836
1	0.0000	-0.9370	-1.1200	0.0809	0.0860	0.0416	0.0291	0.0990	-0.0022	0.0980	0.0308	0.0836

Dipole mement (in D) 2.31 (DEN) 1.79 0.14 1.47 2.37 2.16 2.31 3.30 6.51 2.35

File TZVPMol096.out
Molecule PMol096 acetaldehyde
SP Mol096 B3LYP/Def2TZVP VAC.
0 7
Dipole -2.7968 -0.3617 0.0000 2.8201
Quadrupole -2.1022 0.9962 1.1060 -0.7782 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-0.3788	-1.6540	0.0000	0.1173	0.1270	0.0470	0.1483	0.1018	0.1118	0.2265	0.0432	0.0911
6	-0.9247	-0.7152	0.0000	-0.2716	-0.2925	-0.0825	-0.5098	-0.2271	-0.3311	-0.7054	-0.0301	-0.2495
6	0.0000	0.4562	0.0000	0.1211	-0.3249	0.1462	0.5088	0.1277	0.5661	0.4345	1.0365	0.2440
8	1.1994	0.3870	0.0000	-0.2589	0.1167	-0.2409	-0.4401	-0.2973	-0.4825	-0.5034	-1.1295	-0.3550
1	-1.5795	-0.6684	0.8713	0.1200	0.1348	0.0492	0.1417	0.1014	0.0933	0.2291	0.0335	0.1011
1	-1.5795	-0.6684	-0.8713	0.1200	0.1348	0.0492	0.1417	0.1014	0.0933	0.2291	0.0335	0.1011
1	-0.5090	1.4489	0.0000	0.0520	0.1041	0.0318	0.0093	0.0920	-0.0510	0.0896	0.0128	0.0673

Dipole mement (in D) 2.82 (DEN) 2.52 0.85 1.96 2.71 2.67 2.83 3.88 6.99 2.81

File TZVPMol097.out
Molecule PMol097 propanal
SP Mol097 B3LYP/Def2TZVP VAC.
0 10
Dipole -1.6270 2.1869 0.0000 2.7257
Quadrupole -1.7094 0.2552 1.4542 2.5263 -0.0003 0.0003

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.4318	-0.4975	-0.0000	-0.3256	-0.3007	-0.0829	-0.3284	-0.2329	-0.1750	-0.5941	0.0231	-0.2503
6	-0.5427	0.7239	0.0000	-0.1214	-0.2927	-0.0469	-0.2998	-0.1524	0.1043	-0.5009	0.0050	-0.1389
6	0.9232	0.4199	-0.0002	0.0907	-0.3008	0.1436	0.4802	0.1265	0.4497	0.4392	1.0234	0.2403
8	1.3956	-0.6854	0.0001	-0.2647	0.1198	-0.2355	-0.4342	-0.2929	-0.4610	-0.5119	-1.1333	-0.3481
1	-2.4843	-0.2225	0.0002	0.1114	0.1184	0.0320	0.1082	0.0836	0.0450	0.2051	0.0000	0.0856
1	-1.2442	-1.1188	-0.8737	0.1155	0.1245	0.0347	0.1175	0.0885	0.0523	0.2126	0.0163	0.0794
1	-1.2440	-1.1190	0.8735	0.1155	0.1245	0.0347	0.1175	0.0885	0.0522	0.2126	0.0164	0.0794
1	-0.7334	1.3733	-0.8616	0.1062	0.1496	0.0446	0.1170	0.0998	-0.0095	0.2221	0.0194	0.0929
1	-0.7332	1.3731	0.8619	0.1062	0.1497	0.0446	0.1170	0.0998	-0.0093	0.2221	0.0195	0.0929
1	1.5823	1.3196	0.0003	0.0662	0.1077	0.0311	0.0050	0.0914	-0.0488	0.0930	0.0106	0.0669

Dipole mement (in D) 2.73 (DEN) 2.58 0.84 1.86 2.64 2.56 2.71 3.80 6.86 2.77

File TZVPMol098.out
Molecule PMol098 butanal
SP Mol098 B3LYP/Def2TZVP VAC.
0 13
Dipole -2.8033 0.5159 0.9983 3.0201
Quadrupole -6.0682 2.8805 3.1877 1.0474 2.2975 -0.0998

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.1169	-0.4423	0.2272	-0.1009	-0.2550	-0.0510	-0.3521	-0.1554	-0.1406	-0.4966	0.0031	-0.1485
6	-1.0217	0.4999	-0.1495	-0.1870	-0.2864	-0.0399	-0.1057	-0.1521	0.2286	-0.3775	0.0525	-0.1335
1	-0.0594	-0.8226	1.2406	0.0966	0.1510	0.0440	0.1211	0.1003	0.0499	0.2186	0.0169	0.0900
1	0.1652	-1.3082	-0.4338	0.0976	0.1419	0.0412	0.1259	0.0997	0.0536	0.2149	0.0268	0.0806
6	-2.3811	-0.1642	-0.0592	-0.3235	-0.3056	-0.0805	-0.3249	-0.2324	-0.2858	-0.5833	0.0176	-0.2452
1	-0.9913	1.3788	0.5004	0.0904	0.1334	0.0291	0.0834	0.0844	-0.0404	0.1946	-0.0100	0.0780
1	-0.8572	0.8762	-1.1620	0.1022	0.1360	0.0321	0.0905	0.0875	-0.0223	0.1982	-0.0039	0.0791
1	-3.1824	0.5176	-0.3391	0.1165	0.1191	0.0332	0.1045	0.0846	0.0701	0.2071	0.0022	0.0870
1	-2.4444	-1.0306	-0.7178	0.1091	0.1193	0.0315	0.1052	0.0833	0.0677	0.1996	-0.0014	0.0839
1	-2.5856	-0.5134	0.9534	0.1041	0.1177	0.0299	0.1023	0.0817	0.0662	0.1967	-0.0050	0.0823
6	1.4465	0.2459	0.2439	0.1034	-0.2971	0.1436	0.4914	0.1270	0.4386	0.4462	1.0269	0.2394
8	2.4419	-0.1416	-0.3055	-0.2547	0.1190	-0.2422	-0.4462	-0.2985	-0.4559	-0.5041	-1.1327	-0.3561
1	1.4564	1.1994	0.8280	0.0465	0.1066	0.0290	0.0046	0.0898	-0.0296	0.0854	0.0076	0.0631

Dipole mement (in D) 3.02 (DEN) 2.64 1.03 2.18 2.91 2.90 3.03 4.00 7.28 2.99

File TZVPMol099.out
Molecule PMol099 E-2-butenal
 SP Mol099 B3LYP/Def2TZVP VAC.
  0 11
Dipole 4.0903 0.9260 -0.0002 4.1938
Quadrupole -4.5767 3.5276 1.0492 -1.6426 0.0006 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-2.4600	-0.2396	0.0001	-0.2768	0.1049	-0.2545	-0.4516	-0.3081	-0.4722	-0.5094	-1.1251	-0.3672
6	-1.3916	0.3243	-0.0001	0.1018	-0.3097	0.1181	0.4440	0.1056	0.5172	0.3827	1.0186	0.2090
1	-1.3290	1.4394	0.0001	0.0474	0.1094	0.0269	0.0044	0.0882	-0.0365	0.0901	0.0058	0.0581
6	-0.0924	-0.3346	-0.0000	-0.0959	-0.1677	-0.0514	-0.2962	-0.1066	-0.3900	-0.3141	-0.0467	-0.0961
1	-0.0821	-1.4198	-0.0000	0.1137	0.1455	0.0487	0.1349	0.1072	0.1953	0.2089	0.0530	0.0837
6	1.0358	0.3816	-0.0000	-0.0642	-0.1447	0.0087	0.0849	-0.0548	0.0575	-0.0748	-0.0335	-0.0251
6	2.4125	-0.1571	0.0000	-0.3166	-0.2788	-0.0739	-0.3882	-0.2210	-0.2344	-0.6391	0.0180	-0.2388
1	0.9362	1.4665	-0.0000	0.1150	0.1450	0.0431	0.0837	0.0996	0.0885	0.1913	0.0336	0.0879
1	2.4293	-1.2446	0.0000	0.1204	0.1282	0.0427	0.1269	0.0953	0.0924	0.2143	0.0211	0.0945
1	2.9696	0.1948	-0.8704	0.1276	0.1339	0.0457	0.1285	0.0972	0.0911	0.2250	0.0275	0.0970
1	2.9695	0.1948	0.8704	0.1276	0.1339	0.0457	0.1285	0.0972	0.0911	0.2250	0.0275	0.0970

Dipole mement (in D)	4.19 (DEN)	3.91	2.17	3.29	4.09	3.99	4.20	5.23	8.14	4.10	

File TZVPMol100.out
Molecule PMol100 acetone
 SP Mol100 B3LYP/Def2TZVP VAC.
  0 10
Dipole 0.0000 0.0000 -3.0256 3.0256
Quadrupole 1.4182 1.9245 -3.3428 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	1.3970	-0.2818	0.1282	-0.2581	-0.4817	-0.3091	-0.5432	-0.5222	-1.1465	-0.3757
6	0.0000	0.0000	0.1888	0.2014	-0.3860	0.1689	0.6851	0.1846	0.7789	0.5742	1.0294	0.3388
6	0.0000	1.2757	-0.6110	-0.3215	-0.2651	-0.0873	-0.5304	-0.2305	-0.5326	-0.7016	-0.0298	-0.2585
6	0.0000	-1.2757	-0.6110	-0.3215	-0.2651	-0.0873	-0.5304	-0.2305	-0.5326	-0.7016	-0.0298	-0.2585
1	0.0000	2.1423	0.0422	0.1273	0.1289	0.0441	0.1471	0.0995	0.1441	0.2296	0.0408	0.0870
1	0.0000	-2.1423	0.0422	0.1273	0.1289	0.0441	0.1471	0.0995	0.1441	0.2296	0.0408	0.0870
1	0.8719	1.3148	-1.2651	0.1172	0.1326	0.0439	0.1408	0.0967	0.1354	0.2230	0.0238	0.0950
1	0.8719	-1.3148	-1.2651	0.1172	0.1326	0.0439	0.1408	0.0967	0.1354	0.2230	0.0238	0.0950
1	-0.8719	1.3148	-1.2651	0.1172	0.1326	0.0439	0.1408	0.0967	0.1353	0.2230	0.0238	0.0950
1	-0.8719	-1.3148	-1.2651	0.1172	0.1326	0.0439	0.1408	0.0967	0.1353	0.2230	0.0238	0.0950

Dipole mement (in D)	3.03 (DEN)	2.62	1.10	2.12	2.86	2.86	3.04	4.19	7.15	2.97	

File TZVPMol101.out
Molecule PMol101 2-butanone
 SP Mol101 B3LYP/Def2TZVP VAC.
  0 13
Dipole 2.8069 -0.6948 0.0000 2.8916

Quadrupole -2.1292 0.6795 1.4498 2.4823 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.6000	-1.9097	0.0000	-0.3085	-0.3002	-0.0852	-0.3251	-0.2352	-0.2509	-0.5885	0.0258	-0.2521
6	0.5009	-0.8747	0.0000	-0.1754	-0.2637	-0.0506	-0.3188	-0.1547	0.0256	-0.4953	0.0063	-0.1471
6	0.0000	0.5518	0.0000	0.1965	-0.3580	0.1679	0.6564	0.1850	0.6416	0.5802	1.0142	0.3364
8	-1.1796	0.8158	0.0000	-0.2898	0.1329	-0.2494	-0.4726	-0.3017	-0.5247	-0.5300	-1.1483	-0.3653
1	1.1641	-0.9928	0.8630	0.1038	0.1474	0.0398	0.1176	0.0957	0.0084	0.2162	0.0101	0.0873
1	1.1641	-0.9928	-0.8630	0.1038	0.1474	0.0398	0.1176	0.0957	0.0084	0.2162	0.0101	0.0873
1	-1.2403	-1.8007	-0.8730	0.1128	0.1238	0.0327	0.1160	0.0868	0.0698	0.2115	0.0145	0.0768
1	-1.2403	-1.8007	0.8730	0.1128	0.1238	0.0327	0.1160	0.0868	0.0698	0.2115	0.0145	0.0768
1	-0.1953	-2.9197	0.0000	0.1076	0.1167	0.0295	0.1048	0.0812	0.0658	0.2020	-0.0047	0.0829
6	1.0595	1.6216	0.0000	-0.3324	-0.2640	-0.0877	-0.5347	-0.2311	-0.4946	-0.6995	-0.0300	-0.2587
1	1.7060	1.5187	-0.8721	0.1194	0.1325	0.0435	0.1381	0.0962	0.1188	0.2231	0.0232	0.0947
1	1.7060	1.5187	0.8721	0.1194	0.1325	0.0435	0.1381	0.0962	0.1188	0.2231	0.0232	0.0947
1	0.6107	2.6097	0.0000	0.1300	0.1288	0.0436	0.1467	0.0990	0.1433	0.2293	0.0401	0.0865

Dipole mement (in D) 2.89 (DEN) 2.57 0.79 2.00 2.75 2.73 2.89 4.09 6.96 2.95

File TZVPMol102.out
Molecule PMol102 cyclopentanone
SP Mol102 B3LYP/Def2TZVP VAC.
0 14
Dipole 0.0000 0.0000 -3.1750 3.1750
Quadrupole 3.2492 3.2995 -6.5487 -0.2087 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.9196	0.1390	-0.3185	0.1644	0.6471	0.1857	0.5691	0.5935	1.0303	0.3253
6	0.0000	1.2293	0.0260	-0.1735	-0.2180	-0.0558	-0.3733	-0.1573	-0.1836	-0.5136	-0.0168	-0.1605
6	0.0000	-1.2293	0.0260	-0.1735	-0.2180	-0.0558	-0.3733	-0.1573	-0.1808	-0.5136	-0.0166	-0.1605
6	-0.3072	-0.7014	-1.3681	-0.1801	-0.2490	-0.0480	-0.1458	-0.1567	-0.0191	-0.3880	0.0331	-0.1479
6	0.3072	0.7014	-1.3681	-0.1801	-0.2490	-0.0480	-0.1458	-0.1567	-0.0164	-0.3880	0.0340	-0.1479
1	-1.0071	1.6545	0.0723	0.1083	0.1537	0.0457	0.1287	0.1027	0.0749	0.2284	0.0250	0.0887
1	1.0071	-1.6545	0.0723	0.1083	0.1537	0.0457	0.1287	0.1027	0.0746	0.2284	0.0250	0.0887
1	0.6736	1.9945	0.4059	0.1178	0.1427	0.0446	0.1295	0.1014	0.0614	0.2330	0.0320	0.0877
1	-0.6736	-1.9945	0.4059	0.1178	0.1427	0.0446	0.1295	0.1014	0.0607	0.2330	0.0320	0.0877
1	0.0738	-1.3341	-2.1675	0.1016	0.1297	0.0331	0.0943	0.0876	0.0169	0.2089	0.0010	0.0839
1	-0.0738	1.3341	-2.1675	0.1016	0.1297	0.0331	0.0943	0.0876	0.0168	0.2089	0.0010	0.0839
1	-1.3882	-0.6304	-1.5098	0.0928	0.1353	0.0301	0.0918	0.0858	0.0294	0.1943	-0.0096	0.0777
1	1.3882	0.6304	-1.5098	0.0928	0.1353	0.0301	0.0918	0.0858	0.0281	0.1943	-0.0096	0.0777
8	0.0000	0.0000	2.1232	-0.2728	0.1293	-0.2641	-0.4980	-0.3129	-0.5319	-0.5197	-1.1604	-0.3849

Dipole mement (in D) 3.17 (DEN) 2.77 0.87 2.27 3.10 2.95 3.20 3.81 7.47 3.06

File TZVPMol103.out
Molecule PMol103 acetophenone
SP Mol103 B3LYP/Def2TZVP VAC.
0 17

Dipole -1.9400 2.4872 0.0001 3.1543
Quadrupole 1.1214 1.5348 -2.6562 6.6346 0.0003 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.4247	1.1851	0.0000	-0.1787	-0.0983	-0.0313	-0.0757	-0.0849	-0.1487	-0.1732	-0.0340	-0.0826
6	0.2073	-0.0593	0.0000	0.0744	-0.1258	-0.0173	-0.0999	-0.0240	0.0053	-0.1622	-0.0370	0.0001
6	-0.5741	-1.2166	-0.0000	-0.1543	-0.0740	-0.0221	-0.0643	-0.0740	-0.0742	-0.1491	-0.0168	-0.0737
6	-1.9544	-1.1320	-0.0000	-0.0859	-0.1319	-0.0339	-0.0993	-0.0896	-0.1310	-0.2080	-0.0194	-0.0793
6	-2.5747	0.1128	-0.0000	-0.0975	-0.1232	-0.0265	-0.0644	-0.0825	-0.0757	-0.1803	-0.0241	-0.0708
6	-1.8090	1.2704	-0.0000	-0.1172	-0.1365	-0.0382	-0.1041	-0.0942	-0.1157	-0.2119	-0.0217	-0.0834
1	0.1638	2.0937	0.0000	0.1230	0.1483	0.0410	0.1017	0.0991	0.1161	0.2094	0.0334	0.0855
1	-0.0658	-2.1723	-0.0000	0.1402	0.1562	0.0450	0.1128	0.1065	0.1077	0.2334	0.0774	0.0722
1	-2.5526	-2.0342	-0.0000	0.1161	0.1447	0.0447	0.0985	0.1008	0.1161	0.2117	0.0364	0.0892
1	-3.6554	0.1797	-0.0001	0.1163	0.1442	0.0451	0.0964	0.1011	0.1080	0.2100	0.0361	0.0898
1	-2.2908	2.2396	-0.0000	0.1138	0.1439	0.0431	0.0973	0.0992	0.1124	0.2108	0.0341	0.0876
6	1.6910	-0.2048	0.0001	0.2231	-0.3148	0.1572	0.6070	0.1810	0.4843	0.5526	1.0074	0.3172
8	2.2074	-1.3033	-0.0000	-0.2982	0.1291	-0.2512	-0.4850	-0.3024	-0.4806	-0.5280	-1.1381	-0.3639
6	2.5277	1.0467	0.0000	-0.3665	-0.2595	-0.0876	-0.5470	-0.2305	-0.2690	-0.6979	-0.0265	-0.2598
1	2.3135	1.6618	-0.8745	0.1281	0.1335	0.0437	0.1376	0.0969	0.0760	0.2246	0.0251	0.0926
1	2.3136	1.6618	0.8746	0.1281	0.1335	0.0437	0.1376	0.0969	0.0760	0.2246	0.0251	0.0926
1	3.5798	0.7821	0.0000	0.1352	0.1307	0.0445	0.1506	0.1004	0.0932	0.2334	0.0430	0.0868

Dipole mement (in D)	3.15 (DEN)	2.35	0.98	2.25	3.23	2.90	3.17	4.23	7.01	3.11

File TZVPMol104.out
Molecule PMol104 cyclobutane-1,2-dione
SP Mol104 B3LYP/Def2TZVP VAC.
0 10
Dipole -3.7181 -1.3874 0.0000 3.9685
Quadrupole -0.9540 -3.6032 4.5572 1.1481 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.6272	-1.1366	0.0000	-0.2013	0.1883	-0.2065	-0.3939	-0.2503	-0.4248	-0.4390	-1.1102	-0.3314
6	0.5486	-0.6327	0.0000	0.1248	-0.2779	0.1584	0.4646	0.1909	0.4374	0.4808	1.0533	0.2986
6	-0.8931	-1.1526	0.0000	-0.1687	-0.2004	-0.0569	-0.3563	-0.1567	-0.2011	-0.5167	-0.0372	-0.1641
6	0.0000	0.8374	0.0000	0.1249	-0.2779	0.1584	0.4646	0.1909	0.4286	0.4808	1.0525	0.2986
6	-1.4298	0.2857	0.0000	-0.1689	-0.2004	-0.0568	-0.3563	-0.1567	-0.1933	-0.5167	-0.0373	-0.1641
1	-1.1271	-1.7498	0.8795	0.1227	0.1450	0.0525	0.1428	0.1080	0.0946	0.2375	0.0473	0.0985
1	-1.1271	-1.7498	-0.8795	0.1227	0.1450	0.0525	0.1428	0.1080	0.0946	0.2375	0.0473	0.0985
1	-1.9979	0.5837	-0.8795	0.1227	0.1450	0.0525	0.1428	0.1080	0.0932	0.2375	0.0473	0.0985
1	-1.9979	0.5837	0.8795	0.1227	0.1450	0.0525	0.1428	0.1080	0.0932	0.2375	0.0473	0.0985
8	0.4848	1.9247	0.0000	-0.2013	0.1883	-0.2065	-0.3939	-0.2503	-0.4224	-0.4390	-1.1102	-0.3314

Dipole mement (in D)	3.97 (DEN)	3.75	1.00	2.79	3.29	3.77	4.03	4.86	10.13	3.95

File TZVPMol105.out
Molecule PMol105 cyclobutanone
SP Mol105 B3LYP/Def2TZVP VAC.

```
    0   11
Dipole          0.0000    0.0000   -3.0180    3.0180
Quadrupole      3.0198    2.4778   -5.4976    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      0.0000    0.0000    1.8675   -0.2539    0.1412   -0.2536   -0.4837   -0.2995   -0.5400   -0.4987   -1.1583   -0.3767
   6      0.0000    0.0000    0.6710    0.1317   -0.3250    0.1629    0.6370    0.1873    0.6644    0.5972    1.0668    0.3186
   6      0.0000    1.0973   -0.3818   -0.1630   -0.2010   -0.0563   -0.3622   -0.1570   -0.3120   -0.5180   -0.0408   -0.1624
   6      0.0000   -1.0973   -0.3818   -0.1630   -0.2010   -0.0563   -0.3622   -0.1570   -0.3120   -0.5180   -0.0408   -0.1624
   6      0.0000    0.0000   -1.4662   -0.1972   -0.2316   -0.0494   -0.1457   -0.1563    0.1532   -0.3916    0.0208   -0.1519
   1      0.8784    1.7417   -0.3444    0.1111    0.1411    0.0465    0.1299    0.1017    0.0911    0.2300    0.0348    0.0917
   1     -0.8784    1.7417   -0.3444    0.1111    0.1411    0.0465    0.1299    0.1017    0.0895    0.2300    0.0348    0.0917
   1     -0.8784   -1.7417   -0.3444    0.1111    0.1411    0.0465    0.1299    0.1017    0.0895    0.2300    0.0348    0.0917
   1      0.8784   -1.7417   -0.3444    0.1111    0.1411    0.0465    0.1299    0.1017    0.0911    0.2300    0.0348    0.0917
   1     -0.8791    0.0000   -2.1052    0.1005    0.1266    0.0333    0.0987    0.0879   -0.0081    0.2045    0.0069    0.0840
   1      0.8791    0.0000   -2.1052    0.1005    0.1266    0.0333    0.0987    0.0879   -0.0068    0.2045    0.0069    0.0840

 Dipole mement (in D)   3.02 (DEN)      2.63      0.91      2.18      2.79      2.86      3.08      3.55      7.32      2.99

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File TZVPMol106.out
Molecule PMol106    cyclopropanone
 SP Mol106 B3LYP/Def2TZVP VAC.
    0    8
Dipole          0.0000    2.9679    0.0000    2.9679
Quadrupole      2.7264   -3.9929    1.2665    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8     -0.0000   -1.5738    0.0000   -0.2348    0.1557   -0.2335   -0.4555   -0.2771   -0.4672   -0.4660   -1.1200   -0.3554
   6      0.0000   -0.3800    0.0000    0.1803   -0.3208    0.1576    0.6327    0.1834    0.5656    0.5824    1.0488    0.3068
   6      0.0000    0.8535    0.7776   -0.2213   -0.1956   -0.0708   -0.3940   -0.1719   -0.3592   -0.5230   -0.0849   -0.1814
   6      0.0000    0.8535   -0.7776   -0.2213   -0.1956   -0.0708   -0.3940   -0.1719   -0.3592   -0.5230   -0.0849   -0.1814
   1     -0.9076    1.1572    1.2836    0.1243    0.1391    0.0544    0.1527    0.1094    0.1547    0.2324    0.0603    0.1029
   1     -0.9076    1.1572   -1.2836    0.1243    0.1391    0.0544    0.1527    0.1094    0.1547    0.2324    0.0603    0.1029
   1      0.9076    1.1572    1.2836    0.1243    0.1391    0.0544    0.1527    0.1094    0.1553    0.2324    0.0603    0.1029
   1      0.9076    1.1572   -1.2836    0.1243    0.1391    0.0544    0.1527    0.1094    0.1553    0.2324    0.0603    0.1029

 Dipole mement (in D)   2.97 (DEN)      2.39      0.90      2.11      2.45      2.78      3.00      3.34      7.20      2.93

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File TZVPMol107.out
Molecule PMol107    cyclopentadienone
 SP Mol107 B3LYP/Def2TZVP VAC.
    0   10
Dipole          0.0000    0.0000   -3.2789    3.2789
Quadrupole     -1.4797    3.9683   -2.4885    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.0000    0.8182    0.2666   -0.2865    0.1510    0.5899    0.1825    0.7717    0.5009    1.0349    0.3006
   6      0.0000    1.1971   -0.0874   -0.2038   -0.1144   -0.0535   -0.2982   -0.1047   -0.4094   -0.2906   -0.0600   -0.1077
   6      0.0000    0.7458   -1.3418   -0.0736   -0.1039   -0.0173   -0.0329   -0.0720   -0.0456   -0.1686   -0.0411   -0.0623
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1	0.0000	1.3380	-2.2459	0.1351	0.1382	0.0538	0.1117	0.1090	0.1345	0.2137	0.0590	0.0995
6	0.0000	-1.1971	-0.0874	-0.2038	-0.1144	-0.0535	-0.2982	-0.1047	-0.4094	-0.2906	-0.0600	-0.1077
6	0.0000	-0.7458	-1.3418	-0.0736	-0.1039	-0.0173	-0.0329	-0.0720	-0.0456	-0.1686	-0.0412	-0.0623
1	0.0000	2.2147	0.2673	0.1322	0.1401	0.0552	0.1431	0.1121	0.1836	0.2254	0.0746	0.0940
1	0.0000	-1.3380	-2.2459	0.1351	0.1382	0.0538	0.1117	0.1090	0.1345	0.2137	0.0590	0.0995
1	0.0000	-2.2147	0.2673	0.1322	0.1401	0.0552	0.1431	0.1121	0.1836	0.2254	0.0746	0.0940
8	0.0000	0.0000	2.0248	-0.2467	0.1663	-0.2273	-0.4373	-0.2713	-0.4978	-0.4607	-1.1000	-0.3476

Dipole mement (in D)	3.28 (DEN)	2.81	0.70	2.37	3.30	2.97	3.31	4.13	7.13	3.21	

File TZVPMol108.out
Molecule PMol108 4-cyclopentene-1,3-dione
SP Mol108 B3LYP/Def2TZVP VAC.
0 11
Dipole 0.0000 0.0000 -1.7546 1.7546
Quadrupole 4.4673 -12.6119 8.1445 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	1.0776	-0.1318	-0.1608	-0.0593	-0.5788	-0.1517	-0.4884	-0.6039	-0.0437	-0.1722
1	-0.8722	0.0000	1.7306	0.1344	0.1635	0.0643	0.1766	0.1227	0.1639	0.2587	0.0708	0.1022
1	0.8722	0.0000	1.7306	0.1344	0.1635	0.0643	0.1766	0.1227	0.1644	0.2587	0.0708	0.1022
6	0.0000	1.1955	0.1483	0.1580	-0.3146	0.1523	0.5999	0.1797	0.6379	0.5204	1.0415	0.3059
6	0.0000	-1.1955	0.1483	0.1580	-0.3146	0.1523	0.5999	0.1797	0.6379	0.5204	1.0415	0.3059
6	0.0000	-0.6690	-1.2391	-0.1190	-0.0657	-0.0089	-0.1797	-0.0595	-0.2295	-0.2185	-0.0545	-0.0617
6	0.0000	0.6690	-1.2391	-0.1190	-0.0657	-0.0089	-0.1797	-0.0595	-0.2295	-0.2185	-0.0546	-0.0617
1	0.0000	-1.3272	-2.0974	0.1494	0.1478	0.0662	0.1478	0.1232	0.1690	0.2291	0.0874	0.1052
1	0.0000	1.3272	-2.0974	0.1494	0.1478	0.0662	0.1478	0.1232	0.1690	0.2291	0.0874	0.1052
8	0.0000	2.3608	0.4599	-0.2569	0.1494	-0.2442	-0.4553	-0.2904	-0.4973	-0.4876	-1.1233	-0.3655
8	0.0000	-2.3608	0.4599	-0.2569	0.1494	-0.2442	-0.4553	-0.2904	-0.4973	-0.4876	-1.1233	-0.3655

Dipole mement (in D)	1.75 (DEN)	0.95	0.10	1.33	2.06	1.55	1.76	2.25	3.64	1.76	

File TZVPMol109.out
Molecule PMol109 3-cyclopentenone
SP Mol109 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -2.8131 2.8131
Quadrupole 1.2193 4.5715 -5.7908 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.8513	0.1138	-0.2932	0.1726	0.6611	0.1959	0.5048	0.6043	1.0458	0.3329
6	0.0000	1.2334	-0.0447	-0.1161	-0.2041	-0.0563	-0.3967	-0.1526	0.0258	-0.5477	-0.0073	-0.1600
6	0.0000	-1.2334	-0.0447	-0.1161	-0.2041	-0.0563	-0.3967	-0.1526	0.0258	-0.5477	-0.0076	-0.1600
6	0.0000	-0.6658	-1.4240	-0.1591	-0.1572	-0.0429	-0.0635	-0.1022	-0.2437	-0.1813	-0.0563	-0.0859
6	0.0000	0.6658	-1.4240	-0.1591	-0.1572	-0.0429	-0.0635	-0.1022	-0.2437	-0.1813	-0.0563	-0.0859
1	-0.8690	1.8577	0.1792	0.1150	0.1527	0.0490	0.1360	0.1054	0.0416	0.2371	0.0393	0.0898
1	0.8690	-1.8577	0.1792	0.1150	0.1527	0.0490	0.1360	0.1054	0.0431	0.2371	0.0393	0.0898
1	0.8690	1.8577	0.1792	0.1150	0.1527	0.0490	0.1360	0.1054	0.0431	0.2371	0.0393	0.0898

1	-0.8690	-1.8577	0.1792	0.1150	0.1527	0.0490	0.1360	0.1054	0.0416	0.2371	0.0393	0.0898
1	0.0000	-1.2812	-2.3135	0.1185	0.1345	0.0434	0.1028	0.0986	0.1441	0.2084	0.0400	0.0893
1	0.0000	1.2812	-2.3135	0.1185	0.1345	0.0434	0.1028	0.0986	0.1441	0.2084	0.0400	0.0893
8	0.0000	0.0000	2.0533	-0.2606	0.1360	-0.2570	-0.4904	-0.3055	-0.5265	-0.5113	-1.1552	-0.3787

Dipole mement (in D) 2.81 (DEN) 2.12 0.09 2.01 2.91 2.58 2.86 3.67 7.10 2.81

File TZVPMol110.out
Molecule PMol110 cyclohexanone
SP Mol110 B3LYP/Def2TZVP VAC.
0 17
Dipole 2.1659 -2.5342 0.0000 3.3337
Quadrupole -0.1665 -3.6038 3.7703 5.0298 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.4127	1.0782	0.0000	0.1440	-0.3283	0.1622	0.6407	0.1821	0.4962	0.5875	1.0045	0.3239
6	0.1553	0.4936	1.2726	-0.1578	-0.2168	-0.0546	-0.3670	-0.1563	-0.1102	-0.4976	-0.0021	-0.1585
6	0.1553	-1.0354	1.2530	-0.1786	-0.2526	-0.0435	-0.1350	-0.1529	0.0611	-0.3791	0.0416	-0.1427
6	0.8266	-1.5757	0.0000	-0.1749	-0.2621	-0.0481	-0.1623	-0.1582	-0.1025	-0.3885	0.0410	-0.1459
6	0.1553	-1.0354	-1.2530	-0.1786	-0.2526	-0.0435	-0.1350	-0.1529	0.0611	-0.3791	0.0417	-0.1427
6	0.1553	0.4936	-1.2726	-0.1578	-0.2168	-0.0546	-0.3670	-0.1563	-0.1102	-0.4976	-0.0022	-0.1585
1	0.6415	-1.4166	2.1519	0.1006	0.1346	0.0330	0.0929	0.0878	0.0001	0.2072	-0.0028	0.0836
1	1.1900	0.8459	1.3543	0.0930	0.1498	0.0395	0.1168	0.0964	0.0357	0.2140	0.0083	0.0847
1	-0.3902	0.8983	2.1230	0.1077	0.1423	0.0393	0.1230	0.0979	0.0360	0.2266	0.0276	0.0785
1	1.8839	-1.2896	0.0000	0.0821	0.1349	0.0268	0.0860	0.0825	0.0325	0.1881	-0.0182	0.0739
1	0.8071	-2.6666	0.0000	0.1009	0.1353	0.0323	0.0880	0.0871	0.0203	0.2082	-0.0054	0.0827
1	0.6415	-1.4166	-2.1519	0.1006	0.1346	0.0330	0.0929	0.0878	0.0001	0.2072	-0.0028	0.0836
1	-0.8776	-1.3941	-1.2930	0.0962	0.1380	0.0304	0.0898	0.0865	0.0090	0.1942	-0.0087	0.0764
1	1.1900	0.8459	-1.3543	0.0930	0.1498	0.0395	0.1168	0.0964	0.0357	0.2140	0.0083	0.0847
1	-0.3902	0.8983	-2.1230	0.1077	0.1423	0.0393	0.1230	0.0979	0.0360	0.2266	0.0276	0.0785
1	-0.8776	-1.3941	1.2930	0.0962	0.1380	0.0304	0.0898	0.0865	0.0090	0.1942	-0.0087	0.0764
8	-1.2535	1.9469	0.0000	-0.2742	0.1295	-0.2615	-0.4935	-0.3121	-0.5102	-0.5260	-1.1505	-0.3784

Dipole mement (in D) 3.33 (DEN) 2.86 1.10 2.40 3.34 3.12 3.35 4.23 7.56 3.22

File TZVPMol111.out
Molecule PMol111 formic_acid(s-cis)
SP Mol111 B3LYP/Def2TZVP VAC.
0 5
Dipole -1.4859 -0.3664 0.0000 1.5304
Quadrupole -4.8057 4.4672 0.3385 -0.0852 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.1573	0.1197	0.0000	-0.2851	0.0903	-0.2675	-0.5328	-0.3226	-0.5052	-0.5629	-1.1789	-0.3841
6	0.0000	0.4175	0.0000	0.2271	-0.4728	0.1927	0.6818	0.2035	0.5867	0.6269	1.6193	0.3676
1	-0.3967	1.4432	0.0000	0.0919	0.1095	0.0613	0.0396	0.1325	0.0487	0.1086	0.0799	0.0955
8	-1.0261	-0.4459	0.0000	-0.3528	0.0824	-0.1682	-0.6428	-0.3715	-0.5619	-0.6561	-1.1127	-0.3447
1	-0.6527	-1.3389	0.0000	0.3190	0.1906	0.1817	0.4541	0.3582	0.4317	0.4835	0.5926	0.2659

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 Dipole mement (in D)   1.53 (DEN)      1.09      1.70      1.35      1.31      1.39      1.53      1.62      3.51      1.47

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File TZVPMol112.out
Molecule PMol112    formic_acid(s-trans)
 SP Mol112 B3LYP/Def2TZVP VAC.
    0    5
Dipole          2.8932    2.7007    0.0001    3.9578
Quadrupole     -0.0188    0.2452   -0.2263    1.4881    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   8     -1.1708   -0.2186   -0.0000   -0.2547    0.1183   -0.2514   -0.4955   -0.3028   -0.4373   -0.5259   -1.1554   -0.3750
   6     -0.1326    0.3602    0.0000    0.1968   -0.4787    0.1875    0.6828    0.1997    0.5573    0.6213    1.6198    0.3542
   1     -0.0320    1.4622    0.0000    0.0651    0.0930    0.0492    0.0041    0.1181   -0.0069    0.0810    0.0494    0.0885
   8      1.0531   -0.2798   -0.0000   -0.3201    0.0839   -0.1660   -0.6267   -0.3692   -0.4949   -0.6511   -1.0974   -0.3472
   1      1.7690    0.3638   -0.0000    0.3128    0.1835    0.1807    0.4352    0.3542    0.3819    0.4747    0.5836    0.2795

 Dipole mement (in D)   3.96 (DEN)      3.10      1.61      2.47      4.40      3.75      3.93      5.10      8.41      3.59

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File TZVPMol113.out
Molecule PMol113    acetic_acid
 SP Mol113 B3LYP/Def2TZVP VAC.
    0    8
Dipole         -0.7293   -1.5737    0.0002    1.7345
Quadrupole      4.4401   -4.8694    0.4293   -2.2896   -0.0001    0.0005
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6      0.0907    0.1289    0.0001    0.2963   -0.5346    0.2139    0.9016    0.2589    0.7523    0.7650    1.5703    0.4649
   6     -1.3825   -0.1088    0.0000   -0.3293   -0.2574   -0.0796   -0.5652   -0.2203   -0.3987   -0.7064    0.0075   -0.2528
   8      0.6407    1.1973   -0.0001   -0.3061    0.1013   -0.2838   -0.5833   -0.3341   -0.5550   -0.5744   -1.1927   -0.4040
   8      0.7709   -1.0420    0.0000   -0.3744    0.0897   -0.1788   -0.6717   -0.3773   -0.5895   -0.6709   -1.1136   -0.3593
   1      1.7097   -0.8148   -0.0001    0.3177    0.1904    0.1752    0.4508    0.3534    0.4082    0.4857    0.5915    0.2592
   1     -1.6687   -0.6920   -0.8732    0.1313    0.1384    0.0517    0.1569    0.1070    0.1333    0.2351    0.0457    0.0987
   1     -1.9141    0.8354   -0.0002    0.1332    0.1337    0.0496    0.1539    0.1054    0.1162    0.2308    0.0465    0.0946
   1     -1.6688   -0.6915    0.8735    0.1313    0.1384    0.0517    0.1569    0.1070    0.1333    0.2350    0.0457    0.0987

 Dipole mement (in D)   1.73 (DEN)      1.33      1.22      1.59      1.38      1.56      1.76      1.99      4.42      1.73

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File TZVPMol114.out
Molecule PMol114    glyoxylic_acid(trans)
 SP Mol114 B3LYP/Def2TZVP VAC.
    0    7
Dipole         -0.3057   -1.9290    0.0000    1.9531
Quadrupole      3.8077   -6.7936    2.9859    0.0902    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   8     -0.5682    1.6346    0.0000   -0.2562    0.1542   -0.2433   -0.4973   -0.2867   -0.4573   -0.5067   -1.1312   -0.3698
   6      0.0000    0.5806    0.0000    0.2632   -0.5257    0.1988    0.6916    0.2558    0.5630    0.6431    1.6172    0.4327
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6	-0.7469	-0.7503	0.0000	0.1158	-0.2435	0.1589	0.2682	0.1517	0.3351	0.3296	1.0249	0.2422
8	1.3241	0.4352	0.0000	-0.3240	0.1379	-0.1558	-0.6085	-0.3474	-0.4622	-0.6260	-1.1060	-0.3438
1	1.5123	-0.5187	0.0000	0.3337	0.2014	0.1654	0.4333	0.3481	0.3641	0.4951	0.6090	0.2430
8	-0.1536	-1.7947	0.0000	-0.2506	0.1460	-0.1886	-0.3642	-0.2496	-0.3802	-0.4816	-1.1006	-0.2995
1	-1.8493	-0.6636	0.0000	0.1182	0.1297	0.0646	0.0768	0.1281	0.0375	0.1465	0.0864	0.0952

Dipole mement (in D)	1.95 (DEN)	1.44	1.99	1.25	2.51	1.97	1.97	2.50	4.14	1.85

File TZVPMol115.out
Molecule PMol115 propionic_acid(cis)
SP Mol115 B3LYP/Def2TZVP VAC.
0 11
Dipole -1.5661 -0.3757 0.0000 1.6105
Quadrupole -4.9724 4.4649 0.5075 -0.6382 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.1714	0.8385	0.0000	-0.3064	0.1057	-0.2762	-0.5763	-0.3276	-0.5441	-0.5810	-1.1939	-0.3945
6	0.0000	0.5676	0.0000	0.2903	-0.5061	0.2128	0.8770	0.2594	0.6617	0.7692	1.5561	0.4633
6	-0.5893	-0.8109	0.0000	-0.1951	-0.2580	-0.0452	-0.3616	-0.1467	0.0810	-0.5024	0.0393	-0.1428
6	0.4572	-1.9011	0.0000	-0.3046	-0.2948	-0.0820	-0.3244	-0.2319	-0.3538	-0.5868	0.0274	-0.2499
8	-0.9685	1.5131	0.0000	-0.3765	0.0917	-0.1785	-0.6805	-0.3776	-0.6326	-0.6685	-1.1158	-0.3586
1	-0.5191	2.3679	0.0000	0.3156	0.1894	0.1745	0.4508	0.3528	0.4330	0.4849	0.5910	0.2587
1	-1.2539	-0.8841	0.8638	0.1187	0.1525	0.0464	0.1336	0.1051	0.0332	0.2283	0.0320	0.0895
1	-1.2539	-0.8841	-0.8638	0.1187	0.1525	0.0464	0.1336	0.1051	0.0332	0.2283	0.0320	0.0895
1	-0.0054	-2.8857	0.0000	0.1115	0.1186	0.0327	0.1108	0.0845	0.0880	0.2041	0.0002	0.0864
1	1.1011	-1.8299	0.8742	0.1139	0.1243	0.0345	0.1185	0.0885	0.1002	0.2119	0.0160	0.0792
1	1.1011	-1.8299	-0.8742	0.1139	0.1243	0.0345	0.1185	0.0885	0.1002	0.2119	0.0160	0.0792

Dipole mement (in D)	1.61 (DEN)	1.26	0.87	1.45	1.25	1.42	1.60	1.91	4.38	1.66

File TZVPMol116.out
Molecule PMol116 acrylic_acid(s-cis)
SP Mol116 B3LYP/Def2TZVP VAC.
0 9
Dipole -1.2983 -0.8651 0.0000 1.5601
Quadrupole -4.1690 6.2790 -2.1100 -2.2499 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.1425	0.8678	0.0000	-0.3150	0.1008	-0.2813	-0.5860	-0.3308	-0.5493	-0.5798	-1.1871	-0.3983
6	0.0000	0.4851	0.0000	0.3292	-0.5032	0.2006	0.8494	0.2521	0.7379	0.7211	1.5595	0.4455
6	-0.4477	-0.9187	0.0000	-0.1773	-0.1745	-0.0438	-0.2823	-0.0964	-0.2233	-0.3221	-0.0179	-0.0877
6	0.4334	-1.9100	0.0000	-0.1890	-0.1223	-0.0313	-0.1590	-0.1318	-0.2957	-0.2735	-0.0349	-0.1401
8	-1.0582	1.3292	0.0000	-0.3757	0.0981	-0.1744	-0.6730	-0.3713	-0.5917	-0.6592	-1.1087	-0.3549
1	-0.6961	2.2245	0.0000	0.3178	0.1912	0.1771	0.4540	0.3553	0.4146	0.4870	0.5933	0.2608
1	-1.5159	-1.0949	0.0000	0.1301	0.1474	0.0487	0.1383	0.1089	0.1590	0.2179	0.0610	0.0852
1	0.1284	-2.9470	0.0000	0.1316	0.1265	0.0522	0.1238	0.1052	0.1674	0.1973	0.0532	0.1027
1	1.4953	-1.6963	0.0000	0.1482	0.1360	0.0521	0.1350	0.1088	0.1809	0.2112	0.0813	0.0868

Dipole mement (in D) 1.56 (DEN) 1.05 0.50 1.45 1.27 1.32 1.57 1.95 4.35 1.66

File TZVPMol117.out
Molecule PMol117 acrylic_acid(s-trans)
SP Mol117 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.8700 -1.9897 0.0000 2.1716
Quadrupole 2.4065 -0.7596 -1.6469 5.0957 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.4597	1.6805	0.0000	-0.3108	0.1044	-0.2816	-0.5789	-0.3303	-0.5480	-0.5665	-1.1767	-0.4006
6	0.0000	0.5655	0.0000	0.3295	-0.5021	0.2001	0.8453	0.2512	0.7105	0.7184	1.5538	0.4436
6	-0.8082	-0.6623	0.0000	-0.1717	-0.1684	-0.0401	-0.2758	-0.0926	-0.2006	-0.3109	-0.0119	-0.0837
6	-0.3056	-1.8908	0.0000	-0.1929	-0.1333	-0.0370	-0.1606	-0.1375	-0.2914	-0.2858	-0.0386	-0.1463
8	1.3321	0.3250	0.0000	-0.3803	0.0961	-0.1712	-0.6818	-0.3696	-0.5635	-0.6711	-1.1159	-0.3517
1	1.7618	1.1891	0.0000	0.3184	0.1925	0.1772	0.4563	0.3560	0.4083	0.4895	0.5956	0.2630
1	-1.8752	-0.4815	0.0000	0.1332	0.1527	0.0526	0.1363	0.1121	0.1424	0.2209	0.0653	0.0883
1	-0.9455	-2.7629	0.0000	0.1301	0.1266	0.0516	0.1228	0.1045	0.1672	0.1979	0.0528	0.1019
1	0.7626	-2.0628	0.0000	0.1445	0.1315	0.0485	0.1364	0.1062	0.1751	0.2076	0.0750	0.0856

Dipole mement (in D) 2.17 (DEN) 1.68 1.64 1.94 1.96 1.88 2.22 2.55 4.82 1.94

File TZVPMol118.out
Molecule PMol118 2-methoxyethanoic_acid(g
SP Mol118 B3LYP/Def2TZVP VAC.
0 12
Dipole 5.1108 -0.0627 0.0007 5.1112
Quadrupole -3.9163 1.5481 2.3683 -1.8893 -0.0015 -0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-2.1631	-0.7772	-0.0001	-0.2939	0.1228	-0.2788	-0.5629	-0.3244	-0.5305	-0.5528	-1.1785	-0.4071
6	-1.1852	-0.0870	0.0002	0.2648	-0.5219	0.2036	0.8230	0.2557	0.7514	0.7409	1.6258	0.4446
6	0.2124	-0.6651	0.0002	-0.0242	-0.2964	0.0246	-0.1555	-0.0475	-0.3202	-0.1871	0.4894	-0.0082
8	1.1637	0.3703	0.0000	-0.3513	0.1258	-0.1464	-0.2766	-0.2625	-0.1658	-0.5184	-1.0842	-0.2575
8	-1.2461	1.2513	-0.0002	-0.3401	0.1207	-0.1717	-0.6404	-0.3650	-0.5160	-0.6444	-1.1167	-0.3587
1	-0.3384	1.5925	-0.0002	0.3320	0.1908	0.1520	0.4286	0.3404	0.3487	0.4973	0.6125	0.2337
1	0.3180	-1.3096	-0.8809	0.1139	0.1377	0.0473	0.1026	0.1126	0.1488	0.1933	0.0446	0.0883
1	0.3181	-1.3095	0.8813	0.1139	0.1377	0.0472	0.1025	0.1126	0.1486	0.1933	0.0446	0.0883
6	2.4923	-0.0973	-0.0000	-0.1684	-0.3397	0.0038	-0.0789	-0.1188	-0.2031	-0.2447	0.4934	-0.0969
1	2.7016	-0.7015	-0.8885	0.1114	0.1043	0.0352	0.0781	0.0942	0.1116	0.1644	0.0146	0.0869
1	2.7017	-0.7014	0.8885	0.1114	0.1043	0.0352	0.0781	0.0942	0.1116	0.1644	0.0146	0.0869
1	3.1457	0.7705	-0.0001	0.1306	0.1139	0.0479	0.1015	0.1084	0.1150	0.1938	0.0393	0.0997

Dipole mement (in D) 5.11 (DEN) 4.30 2.23 3.55 5.53 5.05 5.16 6.48 10.45 4.95

File TZVPMol119.out
Molecule PMol119 acetoacetic_acid

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 SP Mol119 B3LYP/Def2TZVP VAC.
    0   10
Dipole         -2.3208    0.5312    0.0004    2.3808
Quadrupole     -0.5541   -2.4894    3.0435    6.2884    0.0002    0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      1.0077   -1.4527   -0.0000   -0.2685    0.1429   -0.2498   -0.4924   -0.2944   -0.4616   -0.5245   -1.1473   -0.3742
   6      0.7606   -0.2800    0.0000    0.2609   -0.4935    0.1971    0.6739    0.2552    0.5609    0.6535    1.6104    0.4299
   6     -0.6741    0.2823    0.0001    0.1794   -0.3201    0.1724    0.4776    0.1988    0.4651    0.4796    0.9956    0.3308
   8      1.6821    0.6806   -0.0001   -0.3284    0.1355   -0.1609   -0.6076   -0.3516   -0.4931   -0.6272   -1.1122   -0.3482
   1      1.1967    1.5253   -0.0000    0.3342    0.2018    0.1583    0.4284    0.3431    0.3749    0.4975    0.6120    0.2347
   8     -0.8123    1.4849   -0.0000   -0.2939    0.1442   -0.2117   -0.4284   -0.2694   -0.4522   -0.5133   -1.1242   -0.3254
   6     -1.7734   -0.7131    0.0000   -0.3102   -0.2450   -0.0771   -0.5458   -0.2186   -0.3800   -0.7014   -0.0124   -0.2512
   1     -1.6766   -1.3685    0.8658    0.1443    0.1503    0.0599    0.1674    0.1147    0.1240    0.2517    0.0643    0.1033
   1     -1.6765   -1.3686   -0.8657    0.1444    0.1503    0.0599    0.1674    0.1147    0.1240    0.2517    0.0643    0.1033
   1     -2.7419   -0.2255   -0.0000    0.1378    0.1336    0.0519    0.1594    0.1073    0.1381    0.2323    0.0501    0.0969

 Dipole mement (in D)   2.38 (DEN)      2.01      1.02      1.62      2.51      2.42      2.39      3.06      5.63      2.31

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File TZVPMol120.out
Molecule PMol120    methyl_acetate
 SP Mol120 B3LYP/Def2TZVP VAC.
    0   11
Dipole          1.6360   -0.9194    0.0000    1.8766
Quadrupole     -3.1751    2.8192    0.3559    4.6395    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1      0.7314    2.4902    0.0000    0.1323    0.1324    0.0477    0.1528    0.1035    0.1866    0.2288    0.0431    0.0922
   6      1.1231    1.4795    0.0000   -0.3333   -0.2565   -0.0823   -0.5723   -0.2227   -0.6864   -0.6951    0.0081   -0.2554
   6      0.0000    0.4935    0.0000    0.3233   -0.5106    0.2113    0.8403    0.2611    0.8962    0.7622    1.5628    0.4648
   8     -1.1742    0.7549    0.0000   -0.3235    0.1085   -0.2742   -0.5705   -0.3248   -0.5743   -0.5784   -1.1887   -0.3929
   1      1.7553    1.3329    0.8737    0.1280    0.1364    0.0491    0.1503    0.1044    0.1827    0.2324    0.0412    0.0955
   1      1.7553    1.3329   -0.8737    0.1280    0.1364    0.0491    0.1503    0.1044    0.1827    0.2324    0.0412    0.0955
   8      0.4779   -0.7685    0.0000   -0.2656    0.2314   -0.1264   -0.3451   -0.2152   -0.4045   -0.4830   -1.0820   -0.2487
   6     -0.5201   -1.7885    0.0000   -0.1624   -0.3094    0.0010   -0.1040   -0.1210    0.0042   -0.2584    0.4559   -0.1106
   1      0.0142   -2.7325    0.0000    0.1235    0.1100    0.0441    0.1008    0.1052    0.0804    0.1870    0.0340    0.0940
   1     -1.1521   -1.7110   -0.8829    0.1248    0.1107    0.0403    0.0987    0.1026    0.0662    0.1860    0.0422    0.0828
   1     -1.1521   -1.7110    0.8829    0.1248    0.1107    0.0403    0.0987    0.1026    0.0662    0.1860    0.0422    0.0828

 Dipole mement (in D)   1.88 (DEN)      1.37      1.15      1.52      1.97      1.64      1.87      2.01      3.55      1.66

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File TZVPMol121.out
Molecule PMol121    methyl_formate
 SP Mol121 B3LYP/Def2TZVP VAC.
    0    8
Dipole          1.6950    0.8660    0.0000    1.9034
Quadrupole      0.3582   -0.9753    0.6172   -4.5739    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
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8	-1.2915	-0.6711	-0.0000	-0.3019	0.0937	-0.2625	-0.5253	-0.3179	-0.5164	-0.5698	-1.1773	-0.3775
6	-0.8250	0.4314	0.0000	0.2270	-0.4583	0.1863	0.6221	0.2018	0.6605	0.6235	1.6093	0.3639
8	0.4770	0.7306	0.0000	-0.2457	0.2207	-0.1199	-0.3244	-0.2140	-0.3687	-0.4692	-1.0808	-0.2379
6	1.3545	-0.4012	-0.0000	-0.1612	-0.3041	0.0052	-0.1109	-0.1173	0.0016	-0.2676	0.4428	-0.1085
1	1.1883	-1.0137	-0.8839	0.1291	0.1120	0.0438	0.1030	0.1058	0.0802	0.1889	0.0470	0.0869
1	2.3616	0.0000	-0.0000	0.1279	0.1117	0.0476	0.1059	0.1086	0.0819	0.1907	0.0407	0.0976
1	1.1883	-1.0137	0.8839	0.1291	0.1120	0.0438	0.1030	0.1058	0.0802	0.1889	0.0470	0.0869
1	-1.3992	1.3698	-0.0000	0.0956	0.1122	0.0559	0.0267	0.1275	-0.0192	0.1147	0.0717	0.0886

Dipole mement (in D)	1.90 (DEN)	1.66	1.57	1.51	1.96	1.67	1.91	2.01	3.11	1.58

File TZVPMol122.out
Molecule PMol122 ethyl_formate(cis)
SP Mol122 B3LYP/Def2TZVP VAC.
0 11
Dipole -1.5191 -1.2218 -0.2323 1.9633
Quadrupole 1.5575 -2.6498 1.0922 -3.1460 -2.2804 -0.9946

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.4514	0.8975	0.2408	-0.3121	0.0875	-0.2621	-0.5300	-0.3192	-0.4913	-0.5780	-1.1819	-0.3740
6	1.3117	-0.1888	-0.2452	0.2247	-0.4598	0.1864	0.6314	0.2019	0.5610	0.6261	1.6116	0.3656
8	0.2170	-0.9495	-0.1833	-0.2515	0.2389	-0.1212	-0.3528	-0.2115	-0.4268	-0.4752	-1.0793	-0.2415
6	-0.9040	-0.3850	0.5365	0.0085	-0.3003	0.0365	0.1067	-0.0488	0.3559	-0.0848	0.4366	-0.0025
6	-1.6927	0.5549	-0.3339	-0.3482	-0.3062	-0.0853	-0.4082	-0.2340	-0.3155	-0.6201	0.0160	-0.2537
1	2.0795	-0.7296	-0.8192	0.0942	0.1118	0.0538	0.0236	0.1255	0.0235	0.1135	0.0682	0.0867
1	-0.5263	0.1160	1.4275	0.1139	0.1289	0.0384	0.0842	0.1061	0.0130	0.1940	0.0494	0.0763
1	-1.4896	-1.2501	0.8401	0.1100	0.1263	0.0420	0.0824	0.1062	0.0050	0.1858	0.0283	0.0883
1	-2.0415	0.0562	-1.2365	0.1109	0.1206	0.0345	0.1160	0.0885	0.0948	0.2063	0.0101	0.0826
1	-1.0936	1.4161	-0.6219	0.1387	0.1264	0.0367	0.1263	0.0928	0.1140	0.2194	0.0296	0.0782
1	-2.5652	0.9199	0.2057	0.1109	0.1260	0.0404	0.1204	0.0924	0.0664	0.2130	0.0115	0.0941

Dipole mement (in D)	1.96 (DEN)	1.75	1.77	1.54	1.98	1.73	1.93	2.12	3.06	1.61

File TZVPMol123.out
Molecule PMol123 ethyl_formate(trans)
SP Mol123 B3LYP/Def2TZVP VAC.
0 11
Dipole -2.0934 0.5640 0.0000 2.1680
Quadrupole -2.5957 1.2213 1.3744 4.8296 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.9788	-0.3835	0.0000	-0.3047	0.0902	-0.2651	-0.5345	-0.3207	-0.5379	-0.5732	-1.1788	-0.3790
6	1.3317	0.6247	0.0000	0.2186	-0.4588	0.1843	0.6228	0.2000	0.6556	0.6286	1.6114	0.3628
8	0.0000	0.7029	0.0000	-0.2459	0.2382	-0.1187	-0.3445	-0.2086	-0.4446	-0.4782	-1.0809	-0.2399
6	-0.6942	-0.5643	0.0000	-0.0271	-0.3009	0.0361	0.1064	-0.0486	0.3958	-0.0833	0.4377	-0.0021
6	-2.1665	-0.2783	0.0000	-0.2969	-0.3045	-0.0828	-0.3927	-0.2313	-0.4047	-0.6090	0.0270	-0.2495
1	1.7435	1.6455	0.0000	0.0941	0.1112	0.0537	0.0241	0.1253	-0.0078	0.1125	0.0681	0.0865
1	-0.3764	-1.1313	0.8764	0.1123	0.1272	0.0392	0.0817	0.1048	0.0077	0.1859	0.0368	0.0785

1	-0.3764	-1.1313	-0.8764	0.1123	0.1272	0.0392	0.0817	0.1048	0.0077	0.1859	0.0368	0.0785
1	-2.7280	-1.2106	0.0000	0.1105	0.1257	0.0405	0.1184	0.0926	0.0895	0.2128	0.0122	0.0944
1	-2.4593	0.2900	-0.8808	0.1134	0.1222	0.0368	0.1183	0.0909	0.1194	0.2091	0.0144	0.0849
1	-2.4593	0.2900	0.8808	0.1134	0.1222	0.0368	0.1183	0.0909	0.1194	0.2091	0.0144	0.0849

Dipole mement (in D) 2.17 (DEN) 2.07 2.01 1.77 2.00 1.95 2.20 2.34 3.51 1.70

File TZVPMol124.out
Molecule PMol124 ethyl_acetate
SP Mol124 B3LYP/Def2TZVP VAC.
0 14
Dipole -0.9870 -1.7835 0.0000 2.0384
Quadrupole 3.3395 -4.1514 0.8119 -5.0232 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.0338	0.1464	-0.0000	0.3161	-0.5099	0.2102	0.8399	0.2601	0.8639	0.7668	1.5667	0.4643
8	1.1853	1.3404	-0.0000	-0.3256	0.1058	-0.2761	-0.5787	-0.3269	-0.5865	-0.5812	-1.1899	-0.3938
8	-0.1749	-0.4492	0.0000	-0.2648	0.2500	-0.1244	-0.3658	-0.2089	-0.4722	-0.4907	-1.0823	-0.2504
6	-1.3031	0.4445	0.0000	-0.0253	-0.3052	0.0328	0.1096	-0.0512	0.3612	-0.0717	0.4522	-0.0034
1	-1.2357	1.0925	-0.8756	0.1077	0.1262	0.0363	0.0785	0.1022	0.0041	0.1810	0.0330	0.0749
1	-1.2357	1.0925	0.8757	0.1077	0.1262	0.0363	0.0785	0.1022	0.0041	0.1810	0.0330	0.0749
6	2.1248	-0.8767	-0.0000	-0.3347	-0.2570	-0.0832	-0.5704	-0.2236	-0.5981	-0.6946	0.0066	-0.2562
1	2.0401	-1.5202	0.8737	0.1270	0.1357	0.0483	0.1491	0.1035	0.1646	0.2314	0.0397	0.0949
1	2.0401	-1.5202	-0.8738	0.1270	0.1357	0.0483	0.1491	0.1035	0.1646	0.2314	0.0397	0.0949
1	3.0927	-0.3888	-0.0000	0.1316	0.1320	0.0470	0.1518	0.1028	0.1625	0.2283	0.0422	0.0914
6	-2.5489	-0.3925	0.0000	-0.2962	-0.3058	-0.0843	-0.3886	-0.2327	-0.3720	-0.6074	0.0260	-0.2505
1	-3.4300	0.2465	0.0000	0.1089	0.1246	0.0389	0.1155	0.0910	0.0847	0.2112	0.0095	0.0927
1	-2.5970	-1.0306	-0.8806	0.1104	0.1209	0.0350	0.1157	0.0890	0.1096	0.2072	0.0113	0.0832
1	-2.5970	-1.0306	0.8807	0.1104	0.1209	0.0350	0.1157	0.0890	0.1096	0.2072	0.0113	0.0832

Dipole mement (in D) 2.04 (DEN) 1.70 1.57 1.67 1.97 1.83 2.07 2.26 3.79 1.69

File TZVPMol125.out
Molecule PMol125 pentyl_formate
SP Mol125 B3LYP/Def2TZVP VAC.
0 20
Dipole 1.9696 -1.3190 0.0000 2.3705
Quadrupole -3.1501 -0.6376 3.7877 6.5949 -0.0001 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.8699	-0.4482	-0.0000	-0.1375	-0.2919	-0.0436	-0.1186	-0.1567	0.2823	-0.3767	0.0563	-0.1354
6	1.5553	0.3138	0.0000	-0.2095	-0.2633	-0.0438	-0.1489	-0.1549	0.0040	-0.3758	0.0426	-0.1397
1	2.9016	-1.1102	0.8702	0.0848	0.1322	0.0270	0.0821	0.0822	-0.0563	0.1901	-0.0161	0.0757
1	2.9016	-1.1102	-0.8702	0.0848	0.1322	0.0270	0.0821	0.0822	-0.0563	0.1901	-0.0162	0.0757
6	0.3371	-0.5937	0.0000	-0.1129	-0.2655	-0.0497	-0.2270	-0.1577	-0.2093	-0.4021	0.0553	-0.1462
1	1.5199	0.9771	0.8708	0.0864	0.1350	0.0277	0.0829	0.0836	-0.0110	0.1882	-0.0162	0.0751
1	1.5199	0.9771	-0.8707	0.0864	0.1350	0.0277	0.0829	0.0836	-0.0110	0.1882	-0.0162	0.0751
6	-0.9485	0.1877	0.0000	-0.0348	-0.2736	0.0330	0.0882	-0.0496	0.4110	-0.0711	0.4332	-0.0072

1	0.3594	-1.2513	-0.8728	0.0919	0.1379	0.0318	0.0960	0.0899	0.0585	0.2003	-0.0002	0.0746
1	0.3594	-1.2513	0.8728	0.0919	0.1379	0.0318	0.0960	0.0899	0.0585	0.2003	-0.0002	0.0746
1	-1.0407	0.8327	0.8768	0.1086	0.1291	0.0373	0.0783	0.1034	-0.0016	0.1820	0.0333	0.0753
1	-1.0407	0.8327	-0.8768	0.1086	0.1291	0.0373	0.0783	0.1034	-0.0016	0.1820	0.0333	0.0753
6	4.0824	0.4614	-0.0000	-0.3261	-0.3089	-0.0838	-0.3293	-0.2356	-0.2792	-0.5840	0.0139	-0.2473
1	4.0929	1.1095	0.8773	0.1026	0.1169	0.0279	0.0978	0.0797	0.0578	0.1958	-0.0079	0.0801
1	5.0148	-0.1010	-0.0000	0.1135	0.1172	0.0302	0.1005	0.0815	0.0602	0.2045	-0.0031	0.0837
1	4.0928	1.1095	-0.8773	0.1026	0.1169	0.0279	0.0978	0.0797	0.0578	0.1958	-0.0079	0.0801
8	-2.0453	-0.7502	0.0000	-0.2446	0.2421	-0.1178	-0.3516	-0.2080	-0.4870	-0.4752	-1.0834	-0.2387
6	-3.2634	-0.2068	0.0000	0.2135	-0.4594	0.1840	0.6245	0.1997	0.6796	0.6288	1.6120	0.3625
8	-3.5133	0.9647	-0.0000	-0.3037	0.0900	-0.2657	-0.5355	-0.3212	-0.5477	-0.5732	-1.1792	-0.3795
1	-4.0093	-1.0164	-0.0000	0.0934	0.1110	0.0534	0.0235	0.1249	-0.0084	0.1122	0.0675	0.0862

Dipole mement (in D)	2.37 (DEN)	2.33	2.20	1.96	2.22	2.15	2.37	2.46	3.70	1.87

File TZVPMol126.out
Molecule PMol126 diethyl_carbonate
SP Mol126 B3LYP/Def2TZVP VAC.
0 18
Dipole 0.1233 -0.4237 0.2241 0.4949
Quadrupole 8.7029 -7.5647 -1.1383 2.2717 0.7726 0.7436

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-2.3741	-0.3460	-0.4789	0.0129	-0.3015	0.0372	0.1170	-0.0473	0.3364	-0.0727	0.4553	-0.0000
6	-2.9858	0.0788	0.8285	-0.3532	-0.3068	-0.0868	-0.4088	-0.2354	-0.2669	-0.6213	0.0143	-0.2550
1	-2.3692	0.4705	-1.2011	0.1098	0.1289	0.0367	0.0825	0.1048	-0.0142	0.1921	0.0471	0.0743
1	-2.8969	-1.1951	-0.9151	0.1086	0.1264	0.0415	0.0828	0.1060	0.0157	0.1839	0.0265	0.0872
1	-2.9680	-0.7333	1.5534	0.1113	0.1204	0.0340	0.1159	0.0880	0.0789	0.2058	0.0091	0.0817
1	-2.4555	0.9316	1.2469	0.1377	0.1259	0.0351	0.1258	0.0915	0.0859	0.2188	0.0286	0.0761
1	-4.0237	0.3718	0.6780	0.1086	0.1250	0.0391	0.1183	0.0911	0.0601	0.2116	0.0089	0.0926
8	-1.0251	-0.8187	-0.3030	-0.2671	0.2641	-0.1268	-0.4204	-0.2048	-0.4638	-0.4718	-1.0769	-0.2606
6	-0.0974	0.1370	-0.2233	0.4299	-0.6438	0.2585	1.0330	0.3444	0.9192	0.9517	2.1921	0.5964
8	-0.2827	1.3237	-0.3107	-0.3679	0.0800	-0.2854	-0.6721	-0.3377	-0.5867	-0.6389	-1.2150	-0.3994
8	1.0795	-0.4614	-0.0347	-0.2593	0.2641	-0.1237	-0.4136	-0.2012	-0.4872	-0.4754	-1.0773	-0.2579
6	2.1989	0.4376	0.0659	-0.0234	-0.3010	0.0365	0.1183	-0.0474	0.4488	-0.0692	0.4557	-0.0000
6	3.4284	-0.3968	0.2738	-0.2976	-0.3034	-0.0829	-0.3898	-0.2314	-0.3213	-0.6088	0.0268	-0.2496
1	2.0204	1.1292	0.8912	0.1063	0.1261	0.0369	0.0784	0.1028	-0.0324	0.1822	0.0329	0.0762
1	2.2512	1.0363	-0.8451	0.1078	0.1264	0.0372	0.0787	0.1031	-0.0319	0.1826	0.0334	0.0761
1	3.5873	-1.0802	-0.5582	0.1138	0.1222	0.0368	0.1190	0.0910	0.0957	0.2092	0.0146	0.0845
1	4.3042	0.2439	0.3558	0.1084	0.1249	0.0393	0.1160	0.0914	0.0664	0.2112	0.0098	0.0931
1	3.3560	-0.9871	1.1853	0.1133	0.1221	0.0367	0.1188	0.0909	0.0973	0.2090	0.0143	0.0844

Dipole mement (in D)	0.49 (DEN)	0.25	1.19	0.78	0.56	0.30	0.53	0.50	0.85	0.27

File TZVPMol127.out
Molecule PMol127 maleic_anhydride
SP Mol127 B3LYP/Def2TZVP VAC.

```
    0    9
Dipole          0.0000    0.0000   -4.2086    4.2086
Quadrupole      3.2607   -7.7109    4.4502    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   8      0.0000    0.0000    0.9644   -0.1985    0.3159   -0.1116   -0.4371   -0.1645   -0.3819   -0.4680   -1.0249   -0.2560
   6      0.0000    1.1263    0.1554    0.2966   -0.4171    0.2104    0.7672    0.2696    0.6945    0.7112    1.5435    0.4251
   6      0.0000   -1.1263    0.1554    0.2966   -0.4171    0.2104    0.7672    0.2696    0.6945    0.7112    1.5445    0.4251
   8      0.0000   -2.2307    0.5980   -0.2181    0.1809   -0.2250   -0.4800   -0.2672   -0.4537   -0.4747   -1.1245   -0.3559
   8      0.0000    2.2307    0.5980   -0.2181    0.1809   -0.2250   -0.4800   -0.2672   -0.4537   -0.4747   -1.1245   -0.3559
   6      0.0000   -0.6643   -1.2493   -0.1382   -0.0749   -0.0070   -0.2404   -0.0550   -0.2344   -0.2426   -0.0152   -0.0604
   6      0.0000    0.6643   -1.2493   -0.1382   -0.0749   -0.0070   -0.2404   -0.0550   -0.2344   -0.2426   -0.0153   -0.0604
   1      0.0000    1.3538   -2.0784    0.1590    0.1531    0.0773    0.1718    0.1348    0.1845    0.2400    0.1081    0.1192
   1      0.0000   -1.3538   -2.0784    0.1590    0.1531    0.0773    0.1718    0.1348    0.1845    0.2400    0.1081    0.1192

 Dipole mement (in D)   4.21 (DEN)      3.25      0.28      2.96      4.18      3.93      4.21      5.71     10.88      4.25

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File TZVPMol128.out
Molecule PMol128    \beta-propiolactone
 SP Mol128 B3LYP/Def2TZVP VAC.
    0    9
Dipole          2.0986   -3.7179    0.0000    4.2693
Quadrupole     -0.0167   -2.5338    2.5505   -0.0078    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   8     -0.0784    1.8063    0.0000   -0.2504    0.1434   -0.2605   -0.5396   -0.3033   -0.5228   -0.5224   -1.1816   -0.3907
   6      0.0000    0.6229    0.0000    0.2750   -0.4669    0.2053    0.8019    0.2609    0.7835    0.7636    1.5880    0.4274
   8     -1.0292   -0.2829    0.0000   -0.2525    0.2377   -0.1401   -0.3553   -0.2109   -0.4249   -0.4596   -0.9893   -0.2647
   6     -0.0940   -1.4026    0.0000    0.0292   -0.2396    0.0378    0.0615   -0.0439    0.3149   -0.0760    0.4137   -0.0110
   6      1.0774   -0.4371    0.0000   -0.2637   -0.2072   -0.0504   -0.4483   -0.1470   -0.5341   -0.5431   -0.0150   -0.1571
   1     -0.2278   -2.0109    0.8920    0.1025    0.1209    0.0472    0.0925    0.1088    0.0231    0.1830    0.0394    0.0939
   1     -0.2278   -2.0109   -0.8920    0.1025    0.1209    0.0472    0.0925    0.1088    0.0231    0.1830    0.0394    0.0939
   1      1.7082   -0.4323   -0.8850    0.1287    0.1454    0.0567    0.1475    0.1133    0.1687    0.2357    0.0528    0.1042
   1      1.7082   -0.4323    0.8850    0.1287    0.1454    0.0567    0.1475    0.1133    0.1687    0.2357    0.0528    0.1042

 Dipole mement (in D)   4.27 (DEN)      3.67      1.37      3.06      4.10      4.08      4.31      5.49      9.82      4.19

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File TZVPMol129.out
Molecule PMol129    \gamma-butyrolactone
 SP Mol129 B3LYP/Def2TZVP VAC.
    0   12
Dipole          4.4038    1.5381    0.4035    4.6821
Quadrupole     -4.2537    1.2592    2.9945   -1.7173   -0.2837   -0.1013
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM        ACP
   8     -2.0755   -0.0297   -0.0718   -0.2743    0.1256   -0.2781   -0.5615   -0.3220   -0.5394   -0.5430   -1.1819   -0.4071
   6     -0.8841    0.0008    0.0028    0.2444   -0.4711    0.2027    0.8111    0.2569    0.6812    0.7597    1.5667    0.4312
   8     -0.1249   -1.1270   -0.0463   -0.2297    0.2595   -0.1296   -0.3616   -0.2067   -0.3691   -0.4625   -1.0437   -0.2599
   6      0.0276    1.1951    0.1692   -0.1955   -0.2203   -0.0490   -0.4078   -0.1481   -0.1331   -0.5157    0.0124   -0.1547
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6	1.3934	0.6632	-0.2213	-0.2022	-0.2525	-0.0484	-0.2158	-0.1544	-0.0434	-0.4204	0.0345	-0.1502
6	1.2628	-0.8108	0.1296	-0.0088	-0.2686	0.0355	0.0788	-0.0463	0.0808	-0.0717	0.4540	-0.0060
1	-0.0134	1.4966	1.2183	0.1178	0.1546	0.0505	0.1356	0.1084	0.0680	0.2309	0.0346	0.0951
1	-0.3336	2.0357	-0.4159	0.1235	0.1482	0.0523	0.1435	0.1100	0.0559	0.2386	0.0453	0.0967
1	1.5564	0.7819	-1.2926	0.1065	0.1392	0.0386	0.1064	0.0956	0.0522	0.2064	0.0093	0.0868
1	2.2248	1.1411	0.2913	0.1091	0.1355	0.0416	0.1112	0.0967	0.0281	0.2158	0.0155	0.0932
1	1.8383	-1.4784	-0.5078	0.1118	0.1261	0.0463	0.0870	0.1093	0.0633	0.1914	0.0360	0.0928
1	1.5320	-1.0135	1.1698	0.0974	0.1237	0.0377	0.0731	0.1006	0.0554	0.1706	0.0177	0.0823

Dipole mement (in D)	4.68 (DEN)	4.11	1.52	3.34	4.56	4.46	4.72	6.05	10.52	4.52	

File TZVPMol130.out
Molecule PMol130 2-methoxyethanol_(gauche
SP Mol130 B3LYP/Def2TZVP VAC.
0 13
Dipole 1.1526 -1.1717 -1.1344 1.9971
Quadrupole -1.2020 -0.0199 1.2219 -0.5178 3.7269 1.5055

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.1389	0.5050	-0.0514	-0.3121	0.1469	-0.1624	-0.3008	-0.2703	-0.4061	-0.4909	-1.0668	-0.2747
6	0.0232	-0.3430	0.0413	-0.0259	-0.3462	0.0161	0.0575	-0.0628	0.1509	-0.0825	0.5146	-0.0062
6	-1.2262	0.5074	-0.0032	0.0259	-0.3475	0.0212	0.0879	-0.0622	0.2339	-0.0713	0.5298	-0.0053
1	0.0478	-0.9293	0.9709	0.0832	0.1165	0.0259	0.0536	0.0903	0.0250	0.1557	0.0028	0.0684
1	0.0188	-1.0688	-0.7891	0.0544	0.1093	0.0191	0.0364	0.0830	0.0091	0.1373	-0.0209	0.0641
1	-1.2438	1.1832	0.8515	0.0977	0.1274	0.0401	0.0838	0.1064	0.0608	0.1784	0.0283	0.0807
1	-1.2156	1.1322	-0.9032	0.0874	0.1141	0.0279	0.0547	0.0919	-0.0084	0.1567	0.0053	0.0701
6	2.3506	-0.1980	0.0061	-0.1674	-0.3574	-0.0050	-0.0703	-0.1266	0.0675	-0.2429	0.5105	-0.1009
1	2.4567	-0.7473	0.9493	0.0987	0.0984	0.0271	0.0612	0.0858	0.0267	0.1556	0.0005	0.0776
1	2.4421	-0.9170	-0.8175	0.0960	0.0975	0.0257	0.0592	0.0844	0.0242	0.1537	-0.0022	0.0761
1	3.1584	0.5257	-0.0706	0.1218	0.1099	0.0412	0.0906	0.1017	0.0663	0.1869	0.0271	0.0903
8	-2.3972	-0.2787	0.0848	-0.4529	-0.0351	-0.2303	-0.6197	-0.4490	-0.6360	-0.6880	-1.0824	-0.3963
1	-2.4838	-0.7873	-0.7236	0.2932	0.1661	0.1533	0.4061	0.3276	0.3861	0.4514	0.5541	0.2560

Dipole mement (in D)	2.00 (DEN)	1.75	0.69	0.97	2.22	2.08	2.04	3.27	4.50	1.90	

File TZVPMol131.out
Molecule PMol131 benzyl_alcohol
SP Mol131 B3LYP/Def2TZVP VAC.
0 16
Dipole -1.1577 -1.3261 -0.0004 1.7603
Quadrupole 7.0030 -0.2664 -6.7367 3.3123 0.0019 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.8692	-0.9962	-0.0000	-0.0947	-0.1430	-0.0428	-0.0841	-0.0987	-0.0446	-0.2016	-0.0262	-0.0864
6	0.5159	-1.2918	-0.0000	-0.2088	-0.1171	-0.0465	-0.1558	-0.1002	-0.3248	-0.2059	-0.0381	-0.0959
6	-0.4349	-0.2725	0.0000	0.1517	-0.1504	-0.0006	0.0801	-0.0136	0.3109	-0.0480	-0.0160	0.0277
6	-0.0069	1.0494	0.0000	-0.1842	-0.1079	-0.0427	-0.1354	-0.0952	-0.2802	-0.2032	-0.0231	-0.0950
6	1.3509	1.3456	0.0000	-0.0854	-0.1390	-0.0401	-0.0832	-0.0958	-0.0634	-0.1980	-0.0264	-0.0839

6	2.2921	0.3277	-0.0000	-0.1223	-0.1467	-0.0458	-0.1059	-0.1019	-0.2299	-0.2161	-0.0299	-0.0898
1	2.5959	-1.7989	-0.0001	0.1050	0.1412	0.0387	0.0917	0.0948	0.1192	0.2061	0.0258	0.0824
1	0.1898	-2.3268	-0.0000	0.0974	0.1435	0.0366	0.0896	0.0934	0.1333	0.2010	0.0173	0.0799
1	-0.7436	1.8405	0.0001	0.1314	0.1502	0.0362	0.1152	0.0990	0.1707	0.2280	0.0634	0.0662
1	1.6725	2.3796	0.0000	0.1060	0.1416	0.0392	0.0913	0.0953	0.1183	0.2059	0.0263	0.0829
1	3.3492	0.5609	-0.0000	0.1055	0.1404	0.0384	0.0914	0.0944	0.1430	0.2064	0.0257	0.0821
6	-1.8907	-0.6287	0.0001	-0.0346	-0.3015	0.0255	0.1103	-0.0534	0.1400	-0.0701	0.5171	-0.0021
1	-2.1114	-1.2496	-0.8791	0.0926	0.1230	0.0290	0.0519	0.0910	0.0147	0.1642	0.0046	0.0728
1	-2.1113	-1.2493	0.8795	0.0926	0.1230	0.0290	0.0519	0.0910	0.0147	0.1642	0.0046	0.0728
8	-2.6769	0.5441	-0.0001	-0.4485	-0.0253	-0.2147	-0.6276	-0.4348	-0.6418	-0.6948	-1.0869	-0.3814
1	-3.6001	0.2901	-0.0004	0.2963	0.1680	0.1601	0.4182	0.3344	0.4199	0.4620	0.5624	0.2674

Dipole mement (in D)	1.76 (DEN)	1.60	1.36	1.03	2.02	1.84	1.74	2.48	3.17	1.79

File TZVPMol132.out
Molecule PMol132 diketene
SP Mol132 B3LYP/Def2TZVP VAC.
0 10
Dipole 2.6814 2.3529 -0.0012 3.5674
Quadrupole -3.7694 2.5398 1.2296 -1.1698 0.0017 0.0016

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0463	-0.0019	-0.0007	0.2498	-0.4198	0.2170	0.8021	0.2732	0.6871	0.7686	1.5591	0.4321
8	-2.2137	-0.1839	0.0001	-0.2237	0.1641	-0.2409	-0.5110	-0.2839	-0.4653	-0.5013	-1.1688	-0.3727
6	-0.0536	1.1379	-0.0000	-0.2106	-0.1600	-0.0457	-0.5170	-0.1368	-0.4828	-0.5661	0.0016	-0.1545
1	-0.0879	1.7694	-0.8854	0.1350	0.1554	0.0645	0.1687	0.1213	0.1737	0.2481	0.0703	0.1090
1	-0.0882	1.7690	0.8857	0.1352	0.1555	0.0645	0.1689	0.1214	0.1740	0.2482	0.0705	0.1091
8	-0.0394	-0.9653	0.0005	-0.2355	0.3027	-0.1187	-0.3463	-0.1757	-0.3575	-0.4509	-1.0002	-0.2537
6	2.2515	-0.1520	-0.0001	-0.3120	-0.2000	-0.1081	-0.4497	-0.2051	-0.7480	-0.4624	-0.0107	-0.2223
1	2.9163	0.6974	-0.0003	0.1288	0.1331	0.0465	0.1488	0.1007	0.2510	0.2146	0.0544	0.0941
1	2.6798	-1.1426	0.0001	0.1360	0.1341	0.0509	0.1569	0.1063	0.2712	0.2207	0.0672	0.0929
6	0.9492	0.0327	-0.0000	0.1969	-0.2651	0.0699	0.3787	0.0785	0.4967	0.2805	0.3565	0.1659

Dipole mement (in D)	3.57 (DEN)	3.23	0.44	2.47	3.22	3.41	3.60	5.06	10.35	3.65

File TZVPMol133.out
Molecule PMol133 3-oxetanone
SP Mol133 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0000 0.0000 -1.0107 1.0107
Quadrupole 3.0690 5.4248 -8.4938 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	1.8450	-0.2315	0.1599	-0.2345	-0.4592	-0.2799	-0.4519	-0.4778	-1.1453	-0.3600
6	0.0000	0.0000	0.6536	0.1076	-0.3320	0.1634	0.5453	0.1942	0.3605	0.5448	1.0946	0.3203
6	0.0000	1.0452	-0.4419	0.0160	-0.2394	0.0248	-0.1068	-0.0487	0.1885	-0.1867	0.4067	-0.0195
6	0.0000	-1.0452	-0.4419	0.0160	-0.2394	0.0248	-0.1068	-0.0487	0.1885	-0.1867	0.4072	-0.0195
8	0.0000	0.0000	-1.4275	-0.3382	0.1308	-0.1868	-0.2975	-0.2707	-0.4312	-0.4803	-0.9687	-0.2968

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   1      0.8898    1.6801   -0.4897    0.1075    0.1300    0.0521    0.1063    0.1135    0.0373    0.1966    0.0511    0.0939
   1      0.8898   -1.6801   -0.4897    0.1075    0.1300    0.0521    0.1063    0.1135    0.0373    0.1966    0.0511    0.0939
   1     -0.8898    1.6801   -0.4897    0.1075    0.1300    0.0521    0.1063    0.1135    0.0355    0.1966    0.0511    0.0939
   1     -0.8898   -1.6801   -0.4897    0.1075    0.1300    0.0521    0.1063    0.1135    0.0355    0.1966    0.0511    0.0939

 Dipole mement (in D)   1.01 (DEN)      0.48      0.73      0.88      0.87      0.88      1.06      0.29      2.28      0.95

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File TZVPMol134.out
Molecule PMol134    2-furanone
 SP Mol134 B3LYP/Def2TZVP VAC.
    0   10
Dipole         -4.8233    1.4766   -0.0002    5.0443
Quadrupole     -2.2470    1.7029    0.5441    1.5994   -0.0006    0.0002
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      2.0342   -0.0420    0.0001   -0.2788    0.1270   -0.2772   -0.5539   -0.3189   -0.5405   -0.5373   -1.1727   -0.4063
   6      0.8404    0.0265   -0.0001    0.2811   -0.4550    0.1896    0.7723    0.2479    0.7635    0.7067    1.5395    0.4074
   8      0.0402   -1.0936    0.0000   -0.2441    0.2633   -0.1289   -0.3501   -0.2031   -0.3960   -0.4537   -1.0290   -0.2594
   6     -0.0514    1.1969    0.0000   -0.1773   -0.1217   -0.0421   -0.3278   -0.0911   -0.3224   -0.3083   -0.0277   -0.0949
   6     -1.3116    0.7767   -0.0000   -0.1330   -0.1178   -0.0096   -0.0540   -0.0660   -0.1225   -0.1456   -0.0458   -0.0526
   6     -1.3230   -0.7069    0.0000    0.0404   -0.2638    0.0351    0.0286   -0.0403    0.1849   -0.1158    0.4783   -0.0008
   1      0.3230    2.2071    0.0001    0.1407    0.1475    0.0641    0.1583    0.1218    0.1738    0.2333    0.0845    0.1046
   1     -2.2113    1.3745    0.0000    0.1377    0.1426    0.0624    0.1268    0.1180    0.1383    0.2199    0.0715    0.1106
   1     -1.8166   -1.1281    0.8809    0.1167    0.1389    0.0533    0.1000    0.1159    0.0604    0.2004    0.0505    0.0958
   1     -1.8166   -1.1281   -0.8808    0.1166    0.1389    0.0533    0.1000    0.1159    0.0604    0.2004    0.0505    0.0958

 Dipole mement (in D)   5.04 (DEN)      4.38      1.94      3.72      5.14      4.74      5.06      6.68     10.78      4.95

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File TZVPMol135.out
Molecule PMol135    ketene
 SP Mol135 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000   -1.4796    1.4796
Quadrupole     -1.5238    2.1462   -0.6224    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.0000    0.1015    0.2608   -0.2250    0.1987    0.6880    0.2314    0.7200    0.6955    0.8518    0.3513
   8      0.0000    0.0000    1.2612   -0.1470    0.2323   -0.1563   -0.3730   -0.2008   -0.3528   -0.4358   -1.1359   -0.2882
   6      0.0000    0.0000   -1.2044   -0.4312   -0.3068   -0.1634   -0.7188   -0.2604   -1.0942   -0.7793    0.0795   -0.2751
   1      0.0000    0.9364   -1.7363    0.1587    0.1498    0.0605    0.2019    0.1149    0.3635    0.2598    0.1023    0.1060
   1      0.0000   -0.9364   -1.7363    0.1587    0.1498    0.0605    0.2019    0.1149    0.3635    0.2598    0.1023    0.1060

 Dipole mement (in D)   1.48 (DEN)      0.92      0.57      0.91      1.13      1.51      1.52      2.13      8.63      1.75

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File TZVPMol136.out
Molecule PMol136    methylketene
 SP Mol136 B3LYP/Def2TZVP VAC.
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```
    0    8
Dipole         -1.8278    0.4369    0.0001    1.8793
Quadrupole     -1.8270    2.3580   -0.5311    0.8775   -0.0001    0.0003
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6      0.7632    0.1226   -0.0000    0.2245   -0.2019    0.1847    0.6217    0.2193    0.4729    0.6868    0.8286    0.3294
   8      1.8605   -0.2644    0.0000   -0.1623    0.2202   -0.1689   -0.3810   -0.2129   -0.3090   -0.4462   -1.1388   -0.2990
   6     -0.4687    0.5605   -0.0000   -0.2582   -0.2726   -0.1085   -0.4706   -0.1660   -0.5496   -0.5379    0.1248   -0.1516
   1     -0.5721    1.6373    0.0001    0.1461    0.1632    0.0538    0.1607    0.1109    0.2221    0.2523    0.0775    0.0961
   6     -1.6789   -0.3241    0.0000   -0.3083   -0.2833   -0.0717   -0.2742   -0.2178    0.0475   -0.5824    0.0605   -0.2348
   1     -2.3004   -0.1498    0.8791    0.1200    0.1234    0.0355    0.1138    0.0869    0.0288    0.2077    0.0150    0.0862
   1     -2.3004   -0.1498   -0.8790    0.1200    0.1234    0.0355    0.1138    0.0869    0.0288    0.2077    0.0150    0.0862
   1     -1.4047   -1.3762   -0.0000    0.1183    0.1275    0.0396    0.1158    0.0925    0.0585    0.2120    0.0174    0.0876

 Dipole mement (in D)   1.88 (DEN)      1.45      0.44      1.23      1.63      1.87      1.87      2.39      8.97      2.07

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File TZVPMol137.out
Molecule PMol137    formamide
 SP Mol137 B3LYP/Def2TZVP VAC.
    0    6
Dipole          3.8690    0.8375    0.0030    3.9586
Quadrupole     -0.4920    1.9621   -1.4702   -1.2063    0.0050   -0.0007
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6     -0.1631    0.3841    0.0001    0.1927   -0.4589    0.1382    0.6597    0.1927    0.6135    0.5062    1.4976    0.3299
   8     -1.1928   -0.2447   -0.0001   -0.3321    0.0530   -0.3030   -0.5400   -0.3519   -0.5284   -0.5797   -1.1801   -0.4095
   7      1.0798   -0.1570   -0.0002   -0.3816   -0.0220   -0.1348   -0.8927   -0.5971   -0.8790   -0.7981   -1.1689   -0.5185
   1     -0.1275    1.4920   -0.0001    0.0529    0.1019    0.0376    0.0170    0.1091   -0.0030    0.0920    0.0272    0.0815
   1      1.1883   -1.1566    0.0006    0.2349    0.1646    0.1324    0.3850    0.3257    0.4172    0.3929    0.4169    0.2539
   1      1.9024    0.4165    0.0009    0.2334    0.1614    0.1296    0.3710    0.3214    0.3797    0.3867    0.4072    0.2628

 Dipole mement (in D)   3.96 (DEN)      3.26      2.41      2.89      3.74      3.60      3.93      4.74      6.73      3.41

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File TZVPMol138.out
Molecule PMol138    acetamide
 SP Mol138 B3LYP/Def2TZVP VAC.
    0    9
Dipole         -0.1321   -3.8825   -0.0005    3.8847
Quadrupole      3.4390   -2.3399   -1.0990   -2.3860   -0.0009    0.0010
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6      0.0733    0.1486   -0.0000    0.2931   -0.5130    0.1666    0.8615    0.2543    0.8773    0.6436    1.4683    0.4308
   8      0.3564    1.3284   -0.0000   -0.3518    0.0652   -0.3204   -0.5860   -0.3644   -0.6018   -0.5979   -1.1972   -0.4308
   7      1.0269   -0.8264    0.0001   -0.4199   -0.0035   -0.1415   -0.9286   -0.6001   -1.0045   -0.7995   -1.1606   -0.5331
   1      1.9937   -0.5541   -0.0001    0.2337    0.1656    0.1282    0.3849    0.3227    0.4241    0.3949    0.4143    0.2486
   1      0.8041   -1.8034   -0.0003    0.2285    0.1609    0.1231    0.3728    0.3163    0.4145    0.3840    0.4019    0.2553
   6     -1.3509   -0.3431   -0.0000   -0.3350   -0.2649   -0.0873   -0.5307   -0.2257   -0.5711   -0.6936   -0.0111   -0.2510
   1     -1.8621    0.0554   -0.8735    0.1314    0.1369    0.0492    0.1491    0.1041    0.1599    0.2351    0.0431    0.0958
   1     -1.4477   -1.4268   -0.0006    0.0888    0.1159    0.0328    0.1280    0.0886    0.1418    0.1983   -0.0018    0.0887
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1	-1.8616	0.0543	0.8743	0.1314	0.1369	0.0492	0.1491	0.1041	0.1599	0.2351	0.0431	0.0958

Dipole mement (in D) 3.88 (DEN) 2.97 2.14 2.83 3.63 3.55 3.89 4.68 6.95 3.39

File TZVPMol139.out
Molecule PMol139 N-methylformamide
SP Mol139 B3LYP/Def2TZVP VAC.
0 9
Dipole 4.1860 0.0832 0.0008 4.1868
Quadrupole -4.4913 3.9009 0.5904 -0.9826 -0.0005 -0.0011

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.7292	0.3410	0.0001	0.1645	-0.4383	0.1327	0.5889	0.1893	0.4036	0.5108	1.4810	0.3170
8	-1.8585	-0.0885	-0.0002	-0.3382	0.0469	-0.3115	-0.5548	-0.3603	-0.5202	-0.5873	-1.1870	-0.4172
7	0.3978	-0.4130	-0.0001	-0.2310	0.0798	-0.0805	-0.5503	-0.4514	-0.3536	-0.5897	-1.1522	-0.4124
1	-0.4867	1.4249	-0.0006	0.0447	0.1034	0.0344	0.0122	0.1069	0.0474	0.0880	0.0205	0.0760
1	0.2640	-1.4118	0.0003	0.2106	0.1788	0.1312	0.3368	0.3280	0.3019	0.3908	0.4021	0.2469
6	1.7353	0.1180	0.0002	-0.2140	-0.3153	-0.0263	-0.1411	-0.1160	-0.0930	-0.3976	0.3658	-0.1100
1	2.2959	-0.1862	0.8849	0.1244	0.1121	0.0377	0.1001	0.0979	0.0694	0.1911	0.0194	0.0976
1	2.2965	-0.1871	-0.8838	0.1244	0.1121	0.0377	0.1001	0.0979	0.0695	0.1911	0.0195	0.0976
1	1.6771	1.2048	-0.0004	0.1147	0.1206	0.0447	0.1080	0.1076	0.0750	0.2027	0.0304	0.1046

Dipole mement (in D) 4.19 (DEN) 4.05 2.34 3.22 4.17 3.92 4.19 5.21 7.97 4.10

File TZVPMol140.out
Molecule PMol140 N,N-dimethylformamide
SP Mol010 B3LYP/Def2TZVP VAC.
0 12
Dipole -3.9859 -0.3767 -0.0005 4.0037
Quadrupole -5.2325 4.2367 0.9958 0.0559 -0.0017 -0.0002

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.8630	-0.6426	-0.0003	0.1469	-0.4185	0.1306	0.5023	0.1888	0.3116	0.5138	1.4562	0.3090
8	1.9423	-0.0944	0.0003	-0.3565	0.0444	-0.3033	-0.5503	-0.3550	-0.5003	-0.5988	-1.1895	-0.4049
7	-0.3445	-0.0186	-0.0001	-0.0819	0.1299	-0.0321	-0.1310	-0.3145	0.0934	-0.4060	-1.1415	-0.3046
1	0.7411	-1.7443	0.0003	0.0521	0.1089	0.0335	0.0095	0.1066	0.0337	0.0959	0.0199	0.0752
6	-1.5784	-0.7584	-0.0000	-0.2404	-0.2906	-0.0284	-0.2225	-0.1157	-0.3892	-0.3894	0.3583	-0.1161
1	-2.1794	-0.5288	0.8832	0.1195	0.1137	0.0361	0.0973	0.0970	0.1307	0.1880	0.0151	0.0939
1	-2.1796	-0.5287	-0.8830	0.1195	0.1137	0.0360	0.0973	0.0970	0.1306	0.1880	0.0151	0.0939
1	-1.3631	-1.8251	-0.0001	0.1151	0.1205	0.0431	0.1023	0.1060	0.1257	0.2050	0.0277	0.1026
6	-0.4227	1.4220	-0.0000	-0.2641	-0.2820	-0.0312	-0.2317	-0.1177	-0.2462	-0.4122	0.3337	-0.1221
1	0.5876	1.8204	-0.0001	0.1615	0.1320	0.0452	0.1322	0.1142	0.1283	0.2391	0.0808	0.0875
1	-0.9524	1.7830	-0.8838	0.1142	0.1140	0.0353	0.0973	0.0966	0.0909	0.1884	0.0119	0.0928
1	-0.9522	1.7829	0.8840	0.1142	0.1140	0.0353	0.0973	0.0966	0.0909	0.1884	0.0120	0.0928

Dipole mement (in D) 4.00 (DEN) 3.88 2.41 3.08 3.93 3.82 4.01 5.06 7.30 3.92

File TZVPMol141.out
Molecule PMol141 E-N-methylacetamide
 SP Mol141 B3LYP/Def2TZVP VAC.
    0   12
Dipole -3.7939 1.5418 0.0304 4.0953
Quadrupole -2.2810 1.9063 0.3747 4.8108 -0.0797 -0.1380

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.6255	-0.1569	-0.0033	0.2427	-0.4878	0.1631	0.7903	0.2523	0.6973	0.6474	1.4412	0.4188
8	1.6077	-0.8738	0.0219	-0.3527	0.0603	-0.3231	-0.5936	-0.3673	-0.6033	-0.5997	-1.1953	-0.4304
7	-0.6365	-0.6792	-0.0474	-0.2579	0.0911	-0.0917	-0.5990	-0.4569	-0.4855	-0.5970	-1.1384	-0.4295
1	-0.6693	-1.6837	0.0046	0.2141	0.1812	0.1243	0.3354	0.3230	0.3061	0.3938	0.4014	0.2380
6	0.7054	1.3471	-0.0053	-0.3596	-0.2629	-0.0869	-0.5452	-0.2253	-0.4366	-0.7012	-0.0169	-0.2523
1	0.2866	1.7616	-0.9228	0.1242	0.1302	0.0418	0.1376	0.0968	0.1317	0.2204	0.0215	0.0938
1	0.1438	1.7805	0.8225	0.1186	0.1291	0.0401	0.1361	0.0954	0.1238	0.2181	0.0197	0.0917
1	1.7440	1.6474	0.0725	0.1369	0.1333	0.0468	0.1528	0.1031	0.1310	0.2368	0.0474	0.0896
6	-1.8739	0.0576	0.0229	-0.2437	-0.3184	-0.0290	-0.1271	-0.1192	-0.0878	-0.4026	0.3629	-0.1131
1	-2.6975	-0.5942	-0.2556	0.1283	0.1187	0.0452	0.1131	0.1068	0.0987	0.2064	0.0270	0.1073
1	-2.0819	0.4505	1.0225	0.1259	0.1093	0.0316	0.0926	0.0915	0.0657	0.1824	0.0093	0.0895
1	-1.8738	0.8959	-0.6730	0.1233	0.1159	0.0378	0.1070	0.0998	0.0589	0.1951	0.0215	0.0965

Dipole mement (in D)	4.10 (DEN)	3.89	2.19	3.13	4.21	3.85	4.17	5.27	8.08	4.04

File TZVPMol142.out
Molecule PMol142 Z-N-methylacetamide
 SP Mol142 B3LYP/Def2TZVP VAC.
    0   12
Dipole 0.6602 -3.8293 0.0019 3.8858
Quadrupole 3.5413 -2.9126 -0.6287 0.7339 -0.0009 -0.0066

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.4818	0.1634	0.0002	0.3135	-0.4878	0.1615	0.7797	0.2518	0.7213	0.6398	1.4449	0.4206
8	-0.3709	1.3757	0.0000	-0.3764	0.0630	-0.3160	-0.5858	-0.3605	-0.5597	-0.6115	-1.1961	-0.4248
7	0.6070	-0.6528	-0.0004	-0.3114	0.0875	-0.0874	-0.5826	-0.4558	-0.4071	-0.5873	-1.1467	-0.4258
6	-1.8184	-0.5310	0.0001	-0.3464	-0.2648	-0.0885	-0.5344	-0.2268	-0.7017	-0.6846	-0.0103	-0.2520
1	-2.3822	-0.2169	-0.8756	0.1304	0.1356	0.0476	0.1475	0.1025	0.2003	0.2328	0.0401	0.0941
1	-1.7535	-1.6174	0.0028	0.0891	0.1154	0.0319	0.1207	0.0876	0.1522	0.1968	-0.0045	0.0875
1	-2.3848	-0.2123	0.8723	0.1305	0.1356	0.0476	0.1475	0.1024	0.2004	0.2328	0.0402	0.0941
1	0.4818	-1.6480	0.0016	0.2096	0.1751	0.1207	0.3236	0.3176	0.3031	0.3853	0.3903	0.2479
6	1.9443	-0.1077	0.0001	-0.2043	-0.3077	-0.0321	-0.1403	-0.1211	-0.3312	-0.4025	0.3588	-0.1176
1	2.1162	0.5091	0.8819	0.1281	0.1177	0.0377	0.1101	0.1006	0.1427	0.2016	0.0348	0.0876
1	2.6649	-0.9200	-0.0076	0.1086	0.1126	0.0390	0.1033	0.1008	0.1368	0.1945	0.0133	0.1008
1	2.1108	0.5210	-0.8743	0.1287	0.1180	0.0379	0.1107	0.1009	0.1429	0.2023	0.0357	0.0877

Dipole mement (in D)	3.89 (DEN)	2.88	2.08	2.79	3.80	3.51	3.84	4.70	6.36	3.31

File TZVPMol143.out
Molecule PMol143 N,N-dimethylacetamide

SP Mol143 B3LYP/Def2TZVP VAC.
0 15
Dipole -1.8777 3.3459 0.0000 3.8368
Quadrupole 1.6144 -2.2569 0.6425 4.1813 -0.0008 -0.0011

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.7302	-0.2956	-0.0003	0.2630	-0.4588	0.1637	0.7074	0.2545	0.5799	0.6518	1.4152	0.4138
8	1.0650	-1.4675	0.0006	-0.3768	0.0576	-0.3098	-0.5868	-0.3581	-0.5685	-0.6133	-1.1958	-0.4131
7	-0.5891	0.0799	-0.0022	-0.1043	0.1474	-0.0396	-0.1804	-0.3139	-0.0177	-0.4098	-1.1238	-0.3174
6	1.7569	0.8107	-0.0001	-0.3978	-0.2675	-0.0877	-0.5484	-0.2271	-0.4175	-0.6928	-0.0132	-0.2536
1	1.6710	1.4494	-0.8788	0.1256	0.1276	0.0402	0.1330	0.0950	0.1122	0.2175	0.0178	0.0922
1	1.6685	1.4516	0.8767	0.1257	0.1276	0.0401	0.1330	0.0950	0.1125	0.2174	0.0178	0.0921
1	2.7402	0.3543	0.0018	0.1388	0.1340	0.0456	0.1532	0.1024	0.1284	0.2376	0.0475	0.0877
6	-1.6165	-0.9362	0.0004	-0.2604	-0.2841	-0.0361	-0.2240	-0.1229	-0.3191	-0.4083	0.3310	-0.1268
1	-1.1438	-1.9122	-0.0021	0.1644	0.1318	0.0419	0.1316	0.1123	0.1399	0.2433	0.0863	0.0836
1	-2.2496	-0.8435	0.8860	0.1090	0.1119	0.0317	0.0925	0.0931	0.1099	0.1837	0.0049	0.0888
1	-2.2555	-0.8415	-0.8806	0.1091	0.1119	0.0317	0.0925	0.0931	0.1095	0.1838	0.0050	0.0889
6	-1.0701	1.4388	0.0007	-0.2695	-0.2902	-0.0310	-0.2081	-0.1190	-0.2886	-0.3936	0.3551	-0.1205
1	-1.6979	1.6302	-0.8741	0.1191	0.1142	0.0340	0.0953	0.0951	0.1076	0.1871	0.0113	0.0916
1	-1.6785	1.6351	0.8882	0.1191	0.1140	0.0338	0.0949	0.0949	0.1071	0.1866	0.0109	0.0913
1	-0.2535	2.1509	-0.0106	0.1349	0.1225	0.0417	0.1146	0.1058	0.1043	0.2090	0.0309	0.1017

Dipole mement (in D)	3.84 (DEN)	3.59	2.20	2.90	3.93	3.67	3.87	5.03	7.29	3.77

File TZVPMol144.out
Molecule PMol144 benzamide
SP Mol144 B3LYP/Def2TZVP VAC.
0 16
Dipole -1.5007 3.1251 1.1172 3.6423
Quadrupole 2.6992 2.1328 -4.8321 8.6968 3.0020 0.1670

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.7091	-0.1402	-0.0269	0.2708	-0.4371	0.1613	0.7880	0.2564	0.5203	0.6296	1.4433	0.4140
8	2.2709	-1.2011	-0.2247	-0.3469	0.0767	-0.3028	-0.5776	-0.3470	-0.5079	-0.5912	-1.1820	-0.4085
7	2.4089	1.0183	0.1699	-0.4065	0.0016	-0.1432	-0.9390	-0.6002	-0.7792	-0.7948	-1.1415	-0.5363
1	3.4045	0.9290	0.2707	0.2312	0.1677	0.1285	0.3860	0.3235	0.3844	0.3960	0.4134	0.2480
1	1.9795	1.8282	0.5768	0.2267	0.1609	0.1179	0.3596	0.3118	0.3155	0.3828	0.3983	0.2457
6	0.2209	-0.0223	-0.0120	0.0785	-0.1200	-0.0151	-0.0990	-0.0167	0.1171	-0.1471	-0.0260	0.0107
6	-0.4568	1.1922	-0.1142	-0.1773	-0.1092	-0.0376	-0.0816	-0.0895	-0.2025	-0.1863	-0.0320	-0.0856
6	-1.8432	1.2256	-0.1021	-0.1128	-0.1373	-0.0383	-0.1010	-0.0943	-0.0982	-0.2082	-0.0217	-0.0832
6	-2.5651	0.0460	0.0170	-0.1081	-0.1277	-0.0299	-0.0734	-0.0859	-0.1078	-0.1883	-0.0237	-0.0743
6	-1.8969	-1.1684	0.1133	-0.0786	-0.1311	-0.0333	-0.0929	-0.0891	-0.0948	-0.2050	-0.0197	-0.0787
6	-0.5130	-1.2022	0.0928	-0.1640	-0.0762	-0.0231	-0.0755	-0.0748	-0.1407	-0.1564	-0.0122	-0.0747
1	0.0908	2.1188	-0.2382	0.1014	0.1416	0.0376	0.0986	0.0980	0.1394	0.2011	0.0199	0.0843
1	-2.3605	2.1721	-0.1930	0.1120	0.1437	0.0428	0.0968	0.0989	0.1106	0.2104	0.0334	0.0872
1	-3.6472	0.0732	0.0284	0.1150	0.1439	0.0443	0.0964	0.1004	0.1136	0.2100	0.0351	0.0889
1	-2.4584	-2.0897	0.2014	0.1152	0.1447	0.0447	0.0983	0.1008	0.1133	0.2116	0.0362	0.0892
1	0.0320	-2.1351	0.1546	0.1434	0.1577	0.0463	0.1166	0.1078	0.1169	0.2357	0.0790	0.0734

Dipole mement (in D) 3.64 (DEN) 2.55 1.79 2.66 3.67 3.35 3.66 4.55 6.80 3.35

File TZVPMol145.out
Molecule PMol145 phenylurea
SP Mol145 B3LYP/Def2TZVP VAC.
0 18
Dipole 0.9521 -3.6698 1.0062 3.9225
Quadrupole 7.0371 0.5815 -7.6186 -8.3894 3.9905 -0.5520

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-2.5851	-1.0311	-0.0398	-0.0990	-0.1432	-0.0413	-0.0639	-0.0970	-0.0463	-0.1908	-0.0192	-0.0840
6	-3.0192	0.2869	0.0017	-0.1399	-0.1551	-0.0530	-0.1293	-0.1090	-0.2149	-0.2342	-0.0292	-0.0975
6	-2.0773	1.3044	0.0488	-0.0807	-0.1353	-0.0355	-0.0531	-0.0911	-0.0710	-0.1826	-0.0200	-0.0790
6	-0.7167	1.0333	0.0550	-0.2110	-0.1098	-0.0523	-0.2209	-0.1005	-0.3259	-0.2412	-0.0142	-0.1010
6	-0.2851	-0.2933	0.0129	0.2620	-0.1873	0.0462	0.3567	0.0994	0.6152	0.1451	0.3542	0.1602
6	-1.2320	-1.3199	-0.0340	-0.2234	-0.1337	-0.0625	-0.2224	-0.1108	-0.3957	-0.2453	-0.0323	-0.1055
7	1.0634	-0.6704	0.0301	-0.2897	0.1668	-0.0826	-0.7045	-0.4262	-0.8303	-0.5839	-1.1543	-0.4210
6	2.1818	0.1371	-0.0198	0.3997	-0.5578	0.1929	1.0077	0.3493	0.8390	0.7539	1.8422	0.5351
7	3.3629	-0.5875	-0.0146	-0.4651	-0.0435	-0.1670	-0.9636	-0.6151	-0.8410	-0.8213	-1.0969	-0.5455
8	2.1618	1.3455	-0.1052	-0.3819	0.0627	-0.3024	-0.6164	-0.3465	-0.5662	-0.6191	-1.2055	-0.4006
1	1.2214	-1.6621	-0.0283	0.1952	0.1878	0.1219	0.3433	0.3250	0.4097	0.3820	0.3849	0.2466
1	4.1739	-0.0136	0.1371	0.2414	0.1705	0.1267	0.3822	0.3227	0.3652	0.3948	0.4106	0.2467
1	3.3937	-1.4749	0.4574	0.2180	0.1567	0.1175	0.3631	0.3126	0.3444	0.3718	0.3820	0.2516
1	0.0098	1.8286	0.0851	0.1651	0.1555	0.0368	0.1355	0.1045	0.1945	0.2509	0.1014	0.0628
1	-0.8974	-2.3513	-0.0662	0.0886	0.1384	0.0337	0.1006	0.0932	0.1487	0.1959	0.0094	0.0792
1	-2.4011	2.3372	0.0806	0.1095	0.1442	0.0419	0.0957	0.0981	0.1207	0.2081	0.0304	0.0858
1	-4.0764	0.5159	-0.0035	0.1052	0.1403	0.0382	0.0936	0.0943	0.1321	0.2082	0.0271	0.0819
1	-3.3012	-1.8421	-0.0775	0.1058	0.1427	0.0405	0.0954	0.0967	0.1220	0.2077	0.0286	0.0844

Dipole mement (in D) 3.92 (DEN) 2.68 2.80 3.00 3.77 3.85 3.93 4.58 5.34 3.47

File TZVPMol146.out
Molecule PMol146 nitromethane
SP Mol146 B3LYP/Def2TZVP VAC.
0 7
Dipole 3.5702 -0.1100 0.0000 3.5719
Quadrupole 1.2689 -3.1080 1.8392 -0.0923 0.0002 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.1756	0.0001	-0.0000	0.3821	-0.0862	0.2501	0.7822	0.0661	0.7896	0.5101	0.4816	0.2455
8	-0.6844	1.1070	0.0000	-0.2931	-0.0267	-0.2100	-0.4151	-0.1713	-0.4368	-0.3610	-0.4783	-0.2383
8	-0.7711	-1.0621	0.0000	-0.2971	-0.0233	-0.2050	-0.4087	-0.1660	-0.4260	-0.3533	-0.4725	-0.2323
6	1.3191	-0.0430	-0.0000	-0.2454	-0.2474	-0.0200	-0.4371	-0.1097	-0.4003	-0.4752	0.2391	-0.1224
1	1.6411	-1.0761	-0.0008	0.1513	0.1237	0.0580	0.1572	0.1240	0.1531	0.2230	0.0777	0.1097
1	1.6584	0.4877	-0.8835	0.1510	0.1300	0.0634	0.1608	0.1285	0.1601	0.2282	0.0764	0.1189
1	1.6583	0.4862	0.8844	0.1510	0.1300	0.0634	0.1608	0.1285	0.1602	0.2282	0.0764	0.1189

Dipole mement (in D) 3.57 (DEN) 3.79 1.73 2.58 3.25 3.45 3.57 4.45 6.27 3.42

File TZVPMol147.out
Molecule PMol147 nitroethane
 SP Mol147 B3LYP/Def2TZVP VAC.
  0 10
Dipole 3.3345 -1.6573 0.0000 3.7236
Quadrupole -1.8448 -0.9485 2.7933 -1.0293 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.6531	0.0536	-0.0000	0.3929	-0.0669	0.2475	0.7558	0.0678	0.7256	0.5136	0.4917	0.2411
8	-0.5668	1.2679	0.0000	-0.2989	-0.0158	-0.1952	-0.3975	-0.1572	-0.4190	-0.3581	-0.4781	-0.2222
8	-1.6880	-0.5890	-0.0000	-0.3020	-0.0287	-0.2135	-0.4290	-0.1751	-0.4553	-0.3648	-0.4842	-0.2405
6	0.6306	-0.7546	0.0000	-0.1409	-0.2555	0.0087	-0.2107	-0.0451	0.0584	-0.2827	0.2367	-0.0201
6	1.8635	0.0976	-0.0000	-0.2971	-0.3047	-0.0830	-0.3737	-0.2286	-0.2073	-0.6149	0.0296	-0.2461
1	0.5431	-1.3975	-0.8740	0.1385	0.1443	0.0557	0.1323	0.1245	0.0412	0.2233	0.0615	0.1076
1	0.5431	-1.3975	0.8740	0.1385	0.1443	0.0557	0.1323	0.1245	0.0412	0.2233	0.0615	0.1076
1	2.7439	-0.5425	0.0000	0.1164	0.1283	0.0433	0.1291	0.0956	0.0746	0.2167	0.0180	0.0973
1	1.9080	0.7367	-0.8780	0.1263	0.1274	0.0405	0.1306	0.0968	0.0703	0.2218	0.0318	0.0877
1	1.9080	0.7367	0.8780	0.1263	0.1274	0.0405	0.1306	0.0968	0.0703	0.2218	0.0318	0.0877

 Dipole mement (in D) 3.72 (DEN) 3.93 1.87 2.64 3.40 3.53 3.74 4.64 6.50 3.45

File TZVPMol148.out
Molecule PMol148 1-nitropropane
 SP Mol148 B3LYP/Def2TZVP VAC.
  0 13
Dipole -3.7184 -1.0013 0.0000 3.8509
Quadrupole -3.8994 -0.2521 4.1516 -0.0632 -0.0001 0.0002

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	1.2175	-0.0009	-0.0000	0.4021	-0.0648	0.2478	0.7582	0.0678	0.7845	0.5165	0.4883	0.2413
8	1.3378	1.2107	-0.0001	-0.2998	-0.0158	-0.1953	-0.4058	-0.1577	-0.4441	-0.3589	-0.4787	-0.2215
8	2.1304	-0.8081	0.0000	-0.3043	-0.0289	-0.2141	-0.4284	-0.1757	-0.4548	-0.3653	-0.4848	-0.2411
6	-0.1812	-0.5800	0.0000	-0.1589	-0.2304	0.0055	-0.2491	-0.0458	-0.2314	-0.2765	0.2316	-0.0254
6	-1.2692	0.4593	-0.0000	-0.1370	-0.2953	-0.0481	-0.1600	-0.1551	0.3212	-0.4120	0.0664	-0.1381
1	-0.2087	-1.2304	0.8740	0.1354	0.1460	0.0539	0.1322	0.1232	0.0922	0.2216	0.0582	0.1044
1	-0.2087	-1.2305	-0.8739	0.1354	0.1460	0.0539	0.1322	0.1232	0.0922	0.2216	0.0582	0.1044
1	-1.1511	1.1069	0.8690	0.1091	0.1408	0.0360	0.1092	0.0959	-0.0295	0.2141	0.0196	0.0793
1	-1.1511	1.1067	-0.8691	0.1091	0.1408	0.0360	0.1092	0.0959	-0.0295	0.2141	0.0196	0.0793
6	-2.6402	-0.1924	0.0000	-0.3340	-0.3002	-0.0779	-0.3216	-0.2295	-0.3915	-0.5875	0.0129	-0.2444
1	-2.7872	-0.8217	-0.8780	0.1089	0.1194	0.0319	0.1050	0.0838	0.0970	0.1989	-0.0017	0.0845
1	-2.7872	-0.8216	0.8782	0.1089	0.1194	0.0319	0.1050	0.0838	0.0970	0.1989	-0.0017	0.0845
1	-3.4303	0.5551	-0.0000	0.1252	0.1231	0.0385	0.1140	0.0900	0.0967	0.2144	0.0121	0.0928

 Dipole mement (in D) 3.85 (DEN) 4.08 2.11 2.82 3.59 3.72 3.89 4.77 6.70 3.59

File TZVPMol149.out

Molecule PMol149   2-nitropropane
 SP Mol149 B3LYP/Def2TZVP VAC.
    0   13
Dipole   3.7055   0.0009   -0.9455   3.8242
Quadrupole   -2.1798   3.5072   -1.3275   0.0008   -0.5591   0.0044

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.8496	-0.0003	0.0157	0.3967	-0.0482	0.2465	0.7421	0.0697	0.6699	0.5121	0.4923	0.2368
8	-1.0217	-0.0012	1.2226	-0.3102	-0.0227	-0.2011	-0.4089	-0.1641	-0.4169	-0.3737	-0.4889	-0.2275
8	-1.7286	0.0007	-0.8279	-0.2997	-0.0240	-0.2083	-0.4252	-0.1696	-0.4361	-0.3602	-0.4821	-0.2346
6	1.2650	1.2629	0.0224	-0.3528	-0.2738	-0.0817	-0.4133	-0.2251	-0.3828	-0.6048	0.0145	-0.2459
6	0.6007	0.0003	-0.4746	0.0461	-0.2830	0.0364	0.0357	0.0186	0.3043	-0.0982	0.2471	0.0820
1	0.7510	2.1563	-0.3271	0.1297	0.1273	0.0408	0.1244	0.0961	0.1019	0.2174	0.0206	0.0924
1	1.2879	1.2794	1.1104	0.1358	0.1304	0.0391	0.1332	0.0967	0.1088	0.2226	0.0364	0.0844
1	2.2903	1.3011	-0.3412	0.1151	0.1296	0.0429	0.1316	0.0958	0.1145	0.2157	0.0181	0.0960
6	1.2657	-1.2625	0.0209	-0.3528	-0.2739	-0.0817	-0.4133	-0.2251	-0.3830	-0.6048	0.0147	-0.2459
1	0.5000	0.0009	-1.5580	0.1116	0.1511	0.0443	0.1043	0.1184	-0.0057	0.2183	0.0529	0.0893
1	0.7522	-2.1557	-0.3296	0.1296	0.1273	0.0408	0.1244	0.0961	0.1018	0.2174	0.0206	0.0924
1	2.2910	-1.2997	-0.3428	0.1151	0.1296	0.0429	0.1316	0.0958	0.1146	0.2156	0.0181	0.0960
1	1.2887	-1.2802	1.1089	0.1358	0.1304	0.0391	0.1332	0.0967	0.1088	0.2226	0.0364	0.0844

 Dipole mement (in D)   3.82 (DEN)   3.78   2.11   2.72   3.43   3.63   3.86   4.86   6.61   3.53

File TZVPMol150.out
Molecule PMol150   nitrobenzene
 SP Mol150 B3LYP/Def2TZVP VAC.
    0   14
Dipole   0.0000   0.0000   -4.6364   4.6364
Quadrupole   -0.7995   4.0128   -3.2133   0.0000   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-2.5032	-0.1058	-0.1141	-0.0188	-0.0609	-0.0747	-0.1344	-0.1732	-0.0162	-0.0642
6	0.0000	1.2059	-1.8126	-0.0744	-0.1237	-0.0267	-0.0862	-0.0823	-0.0572	-0.2009	-0.0091	-0.0731
6	0.0000	1.2140	-0.4273	-0.1641	-0.0893	-0.0248	-0.1133	-0.0720	-0.2268	-0.1818	0.0075	-0.0694
6	0.0000	0.0000	0.2396	0.0837	-0.1554	0.0260	0.0071	0.0767	0.1882	0.0195	0.2026	0.1220
6	0.0000	-1.2140	-0.4273	-0.1641	-0.0893	-0.0248	-0.1133	-0.0720	-0.2268	-0.1818	0.0074	-0.0694
6	0.0000	-1.2059	-1.8126	-0.0744	-0.1237	-0.0267	-0.0862	-0.0823	-0.0572	-0.2009	-0.0093	-0.0731
1	0.0000	-2.1310	0.1436	0.1592	0.1585	0.0520	0.1278	0.1166	0.1630	0.2458	0.0962	0.0845
1	0.0000	-2.1424	-2.3541	0.1256	0.1483	0.0504	0.1070	0.1066	0.1217	0.2178	0.0473	0.0957
1	0.0000	2.1424	-2.3541	0.1256	0.1483	0.0504	0.1070	0.1066	0.1217	0.2178	0.0473	0.0957
1	0.0000	2.1310	0.1436	0.1592	0.1585	0.0520	0.1278	0.1166	0.1630	0.2458	0.0962	0.0845
1	0.0000	0.0000	-3.5855	0.1245	0.1476	0.0502	0.1031	0.1063	0.1297	0.2152	0.0455	0.0957
7	0.0000	0.0000	1.7152	0.4238	-0.0242	0.2443	0.7289	0.0797	0.6098	0.5029	0.4434	0.2259
8	0.0000	-1.0846	2.2788	-0.3094	-0.0208	-0.2017	-0.4244	-0.1628	-0.3974	-0.3631	-0.4795	-0.2273
8	0.0000	1.0846	2.2788	-0.3094	-0.0208	-0.2017	-0.4244	-0.1628	-0.3974	-0.3631	-0.4795	-0.2273

 Dipole mement (in D)   4.64 (DEN)   4.71   2.62   3.51   4.60   4.27   4.68   5.75   8.01   4.34

File TZVPMol151.out
Molecule PMol151 methyl_nitrate
 SP Mol151 B3LYP/Def2TZVP VAC.
  0 8
Dipole -0.4803 -2.9692 0.0000 3.0078
Quadrupole -3.2529 1.8010 1.4519 0.1679 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	0.6282	0.0000	0.4882	-0.1430	0.3082	0.9297	0.1668	0.8800	0.6877	0.9021	0.3753
8	-1.2011	0.5647	0.0000	-0.2828	0.0005	-0.1720	-0.4260	-0.1307	-0.3977	-0.3495	-0.4452	-0.2020
8	0.7325	1.5716	0.0000	-0.2540	0.0184	-0.1749	-0.4143	-0.1246	-0.4010	-0.3110	-0.4130	-0.2141
8	0.7120	-0.6128	0.0000	-0.1886	0.1226	-0.1014	-0.2773	-0.1284	-0.3280	-0.3360	-0.6488	-0.1398
6	-0.1524	-1.7437	0.0000	-0.1726	-0.3381	-0.0044	-0.1568	-0.1198	-0.0240	-0.2755	0.4425	-0.1061
1	0.5268	-2.5910	0.0000	0.1383	0.1207	0.0574	0.1279	0.1198	0.1122	0.2045	0.0594	0.1070
1	-0.7797	-1.7661	0.8892	0.1357	0.1094	0.0435	0.1085	0.1085	0.0792	0.1899	0.0516	0.0898
1	-0.7797	-1.7661	-0.8892	0.1357	0.1094	0.0435	0.1085	0.1085	0.0792	0.1899	0.0516	0.0898

Dipole mement (in D)	3.01 (DEN)	3.27	1.20	1.98	2.80	2.80	3.07	3.81	5.28	2.62

File TZVPMol152.out
Molecule PMol152 acetyl_cyanide
 SP Mol152 B3LYP/Def2TZVP VAC.
  0 8
Dipole 3.2664 1.3236 0.0000 3.5244
Quadrupole 2.6339 -6.1394 3.5055 0.6025 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	1.7122	1.7423	0.0000	0.1443	0.1374	0.0576	0.1675	0.1129	0.1533	0.2395	0.0609	0.1027
6	1.4772	0.6831	0.0000	-0.3300	-0.2357	-0.0713	-0.5564	-0.2129	-0.4645	-0.6839	-0.0133	-0.2456
6	0.0000	0.4778	0.0000	0.2936	-0.3534	0.1938	0.5986	0.2231	0.6294	0.4799	1.1442	0.3613
8	-0.8297	1.3493	0.0000	-0.2204	0.1947	-0.2033	-0.4143	-0.2493	-0.4370	-0.4405	-1.0771	-0.3288
1	1.9209	0.2017	0.8722	0.1434	0.1465	0.0599	0.1620	0.1132	0.1450	0.2428	0.0561	0.1087
1	1.9209	0.2017	-0.8722	0.1434	0.1465	0.0599	0.1620	0.1132	0.1450	0.2428	0.0561	0.1087
6	-0.4237	-0.9340	0.0000	-0.2005	-0.1395	0.0725	0.1735	0.1912	0.1825	0.1646	0.8899	0.2160
7	-0.7482	-2.0430	0.0000	0.0262	0.1036	-0.1691	-0.2928	-0.2915	-0.3536	-0.2453	-1.1170	-0.3230

Dipole mement (in D)	3.52 (DEN)	2.70	1.48	2.49	2.85	3.44	3.53	3.90	8.55	3.35

File TZVPMol153.out
Molecule PMol153 dimethylnitrosamine
 SP Mol153 B3LYP/Def2TZVP VAC.
  0 11
Dipole 3.8932 1.6290 0.0000 4.2203
Quadrupole -2.4474 1.3002 1.1472 -1.9003 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-1.7935	-0.2721	-0.0000	-0.3396	-0.0900	-0.2343	-0.3608	-0.1899	-0.2567	-0.4077	-0.5381	-0.2337
7	-0.7094	-0.8338	-0.0000	0.0173	-0.0868	0.0241	0.1584	-0.0487	-0.1938	0.1956	0.3039	0.0168
7	0.3397	-0.0042	0.0000	0.0645	0.0609	0.0169	0.0955	-0.1813	0.4766	-0.1972	-0.6860	-0.1566

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   6      0.1413    1.4293    0.0000   -0.2714   -0.3070   -0.0354   -0.3002   -0.1169   -0.4505   -0.4415    0.3265   -0.1205
   1     -0.4296    1.7342   -0.8769    0.1383    0.1237    0.0432    0.1218    0.1095    0.1537    0.2185    0.0521    0.0945
   1     -0.4296    1.7341    0.8769    0.1383    0.1237    0.0432    0.1218    0.1095    0.1537    0.2185    0.0521    0.0945
   1      1.1104    1.9176    0.0000    0.1246    0.1208    0.0447    0.1192    0.1084    0.1309    0.2041    0.0276    0.1048
   6      1.6479   -0.6025    0.0000   -0.2693   -0.3035   -0.0304   -0.2896   -0.1109   -0.3213   -0.4041    0.3532   -0.1090
   1      1.5172   -1.6811    0.0000    0.1453    0.1267    0.0479    0.1185    0.1167    0.0952    0.2273    0.0651    0.1110
   1      2.2159   -0.3113   -0.8851    0.1260    0.1156    0.0400    0.1077    0.1019    0.1062    0.1932    0.0220    0.0991
   1      2.2159   -0.3113    0.8851    0.1260    0.1156    0.0400    0.1077    0.1019    0.1062    0.1932    0.0220    0.0991

 Dipole mement (in D)   4.22 (DEN)      4.65      2.32      3.04      3.55      4.00      4.15      5.08      6.49      3.99

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File TZVPMol154.out
Molecule PMol154    formaldoxime
 SP Mol154 B3LYP/Def2TZVP VAC.
    0    6
Dipole          0.2106    0.1262    0.0009    0.2455
Quadrupole      4.4366   -2.1187   -2.3179    2.4324   -0.0001   -0.0004
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
   6      1.1233    0.1763   -0.0001   -0.1549   -0.2901   -0.0126   -0.1209   -0.0171    0.0883   -0.1522    0.6295   -0.0046
   7      0.0697   -0.5274   -0.0001   -0.0731   -0.0316   -0.0834   -0.0201   -0.2556   -0.3020   -0.1278   -0.6029   -0.2239
   8     -1.0779    0.2651    0.0001   -0.3299   -0.0641   -0.1754   -0.5065   -0.3194   -0.3701   -0.5460   -0.7437   -0.2618
   1      2.0590   -0.3653    0.0003    0.1295    0.1186    0.0536    0.1119    0.1191    0.0753    0.1894    0.0672    0.1127
   1      1.1214    1.2645    0.0002    0.1084    0.1021    0.0514    0.1212    0.1171    0.1079    0.1704    0.0687    0.0989
   1     -1.7851   -0.3861    0.0003    0.3199    0.1651    0.1665    0.4145    0.3559    0.4006    0.4661    0.5809    0.2787

 Dipole mement (in D)   0.25 (DEN)      0.53      0.95      0.22      0.94      0.24      0.24      1.01      3.12      0.53

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File TZVPMol155.out
Molecule PMol155    fulminic_acid
 SP Mol155 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0000   -3.1476    3.1476
Quadrupole     -0.9210   -0.9210    1.8421    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
   6      0.0000    0.0000   -1.1759   -0.2345   -0.1803   -0.0173   -0.2776    0.0505   -0.4343   -0.0780    0.7568    0.0505
   7      0.0000    0.0000   -0.0179    0.3415    0.0907    0.1070    0.3721   -0.0704    0.4743    0.1922   -0.5652    0.0074
   1      0.0000    0.0000   -2.2338    0.2148    0.1351    0.1171    0.2503    0.1785    0.3267    0.2481    0.2418    0.1728
   8      0.0000    0.0000    1.1768   -0.3218   -0.0455   -0.2067   -0.3448   -0.1585   -0.3667   -0.3624   -0.4335   -0.2307

 Dipole mement (in D)   3.15 (DEN)      2.83      0.70      2.34      3.10      3.09      3.17      4.29      9.27      3.44

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File TZVPMol156.out
Molecule PMol156    1,4-dihydrooxazole
 SP Mol156 B3LYP/Def2TZVP VAC.
    0   10
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Dipole -1.3863 -1.0839 0.0000 1.7597
Quadrupole 4.4014 -5.1845 0.7831 -0.8908 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.4835	-1.1041	0.0000	-0.2790	0.2153	-0.1425	-0.3217	-0.2222	-0.3760	-0.4651	-1.0513	-0.2582
6	-0.9180	-0.7479	0.0000	-0.0118	-0.2596	0.0317	0.0550	-0.0444	0.0540	-0.1038	0.4220	-0.0075
6	-0.9096	0.7871	-0.0000	-0.0891	-0.2834	-0.0130	-0.0504	-0.0576	0.3896	-0.2774	0.3221	-0.0307
6	1.1456	0.0723	-0.0000	0.0955	-0.3602	0.1062	0.3874	0.1718	0.5387	0.3610	1.2355	0.2534
7	0.5075	1.1632	-0.0000	-0.2465	0.0594	-0.2051	-0.4778	-0.3988	-0.6694	-0.4574	-1.1121	-0.4319
1	-1.3756	-1.1900	-0.8843	0.0978	0.1212	0.0405	0.0728	0.1037	0.0439	0.1818	0.0270	0.0869
1	-1.3756	-1.1900	0.8843	0.0978	0.1212	0.0405	0.0728	0.1037	0.0439	0.1818	0.0270	0.0869
1	-1.4010	1.2133	-0.8754	0.1001	0.1275	0.0378	0.0895	0.1022	-0.0251	0.1981	0.0203	0.0938
1	-1.4010	1.2133	0.8754	0.1001	0.1275	0.0378	0.0895	0.1022	-0.0251	0.1981	0.0203	0.0938
1	2.2239	-0.0253	-0.0000	0.1352	0.1312	0.0661	0.0830	0.1393	0.0256	0.1829	0.0892	0.1136

Dipole mement (in D)	1.76 (DEN)	1.48	1.32	0.86	1.48	1.72	1.81	1.71	1.43	1.61

File TZVPMol157.out
Molecule PMol157 oxazole
SP Mol157 B3LYP/Def2TZVP VAC.
0 8
Dipole 0.7388 -1.3667 0.0005 1.5536
Quadrupole 5.2474 -3.4031 -1.8443 0.8359 -0.0003 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.3648	-1.0799	-0.0002	-0.2184	0.3318	-0.0839	-0.2024	-0.1558	-0.1973	-0.3891	-1.0807	-0.2116
6	0.9266	-0.6448	0.0001	0.0081	-0.2531	0.0133	0.0223	-0.0064	-0.0962	0.0399	0.4088	0.0444
6	0.9103	0.7042	0.0001	-0.0913	-0.2504	-0.0259	-0.0229	-0.0080	0.0836	-0.1195	0.3745	0.0238
6	-1.0931	0.0571	0.0002	0.1200	-0.3245	0.0933	0.3009	0.1541	0.3848	0.3030	1.1076	0.2281
7	-0.4014	1.1444	-0.0001	-0.2418	0.1014	-0.1878	-0.4262	-0.3750	-0.5042	-0.4466	-1.0907	-0.4173
1	1.6888	-1.4018	0.0001	0.1457	0.1311	0.0644	0.1154	0.1283	0.1550	0.2084	0.0986	0.1069
1	1.7400	1.3900	0.0001	0.1296	0.1341	0.0565	0.1186	0.1208	0.1111	0.2142	0.0753	0.1076
1	-2.1639	-0.0579	0.0002	0.1481	0.1297	0.0701	0.0942	0.1421	0.0632	0.1898	0.1062	0.1182

Dipole mement (in D)	1.55 (DEN)	0.88	1.42	0.81	1.47	1.49	1.58	1.44	1.98	1.47

File TZVPMol158.out
Molecule PMol158 isoxazole
SP Mol158 B3LYP/Def2TZVP VAC.
0 8
Dipole 0.9613 2.8455 0.0004 3.0035
Quadrupole 3.6823 -1.5578 -2.1245 -1.7292 0.0001 -0.0005

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.5653	-0.9927	-0.0002	-0.1187	0.2685	-0.0540	-0.0604	-0.0689	-0.0507	-0.2560	-0.7391	-0.1063
6	1.0956	0.2336	0.0002	0.0388	-0.2489	0.0428	0.1017	0.0253	0.1581	0.1305	0.4901	0.0849
6	0.1213	1.1735	-0.0001	-0.1793	-0.2039	-0.0789	-0.2989	-0.1233	-0.4233	-0.3670	-0.0291	-0.1166
6	-1.0621	0.4037	0.0001	-0.0466	-0.2584	0.0022	0.0438	0.0346	0.2822	-0.0405	0.5206	0.0646
7	-0.8237	-0.8832	-0.0000	-0.1097	0.0250	-0.1057	-0.1728	-0.2489	-0.3679	-0.1281	-0.5034	-0.2623

1	-2.0880	0.7377	0.0002	0.1349	0.1397	0.0648	0.1232	0.1313	0.0911	0.2178	0.0833	0.1183
1	0.2299	2.2428	-0.0001	0.1314	0.1422	0.0581	0.1466	0.1148	0.1982	0.2347	0.0762	0.1040
1	2.1719	0.2787	0.0002	0.1492	0.1358	0.0707	0.1169	0.1352	0.1124	0.2085	0.1015	0.1134

Dipole mement (in D) 3.00 (DEN) 2.22 1.31 1.40 1.89 2.82 2.91 3.42 8.31 3.01

File TZVPMol159.out
Molecule PMol159 morpholine
SP Mol159 B3LYP/Def2TZVP VAC.
0 15
Dipole 0.2142 1.5390 0.0000 1.5538
Quadrupole -3.7070 0.1654 3.5417 -1.8026 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.6456	-1.2596	0.0000	-0.3242	0.1559	-0.1745	-0.3344	-0.2729	-0.3266	-0.4951	-1.0474	-0.2877
6	-0.0054	-0.7738	1.1654	-0.0085	-0.3222	0.0193	0.0713	-0.0568	0.0201	-0.0768	0.5046	-0.0022
1	1.0299	-1.1416	1.2027	0.0671	0.1181	0.0244	0.0507	0.0898	0.0693	0.1552	0.0014	0.0701
1	-0.5495	-1.1889	2.0131	0.0967	0.1257	0.0382	0.0679	0.1024	0.0614	0.1858	0.0168	0.0833
6	-0.0054	-0.7738	-1.1654	-0.0085	-0.3222	0.0193	0.0713	-0.0568	0.0201	-0.0768	0.5045	-0.0022
1	1.0299	-1.1416	-1.2027	0.0671	0.1181	0.0244	0.0507	0.0898	0.0693	0.1552	0.0014	0.0701
1	-0.5495	-1.1889	-2.0131	0.0967	0.1257	0.0382	0.0679	0.1024	0.0614	0.1858	0.0168	0.0833
6	-0.0054	0.7382	1.1975	-0.0751	-0.3151	-0.0187	-0.0192	-0.0676	0.1108	-0.2437	0.3419	-0.0332
1	-1.0476	1.0895	1.2727	0.0665	0.1150	0.0169	0.0504	0.0814	0.0317	0.1565	-0.0189	0.0649
1	0.5277	1.0927	2.0809	0.0921	0.1291	0.0352	0.0818	0.0997	0.0388	0.1973	0.0052	0.0925
6	-0.0054	0.7382	-1.1975	-0.0751	-0.3151	-0.0187	-0.0192	-0.0676	0.1108	-0.2437	0.3419	-0.0332
1	0.5277	1.0927	-2.0809	0.0921	0.1291	0.0352	0.0818	0.0997	0.0388	0.1973	0.0052	0.0925
1	-1.0476	1.0895	-1.2727	0.0665	0.1150	0.0169	0.0504	0.0814	0.0317	0.1565	-0.0189	0.0649
7	0.6672	1.2238	0.0000	-0.3340	-0.0166	-0.1541	-0.5480	-0.5162	-0.6752	-0.6074	-0.9886	-0.4902
1	0.7029	2.2331	0.0000	0.1807	0.1597	0.0982	0.2766	0.2915	0.3376	0.3540	0.3339	0.2273

Dipole mement (in D) 1.55 (DEN) 1.38 0.66 0.88 1.19 1.45 1.56 2.10 2.76 1.02

File TZVPMol160.out
Molecule PMol160 uracil
SP Mol160 B3LYP/Def2TZVP VAC.
0 12
Dipole 1.3441 4.2472 -0.0005 4.4548
Quadrupole -10.3887 9.0846 1.3041 2.3878 0.0006 0.0006

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.0330	-0.9797	-0.0000	-0.2324	0.2000	-0.0682	-0.7852	-0.4000	-0.5951	-0.6124	-1.1335	-0.4068
6	1.2203	-0.4067	-0.0000	0.2963	-0.5090	0.1993	0.9592	0.3607	0.7637	0.7488	1.8494	0.5304
7	1.1689	0.9828	-0.0001	-0.2345	0.1803	-0.0578	-0.6302	-0.4056	-0.4791	-0.5725	-1.1683	-0.3908
6	0.0051	1.6989	-0.0000	0.0396	-0.1720	0.0392	0.2240	0.0554	0.1089	0.0611	0.4050	0.0897
6	-1.1987	1.1010	-0.0000	-0.2306	-0.1540	-0.0782	-0.4311	-0.1181	-0.5100	-0.3738	-0.0114	-0.1193
6	-1.2913	-0.3439	-0.0002	0.2472	-0.4251	0.1586	0.7879	0.2523	0.7910	0.6068	1.3859	0.4024
8	-2.3076	-1.0036	0.0002	-0.3192	0.0931	-0.2982	-0.5519	-0.3396	-0.5660	-0.5631	-1.1691	-0.4101
8	2.2585	-1.0236	0.0001	-0.3266	0.0766	-0.3143	-0.6111	-0.3522	-0.5740	-0.5905	-1.1931	-0.4214

1	-0.0464	-1.9889	0.0001	0.2355	0.2046	0.1460	0.3901	0.3477	0.3497	0.4232	0.4396	0.2465
1	2.0629	1.4427	-0.0000	0.2365	0.2013	0.1501	0.3713	0.3496	0.3490	0.4185	0.4363	0.2639
1	-2.1115	1.6727	0.0001	0.1377	0.1557	0.0570	0.1584	0.1168	0.2073	0.2391	0.0798	0.0941
1	0.1238	2.7738	0.0000	0.1504	0.1485	0.0667	0.1187	0.1329	0.1547	0.2148	0.0788	0.1214

Dipole mement (in D) 4.45 (DEN) 3.95 2.16 3.47 4.66 4.05 4.49 5.64 9.20 4.44

File TZVPMol205.out
Molecule PMol205 difluoroborane
SP Mol205 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 0.8727 0.8727
Quadrupole 1.7858 -2.0906 0.3048 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	0.4543	0.4630	-0.7264	0.3149	0.9351	0.1004	0.7764	1.1097	2.2754	0.554
1	0.0000	0.0000	1.6336	-0.0187	0.0330	-0.0397	-0.2217	0.0701	-0.1793	-0.1578	-0.6123	-0.052
9	0.0000	1.1234	-0.2169	-0.2221	0.3467	-0.1376	-0.3567	-0.0853	-0.2985	-0.4759	-0.8320	-0.251
9	0.0000	-1.1234	-0.2169	-0.2221	0.3467	-0.1376	-0.3567	-0.0853	-0.2985	-0.4759	-0.8320	-0.251

Dipole mement (in D) 0.87 (DEN) 1.33 2.05 0.66 1.04 0.95 0.91 2.18 1.89 1.32

File TZVPMol206.out
Molecule PMol206 chloroborane
SP Mol206 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 -0.4995 0.4995
Quadrupole 0.7604 -0.9228 0.1623 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	1.0365	-1.7412	0.0119	0.0318	-0.0506	-0.1568	0.0553	-0.1199	-0.0757	-0.6198	-0.063
1	0.0000	-1.0365	-1.7412	0.0119	0.0318	-0.0506	-0.1568	0.0553	-0.1199	-0.0757	-0.6198	-0.063
5	0.0000	0.0000	-1.1771	0.0937	-0.6466	0.1577	0.4542	-0.1263	0.3879	0.2911	1.9351	0.263
17	0.0000	0.0000	0.5511	-0.1175	0.5831	-0.0564	-0.1407	0.0156	-0.1481	-0.1397	-0.6951	-0.138

Dipole mement (in D) 0.50 (DEN) 1.04 4.67 0.19 0.32 0.17 0.58 0.75 2.41 0.80

File TZVPMol207.out
Molecule PMol207 hydroxyborane
SP Mol207 B3LYP/Def2TZVP VAC.
0 5
Dipole -1.5295 -0.5079 0.0000 1.6116
Quadrupole 0.2474 -0.5817 0.3343 2.0487 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0525	0.7091	0.0000	0.0960	-0.4542	0.1694	0.6491	-0.0804	0.5628	0.5994	2.0559	0.315
8	0.0525	-0.6361	0.0000	-0.3675	0.1877	-0.2168	-0.7301	-0.3688	-0.6051	-0.8414	-1.3535	-0.457
1	-0.8257	-1.0213	0.0000	0.3234	0.2064	0.1796	0.4598	0.3629	0.4050	0.4844	0.5853	0.296

1	-0.9689	1.3229	0.0000	-0.0315	0.0252	-0.0695	-0.2006	0.0386	-0.2049	-0.1278	-0.6506	-0.080
1	1.1121	1.2417	0.0000	-0.0204	0.0349	-0.0627	-0.1782	0.0478	-0.1577	-0.1146	-0.6368	-0.074

Dipole mement (in D) 1.61 (DEN) 1.39 2.88 0.87 1.87 1.53 1.58 2.13 2.54 1.24

File TZVPMol208.out
Molecule PMol208 difluorohydroxyborane
SP Mol208 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.4327 -1.9509 0.0000 1.9983
Quadrupole -2.8347 1.6847 1.1500 -2.3962 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0218	0.0000	0.5425	-1.1167	0.3546	1.3017	0.1984	0.9119	1.3565	2.4387	0.725
8	1.1992	-0.5845	0.0000	-0.3878	0.2169	-0.2354	-0.9344	-0.3739	-0.6703	-0.8888	-1.3758	-0.489
1	1.1444	-1.5406	0.0000	0.3325	0.2180	0.1868	0.4915	0.3726	0.4144	0.4955	0.6045	0.301
9	-1.1376	-0.6548	0.0000	-0.2516	0.3290	-0.1586	-0.4419	-0.1055	-0.3549	-0.4882	-0.8398	-0.272
9	-0.0555	1.3335	0.0000	-0.2357	0.3528	-0.1475	-0.4170	-0.0916	-0.3011	-0.4750	-0.8283	-0.265

Dipole mement (in D) 2.00 (DEN) 2.28 1.25 1.27 2.16 2.00 1.95 2.57 3.03 1.67

File TZVPMol209.out
Molecule PMol209 dihydroxyborane
SP Mol209 B3LYP/Def2TZVP VAC.
0 6
Dipole 1.5391 -0.3146 0.0000 1.5709
Quadrupole 0.7205 0.1323 -0.8528 3.8143 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.4823	0.0000	0.2286	-0.7979	0.2060	0.9468	0.0113	0.6555	0.9101	2.2144	0.475
1	0.0531	1.6685	0.0000	-0.0419	0.0382	-0.0614	-0.2224	0.0553	-0.1591	-0.1341	-0.6355	-0.076
8	1.1155	-0.2988	0.0000	-0.4179	0.1641	-0.2504	-0.8446	-0.4002	-0.6731	-0.8828	-1.3858	-0.490
1	1.9309	0.2011	0.0000	0.3263	0.2056	0.1755	0.4672	0.3601	0.4005	0.4886	0.5906	0.292
8	-1.2181	-0.1035	0.0000	-0.4114	0.1839	-0.2426	-0.8166	-0.3869	-0.6624	-0.8655	-1.3667	-0.483
1	-1.1632	-1.0626	0.0000	0.3162	0.2061	0.1729	0.4697	0.3604	0.4386	0.4836	0.5830	0.282

Dipole mement (in D) 1.57 (DEN) 1.45 2.78 0.77 1.91 1.48 1.52 2.25 2.65 1.34

File TZVPMol210.out
Molecule PMol210 dihydroxyfluoroborane
SP Mol210 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 1.4012 1.4012
Quadrupole -0.2899 6.3106 -6.0207 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	-0.0262	0.4548	-1.1263	0.3066	1.2953	0.1607	0.8461	1.2799	2.4065	0.688
9	0.0000	0.0000	1.3143	-0.2816	0.2928	-0.1775	-0.4461	-0.1273	-0.3726	-0.4990	-0.8537	-0.268

8	0.0000	1.1632	-0.7133	-0.4105	0.2047	-0.2432	-0.9001	-0.3821	-0.6309	-0.8803	-1.3726	-0.493
1	0.0000	1.9318	-0.1431	0.3238	0.2121	0.1786	0.4754	0.3654	0.3942	0.4898	0.5961	0.292
8	0.0000	-1.1632	-0.7133	-0.4105	0.2047	-0.2432	-0.9001	-0.3821	-0.6309	-0.8803	-1.3725	-0.493
1	0.0000	-1.9318	-0.1431	0.3238	0.2121	0.1786	0.4754	0.3654	0.3942	0.4898	0.5961	0.292

Dipole mement (in D) 1.40 (DEN) 0.53 0.30 0.26 2.53 1.29 1.32 2.05 2.89 1.09

File TZVPMol211.out
Molecule PMol211 boranamine
SP Mol211 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 1.9733 1.9733
Quadrupole -1.0726 0.5432 0.5294 0.0000 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	-0.7758	0.0092	-0.4664	0.0888	0.5628	-0.1285	0.4236	0.4040	1.9931	0.299
7	0.0000	0.0000	0.6079	-0.4136	0.0384	-0.1861	-0.9552	-0.5828	-0.8364	-0.9942	-1.4688	-0.668
1	0.0000	0.8366	1.1644	0.2291	0.1755	0.1203	0.3669	0.3166	0.3570	0.3829	0.3819	0.259
1	0.0000	1.0379	-1.3524	-0.0268	0.0385	-0.0716	-0.1707	0.0391	-0.1506	-0.0878	-0.6439	-0.075
1	0.0000	-1.0379	-1.3524	-0.0268	0.0385	-0.0716	-0.1707	0.0391	-0.1506	-0.0878	-0.6439	-0.075
1	0.0000	-0.8366	1.1644	0.2291	0.1755	0.1203	0.3669	0.3166	0.3570	0.3829	0.3819	0.259

Dipole mement (in D) 1.97 (DEN) 1.67 3.31 1.40 1.44 1.81 1.93 1.02 0.92 0.81

File TZVPMol212.out
Molecule PMol212 difluoroboranamine
SP Mol212 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 2.6976 2.6976
Quadrupole -0.8012 -1.6348 2.4360 0.0000 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	-0.0394	0.5256	-1.0697	0.2965	1.2244	0.1754	0.9972	1.2701	2.3940	0.716
7	0.0000	0.0000	1.3520	-0.4613	0.0524	-0.2188	-1.1849	-0.6061	-1.1757	-1.0976	-1.5194	-0.704
1	0.0000	0.8425	1.8942	0.2353	0.1847	0.1263	0.3948	0.3251	0.4434	0.3961	0.4027	0.264
9	0.0000	1.1337	-0.7253	-0.2674	0.3239	-0.1651	-0.4146	-0.1098	-0.3542	-0.4824	-0.8404	-0.270
9	0.0000	-1.1337	-0.7253	-0.2674	0.3239	-0.1651	-0.4146	-0.1098	-0.3542	-0.4824	-0.8404	-0.270
1	0.0000	-0.8425	1.8942	0.2353	0.1847	0.1263	0.3948	0.3251	0.4434	0.3961	0.4027	0.264

Dipole mement (in D) 2.70 (DEN) 3.05 1.65 1.97 2.15 2.71 2.71 3.20 2.86 1.98

File TZVPMol213.out
Molecule PMol213 difluoro(methyl)borane
SP Mol213 B3LYP/Def2TZVP VAC.
0 7
Dipole 0.0449 -1.6635 0.0000 1.6641
Quadrupole 2.0326 -0.0475 -1.9850 -0.1210 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	-0.0109	0.0781	0.0000	0.4891	-0.8958	0.3184	1.1007	0.1201	0.8797	1.2623	2.2895	0.616
9	-0.0016	0.7791	1.1182	-0.2434	0.3442	-0.1510	-0.3845	-0.0994	-0.3392	-0.4771	-0.8368	-0.265
9	-0.0016	0.7791	-1.1182	-0.2434	0.3442	-0.1510	-0.3845	-0.0994	-0.3392	-0.4771	-0.8368	-0.265
6	-0.0016	-1.4690	0.0000	-0.3988	-0.2510	-0.1544	-0.8353	-0.2311	-0.6775	-1.0353	-0.7094	-0.398
1	1.0324	-1.8212	0.0000	0.1339	0.1602	0.0503	0.1710	0.1075	0.1611	0.2495	0.0348	0.109
1	-0.4696	-1.8894	0.8869	0.1313	0.1491	0.0439	0.1663	0.1011	0.1576	0.2388	0.0295	0.102
1	-0.4696	-1.8894	-0.8869	0.1313	0.1491	0.0439	0.1663	0.1011	0.1576	0.2388	0.0295	0.102
Dipole mement (in D)	1.66 (DEN)			2.38	0.19	1.16	1.09	1.84	1.70	2.31	1.24	1.75

File TZVPMol214.out
Molecule PMol214 ethynyldifluoroborane
SP Mol214 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 -1.9538 0.0000 1.9538
Quadrupole -4.1733 4.4595 -0.2862 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.4711	0.0000	0.4920	-0.8595	0.3273	1.0852	0.1434	0.9267	1.2199	2.3583	0.616
6	-0.0000	-1.0438	0.0000	-0.0927	-0.0004	-0.1145	-0.4784	-0.0445	-0.3575	-0.4268	-0.6527	-0.169
6	-0.0000	-2.2478	0.0000	-0.1583	-0.0102	-0.0407	-0.0504	-0.0880	-0.1863	-0.1115	-0.2343	-0.089
1	0.0000	-3.3115	0.0000	0.2045	0.1323	0.1007	0.1994	0.1544	0.2695	0.2319	0.1814	0.150
9	-1.1236	1.1503	0.0000	-0.2227	0.3689	-0.1364	-0.3779	-0.0827	-0.3262	-0.4567	-0.8266	-0.254
9	1.1236	1.1503	0.0000	-0.2227	0.3689	-0.1364	-0.3779	-0.0827	-0.3262	-0.4567	-0.8266	-0.254
Dipole mement (in D)	1.95 (DEN)			2.43	0.14	1.35	1.95	1.87	1.99	2.63	0.88	2.00

File TZVPMol215.out
Molecule PMol215 difluoro(vinyl)borane
SP Mol215 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.5739 -1.9622 0.0000 2.0444
Quadrupole -0.6501 0.7096 -0.0596 0.3524 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.5166	0.0000	0.5227	-0.8688	0.2985	1.0407	0.1086	0.8149	1.2252	2.2984	0.590
6	-0.7104	-0.8468	0.0000	-0.2292	-0.1282	-0.1107	-0.5690	-0.0978	-0.4236	-0.6140	-0.7070	-0.223
6	-0.0405	-1.9986	0.0000	-0.1723	-0.1124	-0.0290	-0.0846	-0.1236	-0.1979	-0.2624	-0.0575	-0.126
1	1.0439	-2.0206	0.0000	0.1343	0.1325	0.0465	0.1119	0.1019	0.1279	0.1942	0.0538	0.096
1	-0.5329	-2.9641	0.0000	0.1256	0.1229	0.0479	0.1159	0.1004	0.1545	0.1894	0.0445	0.098
1	-1.7957	-0.8739	0.0000	0.1099	0.1578	0.0432	0.1463	0.1034	0.1650	0.2163	0.0368	0.094
9	-0.6737	1.6503	0.0000	-0.2377	0.3490	-0.1491	-0.3807	-0.0968	-0.3303	-0.4719	-0.8343	-0.264
9	1.3170	0.6106	0.0000	-0.2534	0.3473	-0.1474	-0.3806	-0.0961	-0.3103	-0.4768	-0.8360	-0.263
Dipole mement (in D)	2.04 (DEN)			2.38	0.70	1.50	1.79	2.13	2.10	2.67	1.29	2.08

File TZVPMol216.out
Molecule PMol216 difluoro(ethyl)borane
 SP Mol216 B3LYP/Def2TZVP VAC.
  0 10
Dipole -1.4714 -0.7819 -0.0003 1.6662
Quadrupole -1.7320 -0.9304 2.6624 0.6869 0.0000 -0.0005

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.6049	-0.0131	-0.0001	0.4895	-0.8702	0.3146	1.0736	0.1157	0.7499	1.2672	2.2760	0.612
6	-0.7555	-0.7593	-0.0001	-0.2711	-0.2346	-0.1153	-0.6549	-0.1533	-0.1831	-0.8140	-0.6637	-0.289
6	-1.9977	0.1185	0.0002	-0.3062	-0.2880	-0.0808	-0.2687	-0.2260	-0.0379	-0.5783	0.0234	-0.241
1	-2.9129	-0.4709	0.0001	0.1120	0.1162	0.0304	0.1092	0.0820	0.0321	0.2008	-0.0018	0.084
1	-2.0288	0.7683	-0.8734	0.1118	0.1227	0.0313	0.1072	0.0845	0.0071	0.2032	0.0019	0.084
1	-2.0287	0.7679	0.8741	0.1118	0.1227	0.0313	0.1072	0.0845	0.0071	0.2032	0.0019	0.084
1	-0.7583	-1.4390	-0.8584	0.1179	0.1692	0.0431	0.1448	0.1039	0.0364	0.2361	0.0176	0.098
1	-0.7582	-1.4394	0.8577	0.1180	0.1692	0.0431	0.1448	0.1039	0.0364	0.2361	0.0176	0.098
9	1.7513	-0.6682	-0.0001	-0.2392	0.3441	-0.1518	-0.3874	-0.1005	-0.3392	-0.4769	-0.8381	-0.266
9	0.6911	1.3042	0.0001	-0.2445	0.3487	-0.1458	-0.3759	-0.0948	-0.3090	-0.4773	-0.8349	-0.263

 Dipole mement (in D) 1.67 (DEN) 2.33 0.17 1.12 1.17 1.85 1.71 2.20 1.26 1.71

File TZVPMol217.out
Molecule PMol217 diaminoborane
 SP Mol217 B3LYP/Def2TZVP VAC.
  0 8
Dipole 0.0000 0.0000 -1.3600 1.3600
Quadrupole -4.3617 4.1098 0.2520 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	0.4994	0.1921	-0.7374	0.0996	0.8464	-0.0284	0.7912	0.6507	2.1256	0.479
7	0.0000	1.2359	-0.1755	-0.5022	0.0070	-0.2268	-1.0447	-0.6184	-1.1228	-1.0370	-1.4854	-0.698
1	0.0000	1.3422	-1.1739	0.2037	0.1637	0.1053	0.3596	0.3034	0.4291	0.3729	0.3642	0.246
7	0.0000	-1.2359	-0.1755	-0.5022	0.0070	-0.2268	-1.0447	-0.6184	-1.1228	-1.0370	-1.4854	-0.698
1	0.0000	0.0000	1.6896	-0.0454	0.0503	-0.0762	-0.1999	0.0422	-0.1861	-0.0920	-0.6422	-0.076
1	0.0000	2.1121	0.3091	0.2251	0.1728	0.1098	0.3618	0.3080	0.3912	0.3848	0.3791	0.251
1	0.0000	-2.1121	0.3091	0.2251	0.1728	0.1098	0.3618	0.3080	0.3912	0.3848	0.3791	0.251
1	0.0000	-1.3422	-1.1739	0.2037	0.1637	0.1053	0.3596	0.3034	0.4291	0.3729	0.3642	0.246

 Dipole mement (in D) 1.36 (DEN) 0.69 2.71 0.86 0.81 1.19 1.40 0.50 0.59 0.32

File TZVPMol218.out
Molecule PMol218 BH3B‡CO_adduct
 SP Mol218 B3LYP/Def2TZVP VAC.
  0 6
Dipole 0.0000 0.0000 1.3128 1.3128
Quadrupole 1.1877 1.1877 -2.3754 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP

8	0.0000	0.0000	1.3095	-0.0181	0.3397	-0.0612	-0.2536	-0.1062	-0.1644	-0.3926	-1.1342	-0.201
1	0.0000	1.1605	-1.6352	0.0090	0.1086	-0.0408	-0.0442	0.0615	-0.0554	0.0840	-0.5038	-0.054
1	-1.0050	-0.5802	-1.6352	0.0090	0.1086	-0.0408	-0.0442	0.0615	-0.0557	0.0840	-0.5038	-0.054
1	1.0050	-0.5802	-1.6352	0.0090	0.1086	-0.0408	-0.0442	0.0615	-0.0554	0.0840	-0.5038	-0.054
5	0.0000	0.0000	-1.3260	-0.3366	-0.6910	-0.0957	-0.2558	-0.4639	-0.1048	-0.6674	1.7536	0.017
6	0.0000	0.0000	0.1766	0.3277	0.0256	0.2793	0.6418	0.3857	0.4357	0.8078	0.8936	0.379

Dipole mement (in D)	1.31 (DEN)	2.10	4.00	1.42	1.62	1.16	1.31	0.49	5.67	0.43	

File TZVPMol219.out

Molecule PMol219 BH3‡NH3_adduct

SP Mol219 B3LYP/Def2TZVP VAC.

0 8

Dipole 0.0000 0.0000 5.4080 5.4080

Quadrupole 0.1022 0.1022 -0.2045 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	-0.9281	-0.1903	-0.7467	-0.0911	0.1988	-0.4042	0.3063	-0.2089	1.8515	0.025
7	0.0000	0.0000	0.7235	-0.4292	0.0930	-0.0350	-0.8506	-0.6091	-0.3766	-0.8053	-1.0945	-0.532
1	0.0000	0.9424	1.0943	0.2692	0.1876	0.1532	0.3860	0.3431	0.2518	0.3957	0.3949	0.284
1	0.0000	-1.1624	-1.2357	-0.0627	0.0303	-0.1111	-0.1688	-0.0054	-0.2282	-0.0576	-0.6471	-0.115
1	0.8162	-0.4712	1.0943	0.2692	0.1876	0.1532	0.3860	0.3431	0.2518	0.3957	0.3949	0.284
1	-0.8162	-0.4712	1.0943	0.2692	0.1876	0.1532	0.3860	0.3431	0.2516	0.3957	0.3949	0.284
1	-1.0066	0.5812	-1.2357	-0.0627	0.0303	-0.1111	-0.1688	-0.0054	-0.2285	-0.0576	-0.6471	-0.115
1	1.0066	0.5812	-1.2357	-0.0627	0.0303	-0.1111	-0.1688	-0.0054	-0.2282	-0.0576	-0.6471	-0.115

Dipole mement (in D)	5.41 (DEN)	4.72	6.07	4.68	5.25	5.19	5.36	5.40	5.69	4.58	

File TZVPMol220.out

Molecule PMol220 BF3‡NH3_adduct

SP Mol220 B3LYP/Def2TZVP VAC.

0 8

Dipole 0.0000 0.0000 6.0093 6.0093

Quadrupole -3.3023 -3.3023 6.6046 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
5	0.0000	0.0000	-0.2265	0.5984	-1.4260	0.2440	1.2556	0.0796	0.9637	1.2562	2.4407	0.640
7	0.0000	0.0000	1.4762	-0.4576	0.1074	-0.0567	-1.0747	-0.6146	-0.7326	-0.8930	-1.1084	-0.553
1	0.8205	0.4737	1.8350	0.2727	0.1920	0.1580	0.4096	0.3492	0.3406	0.4056	0.4106	0.285
1	0.0000	-0.9475	1.8350	0.2727	0.1920	0.1580	0.4096	0.3492	0.3400	0.4056	0.4106	0.285
1	-0.8205	0.4737	1.8350	0.2727	0.1920	0.1580	0.4096	0.3492	0.3402	0.4056	0.4106	0.285
9	0.0000	1.3232	-0.5447	-0.3196	0.2476	-0.2204	-0.4699	-0.1708	-0.4175	-0.5266	-0.8545	-0.314
9	-1.1459	-0.6616	-0.5447	-0.3196	0.2476	-0.2204	-0.4699	-0.1708	-0.4169	-0.5266	-0.8545	-0.314
9	1.1459	-0.6616	-0.5447	-0.3196	0.2476	-0.2204	-0.4699	-0.1708	-0.4175	-0.5266	-0.8545	-0.314

Dipole mement (in D)	6.01 (DEN)	5.82	5.45	5.24	5.53	6.13	6.03	7.16	7.05	5.39	

File TZVPMol221.out
Molecule PMol221 hydrogen_fluoride
 SP Mol221 B3LYP/Def2TZVP VAC.
  0 2
Dipole 0.0000 0.0000 -1.9213 1.9213
Quadrupole -0.6854 -0.6854 1.3708 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	0.0917	-0.4000	-0.1802	-0.2211	-0.5198	-0.2900	-0.4416	-0.5460	-0.7093	-0.3108
1	0.0000	0.0000	-0.8255	0.4000	0.1802	0.2211	0.5198	0.2900	0.4416	0.5460	0.7093	0.3108

 Dipole mement (in D) 1.92 (DEN) 1.76 0.79 0.97 2.29 1.28 1.95 2.41 3.12 1.37

File TZVPMol222.out
Molecule PMol222 fluorocyclohexane(axial)
 SP Mol222 B3LYP/Def2TZVP VAC.
  0 18
Dipole -1.7820 -0.0794 0.0000 1.7838
Quadrupole -2.9394 1.5990 1.3404 1.6531 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.2837	0.9075	1.2549	-0.1729	-0.2578	-0.0493	-0.1530	-0.1587	0.0717	-0.3906	0.0408	-0.1479
6	-0.9501	1.4548	0.0000	-0.1731	-0.2602	-0.0487	-0.1501	-0.1587	-0.0498	-0.3849	0.0397	-0.1460
6	-0.2837	0.9075	-1.2549	-0.1729	-0.2578	-0.0493	-0.1530	-0.1587	0.0717	-0.3906	0.0408	-0.1479
6	-0.2837	-0.6153	-1.2595	-0.1684	-0.2417	-0.0546	-0.2812	-0.1603	-0.1511	-0.4208	0.0393	-0.1542
6	0.3372	-1.1811	0.0000	0.1627	-0.3203	0.0804	0.3025	0.0326	0.2941	0.2101	0.5236	0.1156
6	-0.2837	-0.6153	1.2595	-0.1684	-0.2417	-0.0546	-0.2812	-0.1603	-0.1511	-0.4208	0.0394	-0.1542
1	-0.7782	1.2834	-2.1517	0.0923	0.1320	0.0286	0.0849	0.0834	-0.0103	0.2024	-0.0125	0.0787
1	-2.0096	1.1742	0.0000	0.0753	0.1325	0.0231	0.0777	0.0787	0.0200	0.1836	-0.0251	0.0698
1	0.7485	1.2640	1.3024	0.0953	0.1392	0.0284	0.0904	0.0854	0.0130	0.2013	0.0002	0.0704
1	-0.7782	1.2834	2.1517	0.0923	0.1320	0.0286	0.0849	0.0834	-0.0103	0.2024	-0.0125	0.0787
1	-1.3104	-0.9895	-1.3217	0.0802	0.1417	0.0317	0.0972	0.0879	0.0380	0.1979	-0.0106	0.0791
1	0.2434	-1.0088	-2.1295	0.0976	0.1382	0.0333	0.0991	0.0893	0.0480	0.2124	0.0037	0.0795
1	0.2885	-2.2744	0.0000	0.0639	0.1337	0.0332	0.0396	0.0922	0.0039	0.1619	0.0120	0.0776
1	-1.3104	-0.9895	1.3217	0.0802	0.1417	0.0317	0.0972	0.0879	0.0380	0.1979	-0.0106	0.0791
1	0.2434	-1.0088	2.1295	0.0976	0.1382	0.0333	0.0991	0.0893	0.0480	0.2124	0.0037	0.0795
1	0.7485	1.2640	-1.3024	0.0953	0.1392	0.0284	0.0904	0.0854	0.0130	0.2013	0.0002	0.0704
1	-0.9260	2.5457	0.0000	0.0934	0.1323	0.0290	0.0818	0.0837	-0.0022	0.2037	-0.0116	0.0791
9	1.7030	-0.8546	0.0000	-0.2703	0.0787	-0.1532	-0.2260	-0.1822	-0.2846	-0.3794	-0.6610	-0.2073

 Dipole mement (in D) 1.78 (DEN) 2.07 0.60 1.26 1.54 1.76 1.78 3.34 4.43 1.87

File TZVPMol223.out
Molecule PMol223 fluorocyclohexane(equato
 SP Mol223 B3LYP/Def2TZVP VAC.
  0 18
Dipole 0.1753 -2.1264 0.0000 2.1336

Quadrupole 2.3257 -4.7361 2.4104 1.0614 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.5743	0.9009	0.0000	0.1530	-0.3296	0.0778	0.3071	0.0309	0.3530	0.2161	0.5398	0.1145
6	0.0885	0.3765	1.2529	-0.1647	-0.2394	-0.0559	-0.2891	-0.1617	-0.1842	-0.4202	0.0384	-0.1559
6	0.0885	-1.1474	1.2557	-0.1867	-0.2558	-0.0456	-0.1422	-0.1558	-0.0034	-0.3858	0.0383	-0.1438
6	0.7476	-1.7018	0.0000	-0.1602	-0.2609	-0.0483	-0.1592	-0.1587	-0.0566	-0.3868	0.0404	-0.1461
6	0.0885	-1.1474	-1.2557	-0.1867	-0.2558	-0.0456	-0.1422	-0.1558	-0.0034	-0.3858	0.0381	-0.1438
6	0.0885	0.3765	-1.2529	-0.1647	-0.2394	-0.0559	-0.2891	-0.1617	-0.1842	-0.4202	0.0380	-0.1559
1	0.5862	-1.5202	2.1517	0.0976	0.1339	0.0314	0.0888	0.0862	0.0222	0.2073	-0.0061	0.0818
1	1.1159	0.7519	1.2799	0.0847	0.1398	0.0310	0.1010	0.0881	0.0733	0.1980	-0.0023	0.0740
1	-1.6384	0.6278	0.0000	0.0538	0.1352	0.0305	0.0402	0.0906	0.0196	0.1449	0.0055	0.0716
1	1.8084	-1.4308	0.0000	0.0813	0.1350	0.0267	0.0842	0.0825	0.0301	0.1892	-0.0176	0.0740
1	0.7121	-2.7923	0.0000	0.0953	0.1329	0.0295	0.0830	0.0842	0.0166	0.2045	-0.0105	0.0797
1	0.5862	-1.5202	-2.1517	0.0976	0.1339	0.0314	0.0888	0.0862	0.0222	0.2073	-0.0061	0.0818
1	1.1159	0.7519	-1.2799	0.0847	0.1398	0.0310	0.1010	0.0881	0.0733	0.1980	-0.0023	0.0740
1	-0.4160	0.7759	-2.1333	0.1004	0.1367	0.0333	0.0998	0.0892	0.0557	0.2110	0.0029	0.0792
1	-0.9434	-1.5099	1.3116	0.0849	0.1351	0.0264	0.0807	0.0822	0.0156	0.1892	-0.0182	0.0736
1	-0.4160	0.7759	2.1333	0.1004	0.1367	0.0333	0.0998	0.0892	0.0557	0.2110	0.0029	0.0792
1	-0.9434	-1.5099	-1.3116	0.0849	0.1351	0.0264	0.0807	0.0822	0.0156	0.1892	-0.0182	0.0736
9	-0.5256	2.2951	0.0000	-0.2553	0.0867	-0.1571	-0.2334	-0.1855	-0.3208	-0.3670	-0.6633	-0.2113

Dipole mement (in D) 2.13 (DEN) 2.37 0.69 1.56 1.99 2.06 2.16 3.59 4.96 2.12

File TZVPMol224.out
Molecule PMol224 1,2-difluoroethane(gauch
SP Mol224 B3LYP/Def2TZVP VAC.
0 8
Dipole 0.0000 0.0000 2.6748 2.6748
Quadrupole 1.6550 -2.6589 1.0039 1.5925 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.2603	0.7009	0.5110	0.0619	-0.3344	0.0523	0.0552	-0.0313	0.1456	0.0141	0.5740	0.0160
1	-0.0247	1.2010	1.4407	0.0857	0.1242	0.0456	0.0711	0.1014	0.0344	0.1634	0.0320	0.0936
1	1.3492	0.7109	0.4262	0.0980	0.1239	0.0463	0.0771	0.1031	0.0655	0.1698	0.0453	0.0886
6	-0.2603	-0.7009	0.5110	0.0619	-0.3344	0.0523	0.0552	-0.0313	0.1103	0.0141	0.5744	0.0160
1	0.0247	-1.2010	1.4407	0.0857	0.1242	0.0456	0.0711	0.1014	0.0424	0.1634	0.0320	0.0936
1	-1.3492	-0.7109	0.4262	0.0980	0.1239	0.0463	0.0771	0.1031	0.0735	0.1698	0.0453	0.0886
9	0.2603	-1.4149	-0.5481	-0.2457	0.0863	-0.1442	-0.2035	-0.1732	-0.2330	-0.3473	-0.6517	-0.1982
9	-0.2603	1.4149	-0.5481	-0.2457	0.0863	-0.1442	-0.2035	-0.1732	-0.2387	-0.3473	-0.6517	-0.1982

Dipole mement (in D) 2.67 (DEN) 3.19 0.13 1.84 2.64 2.58 2.69 4.85 6.88 2.78

File TZVPMol225.out
Molecule PMol225 1-fluoropropane(gauche)
SP Mol225 B3LYP/Def2TZVP VAC.
0 11
Dipole -1.0100 1.4616 0.4534 1.8336

Quadrupole -1.2572 0.2932 0.9640 1.7066 0.6871 -0.0080

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.5208	-0.4787	0.1172	-0.3337	-0.3077	-0.0845	-0.3331	-0.2354	-0.1690	-0.5924	0.0132	-0.2500
1	-1.6380	-0.5311	1.2002	0.0970	0.1170	0.0285	0.0992	0.0805	0.0437	0.1954	-0.0077	0.0804
1	-1.1339	-1.4403	-0.2150	0.1238	0.1222	0.0317	0.1096	0.0847	0.0539	0.2108	0.0157	0.0770
1	-2.5121	-0.3546	-0.3143	0.1113	0.1177	0.0312	0.1052	0.0827	0.0388	0.2047	-0.0017	0.0848
6	-0.5915	0.6511	-0.2823	-0.1436	-0.3025	-0.0493	-0.2140	-0.1595	0.1062	-0.4248	0.0560	-0.1403
1	-0.9907	1.6129	0.0489	0.0832	0.1390	0.0355	0.0972	0.0904	-0.0196	0.2015	-0.0037	0.0855
1	-0.5125	0.7151	-1.3697	0.0939	0.1365	0.0340	0.0979	0.0896	0.0126	0.2018	0.0031	0.0805
6	0.7909	0.5094	0.2963	0.0582	-0.3228	0.0547	0.1411	-0.0325	0.1156	0.0601	0.5511	0.0192
1	1.4374	1.3457	0.0199	0.0929	0.1163	0.0362	0.0537	0.0918	0.0303	0.1575	0.0186	0.0839
1	0.7646	0.4425	1.3885	0.0799	0.1166	0.0344	0.0558	0.0904	0.0430	0.1504	0.0159	0.0811
9	1.3904	-0.6534	-0.1717	-0.2628	0.0675	-0.1525	-0.2127	-0.1825	-0.2554	-0.3650	-0.6596	-0.2021

Dipole mement (in D) 1.83 (DEN) 2.14 0.44 1.27 1.69 1.76 1.82 3.24 4.51 1.88

File TZVPMol226.out
Molecule PMol226 1-fluoropropane(trans)
SP Mol226 B3LYP/Def2TZVP VAC.
0 11
Dipole 1.8420 0.5851 0.0001 1.9327
Quadrupole -3.1587 1.4471 1.7115 -1.1173 -0.0001 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.8557	0.1391	-0.0000	-0.3508	-0.3049	-0.0798	-0.3239	-0.2316	-0.3169	-0.5904	0.0104	-0.2452
1	1.9903	0.7714	0.8780	0.1062	0.1182	0.0303	0.1003	0.0821	0.0702	0.1979	-0.0042	0.0827
1	1.9903	0.7717	-0.8778	0.1062	0.1182	0.0303	0.1003	0.0821	0.0702	0.1979	-0.0042	0.0827
1	2.6615	-0.5914	-0.0001	0.1181	0.1203	0.0350	0.1104	0.0865	0.0916	0.2110	0.0064	0.0890
6	0.4957	-0.5328	-0.0001	-0.1369	-0.2984	-0.0507	-0.2199	-0.1611	0.1204	-0.4242	0.0569	-0.1427
1	0.3865	-1.1782	0.8733	0.0936	0.1351	0.0340	0.0989	0.0897	0.0052	0.2011	0.0036	0.0798
1	0.3865	-1.1780	-0.8737	0.0936	0.1351	0.0340	0.0989	0.0897	0.0052	0.2011	0.0036	0.0798
6	-0.6182	0.4801	0.0001	0.0651	-0.3249	0.0538	0.1452	-0.0329	0.1999	0.0654	0.5578	0.0187
1	-0.5743	1.1237	0.8843	0.0810	0.1156	0.0342	0.0553	0.0902	0.0229	0.1499	0.0154	0.0804
1	-0.5744	1.1239	-0.8840	0.0810	0.1156	0.0342	0.0553	0.0902	0.0229	0.1499	0.0154	0.0804
9	-1.8518	-0.1513	0.0000	-0.2570	0.0703	-0.1553	-0.2208	-0.1849	-0.2917	-0.3596	-0.6605	-0.2057

Dipole mement (in D) 1.93 (DEN) 2.20 0.57 1.42 1.69 1.91 1.96 3.40 4.70 1.96

File TZVPMol227.out
Molecule PMol227 fluoromethane
SP Mol227 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.0000 -1.8108 0.0000 1.8108
Quadrupole 0.2012 -0.4023 0.2011 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.7480	0.0000	-0.2586	0.0543	-0.1523	-0.1983	-0.1831	-0.2401	-0.3500	-0.6570	-0.1995
6	0.0000	-0.6275	0.0000	-0.0619	-0.3470	0.0295	-0.0302	-0.0967	0.1118	-0.1177	0.5683	-0.0788

1	1.0282	-0.9890	0.0000	0.1068	0.0976	0.0410	0.0762	0.0933	0.0429	0.1559	0.0296	0.0928
1	-0.5141	-0.9890	0.8905	0.1068	0.0976	0.0410	0.0762	0.0933	0.0427	0.1559	0.0296	0.0928
1	-0.5141	-0.9890	-0.8905	0.1068	0.0976	0.0410	0.0762	0.0933	0.0427	0.1559	0.0296	0.0928

Dipole mement (in D) 1.81 (DEN) 2.26 0.15 1.22 1.71 1.70 1.81 3.12 4.49 1.80

File TZVPMol228.out
Molecule PMol228 1,1-difluoroethane
SP Mol228 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.3609 2.1961 0.0000 2.2256
Quadrupole 1.7108 0.3555 -2.0663 0.4799 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	1.2679	0.7165	0.0000	0.0629	0.1175	0.0439	0.0202	0.1039	0.0104	0.1232	0.0522	0.0842
6	0.3210	0.1651	0.0000	0.3177	-0.4885	0.1743	0.5806	0.1517	0.5716	0.5546	1.1387	0.2806
6	-0.8955	1.0337	0.0000	-0.2986	-0.2833	-0.0902	-0.5513	-0.2346	-0.4479	-0.6579	0.0212	-0.2592
9	0.3210	-0.6476	1.0939	-0.2183	0.1316	-0.1335	-0.2417	-0.1600	-0.2684	-0.3416	-0.6552	-0.1948
9	0.3210	-0.6476	-1.0939	-0.2183	0.1316	-0.1335	-0.2417	-0.1600	-0.2684	-0.3416	-0.6552	-0.1948
1	-1.7889	0.4138	0.0000	0.1217	0.1307	0.0468	0.1480	0.1007	0.1571	0.2240	0.0397	0.0913
1	-0.9047	1.6664	-0.8836	0.1164	0.1302	0.0461	0.1429	0.0991	0.1229	0.2196	0.0293	0.0964
1	-0.9047	1.6664	0.8836	0.1164	0.1302	0.0461	0.1429	0.0991	0.1229	0.2196	0.0293	0.0964

Dipole mement (in D) 2.23 (DEN) 2.52 0.68 1.53 1.88 2.12 2.24 3.71 5.85 2.17

File TZVPMol229.out
Molecule PMol229 fluoroethane
SP Mol229 B3LYP/Def2TZVP VAC.
0 8
Dipole -1.7648 0.7043 0.0000 1.9001
Quadrupole -1.6946 0.8548 0.8397 0.2751 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1200	-0.4454	0.0000	-0.3040	-0.3121	-0.0863	-0.4194	-0.2354	-0.2545	-0.6293	0.0174	-0.2510
1	-1.0767	-1.0817	0.8818	0.1133	0.1215	0.0375	0.1195	0.0899	0.0809	0.2092	0.0152	0.0872
1	-1.0767	-1.0817	-0.8818	0.1133	0.1215	0.0375	0.1195	0.0899	0.0809	0.2092	0.0152	0.0872
1	-2.0810	0.0668	0.0000	0.1008	0.1250	0.0394	0.1194	0.0910	0.0530	0.2098	0.0096	0.0930
6	0.0000	0.5528	0.0000	0.0644	-0.3492	0.0568	0.1638	-0.0320	0.3675	0.0576	0.5632	0.0238
1	-0.0256	1.1951	-0.8839	0.0862	0.1141	0.0361	0.0570	0.0915	-0.0131	0.1526	0.0188	0.0837
1	-0.0256	1.1951	0.8839	0.0862	0.1141	0.0361	0.0570	0.0915	-0.0131	0.1526	0.0188	0.0837
9	1.2228	-0.1042	0.0000	-0.2604	0.0653	-0.1570	-0.2167	-0.1865	-0.3015	-0.3617	-0.6586	-0.2077

Dipole mement (in D) 1.90 (DEN) 2.24 0.51 1.33 1.71 1.81 1.90 3.31 4.61 1.89

File TZVPMol230.out
Molecule PMol230 2-fluoropropane
SP Mol230 B3LYP/Def2TZVP VAC.

```
    0   11
Dipole         -1.5079   -1.2048    0.0000    1.9301
Quadrupole     -0.2854   -0.7533    1.0387   -1.5785    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -0.2792   -0.5811    1.2623   -0.3129   -0.2849   -0.0888   -0.4551   -0.2360   -0.4501   -0.6214    0.0147   -0.2560
   6     -0.2792    0.2399    0.0000    0.1727   -0.3831    0.0848    0.3500    0.0329    0.5746    0.2077    0.5527    0.1289
   6     -0.2792   -0.5811   -1.2623   -0.3129   -0.2849   -0.0888   -0.4551   -0.2360   -0.4501   -0.6214    0.0146   -0.2560
   9      0.8702    1.0405    0.0000   -0.2627    0.0772   -0.1593   -0.2260   -0.1877   -0.3298   -0.3714   -0.6592   -0.2138
   1     -1.1263    0.9348    0.0000    0.0618    0.1318    0.0334    0.0454    0.0922   -0.0304    0.1494    0.0124    0.0774
   1     -0.2328    0.0554   -2.1432    0.1189    0.1235    0.0371    0.1226    0.0898    0.1142    0.2148    0.0157    0.0863
   1     -0.2328    0.0554    2.1432    0.1189    0.1235    0.0371    0.1226    0.0898    0.1142    0.2148    0.0157    0.0863
   1      0.5770   -1.2548    1.2812    0.1072    0.1232    0.0354    0.1245    0.0885    0.1252    0.2064    0.0113    0.0841
   1     -1.1845   -1.1835    1.3262    0.1009    0.1253    0.0368    0.1234    0.0891    0.1035    0.2074    0.0057    0.0893
   1     -1.1845   -1.1835   -1.3262    0.1009    0.1253    0.0368    0.1234    0.0891    0.1035    0.2074    0.0057    0.0893
   1      0.5770   -1.2548   -1.2812    0.1072    0.1232    0.0354    0.1245    0.0885    0.1252    0.2064    0.0113    0.0841

 Dipole mement (in D)   1.93 (DEN)      2.20      0.73      1.35      1.65      1.86      1.96      3.46      4.64      1.91

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File TZVPMol231.out
Molecule PMol231    difluoromethane
 SP Mol231 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    1.8809    0.0000    1.8809
Quadrupole     -2.4136    1.2032    1.2104    0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   9      1.0967   -0.2899    0.0000   -0.2166    0.1211   -0.1276   -0.2285   -0.1554   -0.2239   -0.3335   -0.6529   -0.1853
   6      0.0000    0.5001    0.0000    0.2508   -0.4401    0.1564    0.3850    0.0982    0.3707    0.4232    1.1862    0.1823
   9     -1.0967   -0.2899    0.0000   -0.2166    0.1212   -0.1276   -0.2285   -0.1554   -0.2242   -0.3335   -0.6529   -0.1853
   1      0.0000    1.1091    0.9083    0.0912    0.0989    0.0494    0.0359    0.1063    0.0387    0.1218    0.0598    0.0941
   1      0.0000    1.1091   -0.9083    0.0912    0.0989    0.0494    0.0359    0.1063    0.0387    0.1218    0.0598    0.0941

 Dipole mement (in D)   1.88 (DEN)      2.18      0.34      1.26      1.94      1.80      1.93      3.24      5.30      1.96

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File TZVPMol232.out
Molecule PMol232    trifluoromethane
 SP Mol232 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -1.2652    0.9458    0.0000    1.5796
Quadrupole      1.0807    0.0878   -1.1685   -1.6812    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1     -1.1467    0.8571    0.0000    0.0714    0.1056    0.0616   -0.0004    0.1233    0.0803    0.1040    0.1036    0.0991
   6     -0.2710    0.2026    0.0000    0.4652   -0.6432    0.2626    0.8115    0.2725    0.4648    0.8428    1.8385    0.4294
   9      0.8500    0.9231    0.0000   -0.1789    0.1792   -0.1081   -0.2704   -0.1319   -0.1818   -0.3156   -0.6474   -0.1762
   9     -0.2710   -0.5767    1.0809   -0.1789    0.1792   -0.1081   -0.2704   -0.1319   -0.1817   -0.3156   -0.6474   -0.1762
   9     -0.2710   -0.5767   -1.0809   -0.1789    0.1792   -0.1081   -0.2704   -0.1319   -0.1817   -0.3156   -0.6474   -0.1762
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 Dipole mement (in D)   1.58 (DEN)      1.58      0.65      1.05      1.82      1.53      1.64      2.67      4.90      1.70

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File TZVPMol233.out
Molecule PMol233    1,1,1-trifluoroethane
 SP Mol233 B3LYP/Def2TZVP VAC.
    0    8
Dipole         -2.3184   -0.0002    0.0000    2.3184
Quadrupole      1.9607   -0.9804   -0.9803    0.0002    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   1     -1.8339   -1.0227    0.0000    0.1293    0.1371    0.0529    0.1651    0.1072    0.1708    0.2298    0.0489    0.0992
   6     -1.4696   -0.0001    0.0000   -0.3394   -0.2541   -0.0906   -0.6758   -0.2309   -0.5298   -0.6780    0.0408   -0.2645
   6      0.0243    0.0000    0.0000    0.5057   -0.7171    0.2784    1.0248    0.3231    0.6790    0.9560    1.7586    0.5299
   1     -1.8340    0.5111    0.8856    0.1292    0.1371    0.0529    0.1651    0.1072    0.1703    0.2298    0.0489    0.0992
   1     -1.8340    0.5111   -0.8856    0.1292    0.1371    0.0529    0.1651    0.1072    0.1703    0.2298    0.0489    0.0992
   9      0.5250    1.2465    0.0000   -0.1846    0.1866   -0.1156   -0.2814   -0.1379   -0.2206   -0.3224   -0.6487   -0.1877
   9      0.5250   -0.6232   -1.0794   -0.1847    0.1867   -0.1156   -0.2814   -0.1379   -0.2201   -0.3224   -0.6487   -0.1876
   9      0.5250   -0.6232    1.0794   -0.1847    0.1867   -0.1156   -0.2814   -0.1379   -0.2201   -0.3224   -0.6487   -0.1876

 Dipole mement (in D)   2.32 (DEN)      2.36      0.50      1.60      1.60      2.21      2.35      3.61      6.28      2.11

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File TZVPMol234.out
Molecule PMol234    pentafluoroethane
 SP Mol234 B3LYP/Def2TZVP VAC.
    0    8
Dipole         -1.5160   -0.0469    0.0000    1.5167
Quadrupole      3.0244   -1.5508   -1.4736   -0.9423    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   1     -1.6881    0.6111    0.0000    0.0908    0.1331    0.0611    0.0648    0.1232    0.1245    0.1453    0.0941    0.0937
   6     -0.6021    0.7513    0.0000    0.2800   -0.4559    0.1632    0.2769    0.1578    0.2203    0.4737    1.2462    0.2605
   6      0.1193   -0.6031    0.0000    0.4752   -0.7085    0.2667    0.8334    0.3242    0.4100    0.8920    1.8514    0.5116
   9     -0.2318    1.4387    1.0927   -0.1817    0.1830   -0.1038   -0.1943   -0.1287   -0.1608   -0.3059   -0.6392   -0.1747
   9     -0.2318    1.4387   -1.0927   -0.1817    0.1830   -0.1038   -0.1943   -0.1287   -0.1608   -0.3059   -0.6392   -0.1747
   9      1.4369   -0.4480    0.0000   -0.1558    0.2302   -0.0908   -0.2556   -0.1118   -0.1195   -0.2939   -0.6352   -0.1708
   9     -0.2318   -1.2980   -1.0815   -0.1633    0.2176   -0.0964   -0.2655   -0.1180   -0.1568   -0.3026   -0.6392   -0.1728
   9     -0.2318   -1.2980    1.0815   -0.1633    0.2176   -0.0964   -0.2655   -0.1180   -0.1568   -0.3026   -0.6392   -0.1728

 Dipole mement (in D)   1.52 (DEN)      1.60      0.54      1.00      1.59      1.49      1.53      2.72      4.84      1.63

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File TZVPMol235.out
Molecule PMol235    1,1,1,2,2,3,3-heptafluor
 SP Mol235 B3LYP/Def2TZVP VAC.
    0   11
Dipole          1.1404    0.9376    0.0009    1.4763
Quadrupole      2.4815   -0.4100   -2.0715    3.1722    0.0028    0.0015
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
```

6	1.5495	0.1268	0.0002	0.2685	-0.4509	0.1658	0.3796	0.1599	0.2908	0.5036	1.2396	0.2641
6	0.1130	0.6722	0.0003	0.3388	-0.5019	0.1689	0.2879	0.2101	0.1872	0.5238	1.2262	0.3442
1	2.2479	0.9720	0.0009	0.1004	0.1367	0.0610	0.0586	0.1234	0.1235	0.1479	0.0965	0.0921
6	-1.0286	-0.3729	-0.0002	0.4510	-0.6927	0.2670	0.8314	0.3286	0.5480	0.9050	1.8829	0.5088
9	1.7539	-0.6270	-1.0924	-0.1818	0.1857	-0.1028	-0.2034	-0.1279	-0.1778	-0.3062	-0.6398	-0.1753
9	1.7535	-0.6285	1.0919	-0.1818	0.1857	-0.1028	-0.2034	-0.1279	-0.1778	-0.3062	-0.6398	-0.1753
9	-0.0324	1.4427	-1.0924	-0.1697	0.2192	-0.0940	-0.1907	-0.1169	-0.1518	-0.2959	-0.6324	-0.1726
9	-0.0326	1.4419	1.0936	-0.1697	0.2192	-0.0940	-0.1907	-0.1169	-0.1518	-0.2959	-0.6324	-0.1726
9	-0.9579	-1.1401	-1.0809	-0.1517	0.2343	-0.0891	-0.2567	-0.1103	-0.1652	-0.2918	-0.6348	-0.1709
9	-0.9587	-1.1403	1.0805	-0.1517	0.2344	-0.0891	-0.2567	-0.1103	-0.1653	-0.2918	-0.6348	-0.1709
9	-2.1981	0.2593	-0.0006	-0.1524	0.2304	-0.0911	-0.2560	-0.1120	-0.1598	-0.2927	-0.6310	-0.1717

Dipole mement (in D) 1.48 (DEN) 1.53 0.46 0.98 1.58 1.47 1.50 2.49 4.69 1.58

File TZVPMol236.out
Molecule PMol236 2-fluoro-2-methylpropane
SP Mol236 B3LYP/Def2TZVP VAC.
0 14
Dipole -1.9363 0.0001 0.0000 1.9363
Quadrupole -2.2485 1.1245 1.1239 -0.0001 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	1.4116	-0.0000	0.0000	-0.2652	0.0894	-0.1599	-0.2297	-0.1871	-0.3478	-0.3822	-0.6584	-0.2181
6	-0.0018	-0.0000	0.0000	0.2530	-0.4428	0.1131	0.5390	0.0979	0.7624	0.3411	0.5342	0.2360
6	-0.4330	-1.4501	0.0000	-0.3236	-0.2587	-0.0900	-0.4877	-0.2354	-0.5247	-0.6164	0.0152	-0.2602
6	-0.4330	0.7250	1.2557	-0.3237	-0.2587	-0.0900	-0.4877	-0.2354	-0.5108	-0.6164	0.0153	-0.2602
6	-0.4330	0.7250	-1.2557	-0.3237	-0.2587	-0.0900	-0.4877	-0.2354	-0.5108	-0.6164	0.0152	-0.2602
1	-1.5199	-1.5280	0.0000	0.1008	0.1261	0.0350	0.1286	0.0879	0.1211	0.2059	0.0026	0.0865
1	-1.5199	0.7640	1.3232	0.1009	0.1261	0.0350	0.1286	0.0879	0.1184	0.2059	0.0026	0.0865
1	-1.5199	0.7640	-1.3232	0.1009	0.1261	0.0350	0.1286	0.0879	0.1184	0.2059	0.0026	0.0865
1	-0.0566	-1.9645	0.8825	0.1134	0.1252	0.0352	0.1280	0.0886	0.1316	0.2121	0.0119	0.0838
1	-0.0566	1.7465	1.2600	0.1134	0.1252	0.0353	0.1280	0.0886	0.1273	0.2121	0.0119	0.0839
1	-0.0567	0.2181	-2.1425	0.1134	0.1252	0.0352	0.1280	0.0886	0.1280	0.2121	0.0119	0.0838
1	-0.0566	-1.9645	-0.8825	0.1134	0.1252	0.0352	0.1280	0.0886	0.1316	0.2121	0.0119	0.0838
1	-0.0567	0.2181	2.1425	0.1134	0.1252	0.0352	0.1280	0.0886	0.1280	0.2121	0.0119	0.0838
1	-0.0566	1.7465	-1.2600	0.1134	0.1252	0.0353	0.1280	0.0886	0.1273	0.2121	0.0119	0.0839

Dipole mement (in D) 1.94 (DEN) 2.17 0.74 1.35 1.55 1.87 1.97 3.60 4.64 1.89

File TZVPMol237.out
Molecule PMol237 1,2-difluoroethene
SP Mol237 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 2.2792 2.2792
Quadrupole -1.0059 -0.6272 1.6330 0.0000 0.0000 0.0000

Atomic coordinates (in A)				Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6609	0.5716	0.0762	-0.3124	0.0383	0.0412	0.0063	-0.0385	0.1301	0.5663	0.0572

6	0.0000	-0.6609	0.5716	0.0762	-0.3124	0.0383	0.0412	0.0063	-0.0385	0.1301	0.5665	0.0572
1	0.0000	-1.2375	1.4847	0.1145	0.1305	0.0597	0.0977	0.1171	0.1352	0.1722	0.0876	0.1038
1	0.0000	1.2375	1.4847	0.1145	0.1305	0.0597	0.0977	0.1171	0.1352	0.1722	0.0876	0.1038
9	0.0000	1.3815	-0.5461	-0.1906	0.1818	-0.0981	-0.1389	-0.1234	-0.0967	-0.3024	-0.6539	-0.1610
9	0.0000	-1.3815	-0.5461	-0.1906	0.1818	-0.0981	-0.1389	-0.1234	-0.0967	-0.3024	-0.6539	-0.1610

Dipole mement (in D) 2.28 (DEN) 3.05 0.81 1.58 2.35 2.35 2.22 4.76 7.79 2.64

File TZVPMol238.out
Molecule PMol238 3-fluoropropene(eclipsed
SP Mol238 B3LYP/Def2TZVP VAC.
0 9
Dipole -0.8988 1.4714 0.0000 1.7242
Quadrupole 2.6849 -1.4284 -1.2565 -0.3354 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.3201	0.8496	0.0000	-0.2553	-0.2016	-0.0843	-0.2745	-0.1858	-0.4491	-0.3788	-0.0532	-0.1917
1	1.8138	-0.1127	0.0000	0.1304	0.1255	0.0377	0.1183	0.0927	0.1960	0.2031	0.0561	0.0760
1	1.9484	1.7288	0.0000	0.1161	0.1218	0.0390	0.1149	0.0920	0.1769	0.1965	0.0346	0.0880
6	0.0000	0.9448	0.0000	-0.1292	-0.2178	-0.0416	-0.1120	-0.1035	-0.0642	-0.2286	-0.0485	-0.0734
1	-0.4847	1.9165	0.0000	0.1070	0.1432	0.0433	0.1014	0.0990	0.0897	0.1997	0.0295	0.0894
6	-0.9356	-0.2053	0.0000	0.0865	-0.3128	0.0575	0.1153	-0.0239	0.2522	0.0245	0.5693	0.0244
1	-1.5875	-0.1817	0.8805	0.0979	0.1257	0.0427	0.0659	0.0983	0.0245	0.1671	0.0343	0.0875
1	-1.5875	-0.1817	-0.8805	0.0979	0.1257	0.0427	0.0659	0.0983	0.0245	0.1671	0.0343	0.0875
9	-0.2677	-1.4116	0.0000	-0.2513	0.0905	-0.1369	-0.1949	-0.1670	-0.2506	-0.3506	-0.6567	-0.1878

Dipole mement (in D) 1.72 (DEN) 2.08 0.07 1.18 1.72 1.66 1.71 3.19 4.33 1.88

File TZVPMol239.out
Molecule PMol239 3-fluoropropene(gauche)
SP Mol239 B3LYP/Def2TZVP VAC.
0 9
Dipole 1.4963 0.7376 0.8233 1.8603
Quadrupole -1.3942 1.8406 -0.4464 -1.1467 -1.8328 -0.9845

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.6005	0.4348	0.3026	0.0771	-0.3064	0.0534	0.1142	-0.0288	0.2175	0.0190	0.5625	0.0172
1	-0.9137	0.6054	1.3376	0.0900	0.1226	0.0405	0.0632	0.0962	0.0261	0.1651	0.0318	0.0849
1	-0.4715	1.4065	-0.1804	0.0858	0.1222	0.0406	0.0669	0.0972	0.0531	0.1589	0.0299	0.0851
6	0.6405	-0.3748	0.2393	-0.0937	-0.2056	-0.0355	-0.1038	-0.0971	-0.1058	-0.2155	-0.0234	-0.0690
1	0.5575	-1.3923	0.6086	0.1137	0.1418	0.0448	0.1052	0.1012	0.1370	0.2015	0.0405	0.0859
6	1.7989	0.0853	-0.2081	-0.2521	-0.1898	-0.0707	-0.2523	-0.1732	-0.4335	-0.3590	-0.0618	-0.1768
1	2.6954	-0.5197	-0.2074	0.1192	0.1229	0.0429	0.1171	0.0957	0.1829	0.1982	0.0403	0.0924
1	1.8985	1.0957	-0.5881	0.1135	0.1221	0.0394	0.1094	0.0927	0.1828	0.1871	0.0317	0.0876
9	-1.6444	-0.2297	-0.3304	-0.2534	0.0701	-0.1556	-0.2200	-0.1840	-0.2600	-0.3554	-0.6514	-0.2074

Dipole mement (in D) 1.86 (DEN) 2.12 0.36 1.35 1.73 1.82 1.92 3.39 4.62 1.90

File TZVPMol240.out
Molecule PMol240 1,1-difluoro-1-propene
SP Mol240 B3LYP/Def2TZVP VAC.
0 9
Dipole -1.5176 -0.5269 0.0000 1.6065
Quadrupole 0.1263 0.0798 -0.2061 0.4978 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.4839	-0.0590	0.0000	0.3891	-0.4715	0.1730	0.6006	0.2063	0.3791	0.7167	1.0816	0.3309
6	-0.6855	-0.6675	0.0000	-0.2159	-0.2168	-0.0784	-0.3839	-0.1348	-0.3334	-0.3657	0.0813	-0.1199
1	-0.6517	-1.7473	0.0000	0.1256	0.1519	0.0473	0.1403	0.1052	0.1596	0.2201	0.0566	0.0874
6	-1.9950	0.0343	0.0000	-0.3059	-0.2856	-0.0790	-0.3147	-0.2249	-0.0448	-0.6170	0.0390	-0.2435
1	-2.5896	-0.2322	-0.8746	0.1184	0.1266	0.0376	0.1197	0.0892	0.0515	0.2125	0.0154	0.0884
1	-2.5896	-0.2322	0.8746	0.1184	0.1266	0.0376	0.1197	0.0892	0.0515	0.2125	0.0154	0.0884
1	-1.8735	1.1145	-0.0000	0.1253	0.1286	0.0372	0.1183	0.0912	0.0409	0.2193	0.0271	0.0796
9	1.6546	-0.6643	0.0000	-0.1765	0.2201	-0.0899	-0.2054	-0.1126	-0.1745	-0.2963	-0.6584	-0.1586
9	0.6658	1.2477	-0.0000	-0.1784	0.2201	-0.0856	-0.1947	-0.1088	-0.1299	-0.3021	-0.6587	-0.1527

Dipole mement (in D)	1.61 (DEN)	1.99	0.53	1.04	1.11	1.63	1.62	2.74	6.86	1.59	

File TZVPMol241.out
Molecule PMol241 fluoroethene
SP Mol241 B3LYP/Def2TZVP VAC.
0 6
Dipole 1.0999 0.7951 0.0000 1.3572
Quadrupole -0.1695 1.8565 -1.6870 -0.7674 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.4295	0.0000	0.1258	-0.3113	0.0630	0.2234	0.0251	0.1960	0.2308	0.5021	0.0913
6	1.1819	-0.1513	0.0000	-0.2782	-0.2321	-0.1051	-0.4318	-0.2052	-0.5719	-0.4955	-0.0281	-0.2114
1	1.2916	-1.2256	0.0000	0.1290	0.1274	0.0492	0.1501	0.1031	0.2455	0.2109	0.0624	0.0923
9	-1.1416	-0.2669	0.0000	-0.2029	0.1627	-0.1093	-0.1649	-0.1357	-0.1691	-0.3202	-0.6645	-0.1675
1	-0.1787	1.4978	0.0000	0.1039	0.1220	0.0547	0.0794	0.1115	0.1006	0.1624	0.0740	0.0983
1	2.0698	0.4605	0.0000	0.1225	0.1313	0.0476	0.1438	0.1012	0.1989	0.2115	0.0544	0.0970

Dipole mement (in D)	1.36 (DEN)	1.76	0.34	0.92	1.24	1.38	1.33	2.76	4.87	1.50	

File TZVPMol242.out
Molecule PMol242 2-fluoropropene
SP Mol242 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.8127 -1.3486 -0.0002 1.5745
Quadrupole 1.9718 -0.7882 -1.1837 0.1749 0.0001 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.0977	-0.0459	-0.0000	0.2680	-0.3517	0.0988	0.4644	0.0979	0.5218	0.4050	0.4769	0.2054
6	-1.1686	-0.8210	-0.0001	-0.3294	-0.2150	-0.1201	-0.5002	-0.2181	-0.7400	-0.4973	-0.0329	-0.2326
1	-1.0548	-1.8930	-0.0003	0.1173	0.1291	0.0409	0.1462	0.0951	0.2432	0.2060	0.0431	0.0892

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   6      1.3281   -0.4319   -0.0001   -0.3294   -0.2603   -0.0825   -0.4929   -0.2255   -0.4582   -0.6612    0.0342   -0.2499
   9     -0.2515    1.2956    0.0002   -0.2164    0.1714   -0.1156   -0.1853   -0.1407   -0.2291   -0.3313   -0.6660   -0.1782
   1     -2.1639   -0.4046   -0.0001    0.1259    0.1278    0.0434    0.1493    0.0978    0.2503    0.2131    0.0561    0.0854
   1      1.4387   -1.5123   -0.0003    0.1138    0.1332    0.0458    0.1431    0.0988    0.1318    0.2206    0.0258    0.0977
   1      1.8364   -0.0285   -0.8761    0.1251    0.1328    0.0446    0.1377    0.0973    0.1402    0.2226    0.0313    0.0915
   1      1.8364   -0.0289    0.8762    0.1251    0.1328    0.0446    0.1377    0.0973    0.1402    0.2226    0.0313    0.0915

 Dipole mement (in D)   1.57 (DEN)      1.87      0.79      1.13      1.24      1.59      1.59      2.94      4.97      1.63

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File TZVPMol243.out
Molecule PMol243    cis-1-fluoro-1-propene
 SP Mol243 B3LYP/Def2TZVP VAC.
    0    9
Dipole         -0.0771    1.4110    0.0000    1.4131
Quadrupole      2.3047   -0.9515   -1.3532    0.5543    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
   6      0.0000    0.8698    0.0000   -0.1486   -0.2278   -0.0562   -0.1693   -0.1175   -0.1789   -0.2742    0.0024   -0.0903
   6      0.9559   -0.0424    0.0000    0.0912   -0.2894    0.0452    0.1455    0.0089   -0.0822    0.2149    0.4756    0.0662
   9      0.6919   -1.3601    0.0000   -0.2160    0.1516   -0.1131   -0.1637   -0.1399   -0.1143   -0.3297   -0.6675   -0.1681
   6     -1.4601    0.6008    0.0000   -0.3058   -0.2882   -0.0805   -0.3477   -0.2266    0.0916   -0.6321    0.0266   -0.2446
   1      0.3401    1.8979    0.0000    0.1127    0.1477    0.0422    0.1080    0.0986    0.1020    0.2078    0.0352    0.0880
   1      2.0185    0.1595    0.0000    0.1049    0.1229    0.0501    0.0750    0.1071    0.1476    0.1642    0.0693    0.0933
   1     -1.6723   -0.4653    0.0000    0.1291    0.1283    0.0371    0.1190    0.0911    0.0203    0.2205    0.0300    0.0792
   1     -1.9440    1.0400    0.8736    0.1163    0.1274    0.0375    0.1165    0.0891    0.0069    0.2144    0.0142    0.0881
   1     -1.9440    1.0400   -0.8736    0.1163    0.1274    0.0375    0.1165    0.0891    0.0069    0.2144    0.0142    0.0881

 Dipole mement (in D)   1.41 (DEN)      1.88      0.83      0.98      1.31      1.43      1.35      2.85      4.80      1.59

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File TZVPMol244.out
Molecule PMol244    1,1-difluoroethene
 SP Mol244 B3LYP/Def2TZVP VAC.
    0    6
Dipole          0.0000    0.0000    1.1895    1.1895
Quadrupole     -0.8146   -0.3249    1.1395    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
   6      0.0000    0.0000    0.0655    0.4042   -0.5017    0.1875    0.6750    0.2190    0.5436    0.7314    1.1057    0.3534
   6      0.0000    0.0000    1.3808   -0.3449   -0.2288   -0.1291   -0.6337   -0.2249   -0.7347   -0.5928    0.0534   -0.2431
   1      0.0000    0.9340    1.9142    0.1381    0.1362    0.0532    0.1769    0.1081    0.2617    0.2247    0.0768    0.0973
   9      0.0000    1.0723   -0.6948   -0.1677    0.2290   -0.0823   -0.1975   -0.1052   -0.1662   -0.2940   -0.6562   -0.1525
   9      0.0000   -1.0723   -0.6948   -0.1677    0.2290   -0.0823   -0.1975   -0.1052   -0.1662   -0.2940   -0.6562   -0.1525
   1      0.0000   -0.9340    1.9142    0.1381    0.1362    0.0532    0.1769    0.1081    0.2617    0.2247    0.0768    0.0973

 Dipole mement (in D)   1.19 (DEN)      1.50      0.70      0.73      0.58      1.27      1.22      2.39      6.49      1.31

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File TZVPMol245.out
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Molecule PMol245 1,1-difluoroallene
 SP Mol245 B3LYP/Def2TZVP VAC.
  0 7
Dipole 0.0000 0.0000 1.9406 1.9406
Quadrupole 0.2410 -3.0118 2.7708 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.8747	-0.0847	-0.1070	-0.0623	-0.2496	-0.0671	-0.1486	-0.1486	-0.1318	-0.0602
6	0.0000	0.0000	2.1719	-0.2150	-0.1478	-0.0423	-0.1796	-0.1385	-0.2689	-0.3527	0.0719	-0.1447
6	0.0000	0.0000	-0.4204	0.3492	-0.4670	0.1661	0.5564	0.2051	0.3856	0.6624	1.2045	0.3168
1	-0.9215	0.0000	2.7469	0.1422	0.1366	0.0569	0.1350	0.1095	0.1684	0.2085	0.0709	0.1022
1	0.9215	0.0000	2.7469	0.1422	0.1366	0.0569	0.1350	0.1095	0.1691	0.2085	0.0709	0.1022
9	0.0000	1.0799	-1.1806	-0.1670	0.2243	-0.0877	-0.1986	-0.1092	-0.1528	-0.2890	-0.6431	-0.1582
9	0.0000	-1.0799	-1.1806	-0.1670	0.2243	-0.0877	-0.1986	-0.1092	-0.1528	-0.2890	-0.6431	-0.1582

Dipole mement (in D)	1.94 (DEN)	2.34	0.01	1.46	1.77	1.99	1.98	3.14	6.93	2.09	

File TZVPMol246.out
Molecule PMol246 trifluoroethene
 SP Mol246 B3LYP/Def2TZVP VAC.
  0 6
Dipole -1.2290 0.1818 0.0000 1.2424
Quadrupole 1.9297 -2.5188 0.5891 1.1632 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.4311	0.0000	0.3763	-0.4937	0.1678	0.5107	0.2060	0.3416	0.6361	1.1924	0.3240
6	-0.7013	-0.6895	0.0000	0.0059	-0.3015	0.0168	-0.1714	-0.0102	-0.1908	0.0388	0.6436	0.0276
9	-0.0891	-1.8741	0.0000	-0.1913	0.1783	-0.1001	-0.1115	-0.1250	-0.0949	-0.2958	-0.6481	-0.1626
9	1.3064	0.5025	0.0000	-0.1548	0.2474	-0.0718	-0.1763	-0.0939	-0.1013	-0.2790	-0.6454	-0.1456
9	-0.5522	1.6223	0.0000	-0.1664	0.2358	-0.0769	-0.1850	-0.0997	-0.1483	-0.2833	-0.6494	-0.1471
1	-1.7783	-0.7058	0.0000	0.1302	0.1337	0.0643	0.1335	0.1228	0.1937	0.1832	0.1073	0.1038

Dipole mement (in D)	1.24 (DEN)	1.62	0.81	0.83	1.17	1.30	1.22	2.59	5.20	1.45	

File TZVPMol247.out
Molecule PMol247 3,3,3-trifluoropropene
 SP Mol247 B3LYP/Def2TZVP VAC.
  0 9
Dipole 0.3662 -2.4031 0.0000 2.4308
Quadrupole 0.7082 2.3135 -3.0217 -0.2612 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.5228	-1.0503	0.0000	-0.1847	-0.1704	-0.0526	-0.3775	-0.1045	-0.2462	-0.2908	-0.0036	-0.0974
6	-0.2995	-2.0835	0.0000	-0.2207	-0.1483	-0.0478	-0.1754	-0.1485	-0.2811	-0.3195	-0.0242	-0.1576
1	-1.3731	-1.9529	0.0000	0.1432	0.1319	0.0491	0.1281	0.1044	0.1675	0.2084	0.0716	0.0879
6	0.0628	0.3655	0.0000	0.5362	-0.6798	0.2742	0.9939	0.3258	0.6582	0.9283	1.7648	0.5199
1	1.5997	-1.1619	0.0000	0.1331	0.1523	0.0559	0.1485	0.1137	0.1723	0.2191	0.0684	0.0935
1	0.0748	-3.0972	0.0000	0.1321	0.1292	0.0537	0.1332	0.1068	0.1683	0.2034	0.0567	0.1043
9	-1.2698	0.4844	0.0000	-0.1814	0.2035	-0.1014	-0.2742	-0.1242	-0.1968	-0.3158	-0.6492	-0.1725

9	0.5228	1.0257	1.0776	-0.1789	0.1908	-0.1155	-0.2884	-0.1368	-0.2210	-0.3166	-0.6423	-0.1891
9	0.5228	1.0257	-1.0776	-0.1789	0.1908	-0.1155	-0.2884	-0.1368	-0.2210	-0.3166	-0.6423	-0.1891

Dipole mement (in D) 2.43 (DEN) 2.18 0.62 1.73 2.09 2.28 2.49 3.83 6.52 2.22

File TZVPMol248.out
Molecule PMol248 fluoroallene
SP Mol248 B3LYP/Def2TZVP VAC.
0 7
Dipole -0.5548 1.6560 0.0000 1.7465
Quadrupole 0.6761 -0.1388 -0.5373 2.5885 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6221	0.0000	0.0093	-0.1133	-0.0335	-0.0091	-0.0439	0.0548	-0.0438	-0.2335	-0.0195
6	0.5686	1.7881	0.0000	-0.2392	-0.1664	-0.0607	-0.2799	-0.1575	-0.3900	-0.3971	0.0513	-0.1639
6	-0.6157	-0.5217	0.0000	0.0363	-0.2804	0.0405	0.0870	0.0098	-0.0664	0.1475	0.5999	0.0575
1	0.8219	2.3003	0.9222	0.1378	0.1364	0.0551	0.1376	0.1078	0.1888	0.2132	0.0692	0.1005
1	0.8219	2.3003	-0.9222	0.1378	0.1364	0.0551	0.1376	0.1078	0.1888	0.2132	0.0692	0.1005
1	-1.6915	-0.6377	0.0000	0.1189	0.1323	0.0587	0.0941	0.1159	0.1464	0.1804	0.0927	0.0984
9	0.0367	-1.6993	0.0000	-0.2009	0.1550	-0.1152	-0.1673	-0.1399	-0.1223	-0.3135	-0.6491	-0.1736

Dipole mement (in D) 1.75 (DEN) 2.30 0.49 1.30 1.64 1.76 1.80 3.12 5.17 1.85

File TZVPMol249.out
Molecule PMol249 fluorobenzene
SP Mol249 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -1.4796 1.4796
Quadrupole -3.6565 4.7543 -1.0978 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.9257	0.3141	-0.2645	0.0942	0.3851	0.1053	0.4060	0.3805	0.5143	0.1836
6	0.0000	1.2112	0.2595	-0.1906	-0.1202	-0.0521	-0.2727	-0.1034	-0.2757	-0.2751	-0.0063	-0.1023
6	0.0000	-1.2112	0.2595	-0.1906	-0.1202	-0.0521	-0.2727	-0.1034	-0.2757	-0.2751	-0.0064	-0.1023
6	0.0000	1.2016	-1.1284	-0.0956	-0.1320	-0.0325	-0.0425	-0.0882	-0.0748	-0.1868	-0.0160	-0.0766
6	0.0000	-1.2016	-1.1284	-0.0956	-0.1320	-0.0325	-0.0425	-0.0882	-0.0748	-0.1868	-0.0161	-0.0766
6	0.0000	0.0000	-1.8244	-0.1205	-0.1484	-0.0463	-0.1212	-0.1023	-0.1743	-0.2259	-0.0228	-0.0917
1	0.0000	2.1325	0.8255	0.1208	0.1496	0.0500	0.1283	0.1072	0.1618	0.2241	0.0568	0.0879
1	0.0000	-2.1325	0.8255	0.1208	0.1496	0.0500	0.1283	0.1072	0.1618	0.2241	0.0568	0.0879
1	0.0000	2.1406	-1.6666	0.1174	0.1447	0.0448	0.1006	0.1010	0.1238	0.2112	0.0369	0.0892
1	0.0000	-2.1406	-1.6666	0.1174	0.1447	0.0448	0.1006	0.1010	0.1238	0.2112	0.0369	0.0892
1	0.0000	0.0000	-2.9061	0.1131	0.1430	0.0418	0.0971	0.0979	0.1277	0.2112	0.0330	0.0861
9	0.0000	0.0000	2.2676	-0.2106	0.1860	-0.1099	-0.1884	-0.1342	-0.2295	-0.3125	-0.6676	-0.1744

Dipole mement (in D) 1.48 (DEN) 1.78 0.16 1.06 1.44 1.53 1.52 2.95 5.23 1.64

File TZVPMol250.out

Molecule PMol250 (trifluoromethyl)benzene
 SP Mol250 B3LYP/Def2TZVP VAC.
  0 15
Dipole 0.1055 2.8481 0.0000 2.8501
Quadrupole -4.8023 0.8824 3.9199 -0.0982 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0311	0.7414	1.2056	-0.1835	-0.0907	-0.0308	-0.0657	-0.0827	-0.1114	-0.1765	-0.0103	-0.0834
6	0.0311	2.1277	1.2026	-0.0899	-0.1280	-0.0309	-0.0826	-0.0868	-0.1127	-0.2007	-0.0152	-0.0766
6	0.0309	2.8212	0.0000	-0.1116	-0.1248	-0.0274	-0.0733	-0.0834	-0.0864	-0.1887	-0.0196	-0.0724
6	0.0311	2.1277	-1.2026	-0.0899	-0.1280	-0.0309	-0.0826	-0.0868	-0.1127	-0.2007	-0.0156	-0.0766
6	0.0311	0.7414	-1.2056	-0.1835	-0.0907	-0.0308	-0.0657	-0.0827	-0.1114	-0.1765	-0.0102	-0.0834
6	0.0335	0.0508	0.0000	0.0631	-0.1298	-0.0271	-0.2572	-0.0300	-0.0219	-0.1489	0.0106	-0.0100
1	0.0364	0.1935	2.1384	0.1338	0.1532	0.0458	0.1063	0.1046	0.1243	0.2249	0.0598	0.0784
1	0.0338	2.6670	2.1407	0.1188	0.1460	0.0468	0.1004	0.1029	0.1197	0.2137	0.0401	0.0917
1	0.0331	3.9036	0.0000	0.1187	0.1455	0.0466	0.0990	0.1027	0.1129	0.2123	0.0391	0.0915
1	0.0338	2.6670	-2.1407	0.1188	0.1460	0.0468	0.1004	0.1029	0.1197	0.2137	0.0401	0.0917
1	0.0364	0.1935	-2.1384	0.1338	0.1532	0.0458	0.1063	0.1046	0.1243	0.2249	0.0598	0.0784
6	-0.0179	-1.4455	0.0000	0.5172	-0.6397	0.2765	0.9788	0.3305	0.5579	0.9540	1.7580	0.5196
9	0.5767	-1.9738	-1.0802	-0.1828	0.1996	-0.1058	-0.2843	-0.1282	-0.1992	-0.3166	-0.6478	-0.1773
9	0.5767	-1.9738	1.0802	-0.1828	0.1996	-0.1058	-0.2843	-0.1282	-0.1992	-0.3166	-0.6478	-0.1773
9	-1.2866	-1.8984	0.0000	-0.1802	0.1889	-0.1186	-0.2953	-0.1394	-0.2038	-0.3184	-0.6419	-0.1945

Dipole mement (in D)	2.85 (DEN)	2.40	0.70	2.10	2.71	2.67	2.91	4.21	7.16	2.60

File TZVPMol251.out
Molecule PMol251 ortho-fluorotoluene
 SP Mol251 B3LYP/Def2TZVP VAC.
  0 15
Dipole -0.6573 -1.0019 0.0000 1.1983
Quadrupole 1.9880 1.5445 -3.5325 -2.9032 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.6210	-0.6058	-0.0000	0.0261	-0.1547	-0.0060	0.0268	-0.0189	0.1622	-0.0834	0.0152	0.0221
6	0.3656	0.7604	0.0000	0.2893	-0.2335	0.0893	0.3289	0.1023	0.2960	0.3803	0.4944	0.1745
6	-0.4907	-1.4441	-0.0000	-0.1470	-0.1114	-0.0397	-0.1092	-0.0934	-0.2394	-0.1865	-0.0241	-0.0896
6	-0.9059	1.2966	0.0000	-0.2080	-0.1211	-0.0540	-0.2699	-0.1051	-0.2857	-0.2681	-0.0058	-0.1037
6	-1.7842	-0.9391	-0.0000	-0.1217	-0.1479	-0.0481	-0.1182	-0.1041	-0.1724	-0.2183	-0.0244	-0.0930
6	-1.9922	0.4322	-0.0000	-0.0948	-0.1387	-0.0390	-0.0613	-0.0947	-0.1311	-0.1978	-0.0177	-0.0832
9	1.4190	1.5986	0.0000	-0.2152	0.1849	-0.1069	-0.1778	-0.1318	-0.2119	-0.3186	-0.6679	-0.1702
1	-0.3293	-2.5159	-0.0000	0.1092	0.1454	0.0400	0.0988	0.0969	0.1598	0.2058	0.0278	0.0832
1	-1.0296	2.3708	0.0000	0.1167	0.1494	0.0487	0.1266	0.1060	0.1768	0.2231	0.0546	0.0863
1	-2.6274	-1.6170	-0.0000	0.1093	0.1427	0.0407	0.0973	0.0968	0.1446	0.2102	0.0310	0.0847
1	-2.9968	0.8342	-0.0000	0.1140	0.1435	0.0431	0.1004	0.0992	0.1448	0.2107	0.0346	0.0872
6	2.0226	-1.1189	0.0000	-0.3399	-0.2474	-0.0818	-0.4000	-0.2256	-0.4127	-0.6085	0.0258	-0.2517
1	2.5767	-0.7705	0.8719	0.1246	0.1314	0.0385	0.1205	0.0914	0.1270	0.2206	0.0239	0.0827
1	2.0419	-2.2061	-0.0000	0.1128	0.1260	0.0367	0.1165	0.0896	0.1149	0.2101	0.0091	0.0883
1	2.5767	-0.7705	-0.8719	0.1246	0.1314	0.0385	0.1205	0.0914	0.1270	0.2206	0.0239	0.0827

Dipole mement (in D) 1.20 (DEN) 1.39 1.03 0.81 1.12 1.25 1.23 2.71 4.84 1.40

File TZVPMol252.out
Molecule PMol252 meta-fluorotoluene
SP Mol252 B3LYP/Def2TZVP VAC.
0 15
Dipole -1.5930 0.6340 0.0000 1.7145
Quadrupole 0.2379 2.9345 -3.1724 3.2270 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1944	-0.1973	-0.0000	0.1819	-0.1633	0.0132	0.2052	-0.0043	0.3966	0.0019	0.0048	0.0458
6	-0.0429	-0.9846	-0.0000	-0.2745	-0.0954	-0.0585	-0.3356	-0.1075	-0.4888	-0.2767	-0.0140	-0.1144
6	-1.0540	1.1884	-0.0000	-0.1932	-0.1272	-0.0525	-0.1776	-0.1064	-0.3724	-0.2261	-0.0289	-0.1038
6	1.1957	-0.3764	0.0000	0.3471	-0.2636	0.0928	0.3957	0.1039	0.4989	0.3896	0.5124	0.1824
6	0.2035	1.7775	0.0000	-0.0810	-0.1315	-0.0342	-0.0315	-0.0898	-0.0251	-0.1790	-0.0174	-0.0780
6	1.3497	0.9979	0.0000	-0.2175	-0.1262	-0.0581	-0.2851	-0.1093	-0.3949	-0.2851	-0.0083	-0.1082
1	-0.1028	-2.0657	-0.0000	0.1122	0.1516	0.0468	0.1345	0.1048	0.2008	0.2172	0.0489	0.0837
1	-1.9406	1.8105	-0.0000	0.1042	0.1438	0.0373	0.1005	0.0942	0.1689	0.2062	0.0244	0.0805
9	2.2931	-1.1497	0.0000	-0.2123	0.1846	-0.1113	-0.1880	-0.1355	-0.2348	-0.3140	-0.6684	-0.1755
1	0.2932	2.8562	-0.0000	0.1146	0.1445	0.0438	0.1002	0.1000	0.1329	0.2105	0.0351	0.0880
1	2.3404	1.4300	0.0000	0.1184	0.1485	0.0485	0.1279	0.1058	0.1908	0.2238	0.0549	0.0863
6	-2.5444	-0.8423	0.0000	-0.3597	-0.2499	-0.0801	-0.4051	-0.2253	-0.4241	-0.6115	0.0171	-0.2488
1	-2.6822	-1.4795	0.8742	0.1227	0.1293	0.0379	0.1213	0.0901	0.1202	0.2162	0.0154	0.0870
1	-3.3426	-0.1035	-0.0001	0.1145	0.1256	0.0365	0.1163	0.0893	0.1109	0.2108	0.0088	0.0881
1	-2.6821	-1.4796	-0.8741	0.1227	0.1293	0.0379	0.1213	0.0901	0.1202	0.2162	0.0154	0.0870

Dipole mement (in D) 1.71 (DEN) 2.09 0.85 1.31 1.53 1.82 1.76 3.14 5.45 1.85

File TZVPMol253.out
Molecule PMol253 para-fluorotoluene
SP Mol253 B3LYP/Def2TZVP VAC.
0 15
Dipole 1.8803 0.0000 0.0226 1.8804
Quadrupole -1.8361 4.7657 -2.9296 0.0000 0.0650 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.3559	0.0000	-0.0107	0.1484	-0.1747	0.0012	0.1390	-0.0165	0.2634	-0.0395	-0.0001	0.0323
6	0.6377	1.1946	-0.0096	-0.1611	-0.1087	-0.0382	-0.0997	-0.0917	-0.2222	-0.1855	-0.0228	-0.0883
6	0.6377	-1.1946	-0.0096	-0.1611	-0.1087	-0.0382	-0.0997	-0.0917	-0.2222	-0.1855	-0.0227	-0.0883
6	-0.7495	1.2071	-0.0014	-0.1824	-0.1196	-0.0534	-0.2634	-0.1045	-0.2558	-0.2669	-0.0068	-0.1032
6	-0.7495	-1.2071	-0.0014	-0.1824	-0.1196	-0.0534	-0.2634	-0.1045	-0.2558	-0.2669	-0.0069	-0.1032
6	-1.4209	0.0000	0.0038	0.3031	-0.2682	0.0889	0.3733	0.1000	0.3694	0.3714	0.5115	0.1778
1	1.1736	2.1367	-0.0176	0.1095	0.1460	0.0410	0.1036	0.0979	0.1479	0.2061	0.0286	0.0844
1	1.1736	-2.1367	-0.0176	0.1095	0.1460	0.0410	0.1036	0.0979	0.1479	0.2061	0.0286	0.0844
1	-1.3093	2.1323	-0.0034	0.1174	0.1494	0.0491	0.1276	0.1064	0.1646	0.2232	0.0548	0.0868
1	-1.3093	-2.1323	-0.0034	0.1174	0.1494	0.0491	0.1276	0.1064	0.1646	0.2232	0.0548	0.0868
9	-2.7638	0.0000	0.0083	-0.2132	0.1825	-0.1127	-0.1903	-0.1368	-0.2275	-0.3141	-0.6686	-0.1768
6	2.8525	0.0000	0.0113	-0.3612	-0.2538	-0.0817	-0.4014	-0.2268	-0.4074	-0.6077	0.0184	-0.2498

1	3.2358	-0.0000	1.0336	0.1229	0.1284	0.0360	0.1154	0.0878	0.1150	0.2141	0.0133	0.0842
1	3.2636	-0.8801	-0.4803	0.1167	0.1259	0.0357	0.1139	0.0882	0.1091	0.2111	0.0085	0.0864
1	3.2636	0.8801	-0.4803	0.1167	0.1259	0.0357	0.1139	0.0882	0.1091	0.2111	0.0085	0.0864

Dipole mement (in D) 1.88 (DEN) 2.43 0.70 1.45 1.60 2.00 1.92 3.30 5.65 2.00

File TZVPMol254.out
Molecule PMol254 1,3-difluorobenzene
SP Mol254 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 1.4612 1.4612
Quadrupole -1.7768 -3.1413 4.9181 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	1.1794	-0.3044	0.3118	-0.2620	0.1005	0.4259	0.1121	0.4791	0.3994	0.5350	0.1907
6	0.0000	0.0000	-1.0262	-0.2508	-0.0970	-0.0647	-0.4501	-0.1109	-0.4737	-0.3418	0.0143	-0.1210
6	0.0000	1.2087	1.0781	-0.1950	-0.1270	-0.0587	-0.2986	-0.1100	-0.3915	-0.2939	-0.0017	-0.1101
6	0.0000	-1.1794	-0.3044	0.3118	-0.2620	0.1005	0.4259	0.1121	0.4791	0.3994	0.5354	0.1907
6	0.0000	0.0000	1.7599	-0.0876	-0.1233	-0.0254	0.0053	-0.0808	0.0088	-0.1675	-0.0047	-0.0697
6	0.0000	-1.2087	1.0781	-0.1950	-0.1270	-0.0587	-0.2986	-0.1100	-0.3915	-0.2939	-0.0015	-0.1101
1	0.0000	0.0000	-2.1057	0.1350	0.1572	0.0597	0.1654	0.1181	0.2189	0.2398	0.0845	0.0921
1	0.0000	2.1577	1.5942	0.1253	0.1508	0.0515	0.1336	0.1088	0.1898	0.2278	0.0612	0.0898
9	0.0000	-2.3358	-0.9784	-0.2032	0.1959	-0.1028	-0.1759	-0.1272	-0.2198	-0.3063	-0.6645	-0.1682
1	0.0000	0.0000	2.8417	0.1257	0.1478	0.0495	0.1092	0.1058	0.1310	0.2155	0.0457	0.0943
1	0.0000	-2.1577	1.5942	0.1253	0.1508	0.0515	0.1336	0.1088	0.1898	0.2278	0.0612	0.0898
9	0.0000	2.3358	-0.9784	-0.2032	0.1959	-0.1028	-0.1759	-0.1272	-0.2198	-0.3063	-0.6645	-0.1682

Dipole mement (in D) 1.46 (DEN) 1.74 0.22 1.03 1.44 1.51 1.50 2.94 5.26 1.62

File TZVPMol255.out
Molecule PMol255 1,2,3,4-tetrafluorobenze
SP Mol255 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -2.3477 2.3477
Quadrupole 1.2553 -5.3444 4.0892 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6932	0.6838	0.1820	-0.2368	0.0769	0.1275	0.0994	0.1235	0.2703	0.6199	0.1529
6	0.0000	-0.6932	0.6838	0.1820	-0.2368	0.0769	0.1275	0.0994	0.1235	0.2703	0.6197	0.1529
6	0.0000	1.3770	-0.5242	0.2226	-0.2580	0.0818	0.2464	0.0987	0.2549	0.3160	0.5822	0.1642
6	0.0000	-1.3770	-0.5242	0.2226	-0.2580	0.0818	0.2464	0.0987	0.2549	0.3160	0.5820	0.1642
6	0.0000	0.6942	-1.7233	-0.1811	-0.1119	-0.0466	-0.2300	-0.0972	-0.2987	-0.2600	0.0160	-0.0977
6	0.0000	-0.6942	-1.7233	-0.1811	-0.1119	-0.0466	-0.2300	-0.0972	-0.2987	-0.2600	0.0159	-0.0977
9	0.0000	-1.3515	1.8333	-0.1731	0.2352	-0.0802	-0.1325	-0.1029	-0.1259	-0.2722	-0.6415	-0.1559
9	0.0000	2.7087	-0.4969	-0.1883	0.2151	-0.0915	-0.1560	-0.1150	-0.1666	-0.2880	-0.6518	-0.1623
9	0.0000	-2.7087	-0.4969	-0.1883	0.2151	-0.0915	-0.1560	-0.1150	-0.1666	-0.2880	-0.6518	-0.1623
1	0.0000	1.2557	-2.6460	0.1379	0.1564	0.0596	0.1446	0.1171	0.2129	0.2339	0.0754	0.0988
1	0.0000	-1.2557	-2.6460	0.1379	0.1564	0.0596	0.1446	0.1171	0.2129	0.2339	0.0754	0.0988

9	0.0000	1.3515	1.8333	-0.1731	0.2352	-0.0802	-0.1325	-0.1029	-0.1259	-0.2722	-0.6415	-0.1559

Dipole mement (in D) 2.35 (DEN) 2.58 0.74 1.63 1.86 2.47 2.36 4.88 9.23 2.69

File TZVPMol256.out
Molecule PMol256 1,2-difluorobenzene
SP Mol256 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 2.4522 2.4522
Quadrupole -2.5115 3.1360 -0.6245 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6938	-0.5335	0.2351	-0.2533	0.0833	0.2415	0.0998	0.2603	0.3183	0.5615	0.1658
6	0.0000	-0.6938	-0.5335	0.2351	-0.2533	0.0833	0.2415	0.0998	0.2603	0.3183	0.5619	0.1658
6	0.0000	1.3934	0.6568	-0.1786	-0.1133	-0.0467	-0.2367	-0.0977	-0.2427	-0.2602	0.0007	-0.0967
6	0.0000	-1.3934	0.6568	-0.1786	-0.1133	-0.0467	-0.2367	-0.0977	-0.2427	-0.2602	0.0008	-0.0967
6	0.0000	0.6937	1.8564	-0.1100	-0.1395	-0.0391	-0.0782	-0.0948	-0.1451	-0.2057	-0.0107	-0.0845
6	0.0000	-0.6937	1.8564	-0.1100	-0.1395	-0.0391	-0.0782	-0.0948	-0.1451	-0.2057	-0.0108	-0.0845
9	0.0000	-1.3416	-1.6994	-0.1945	0.2077	-0.0976	-0.1637	-0.1210	-0.1878	-0.2941	-0.6560	-0.1678
1	0.0000	2.4743	0.6255	0.1279	0.1526	0.0540	0.1317	0.1113	0.1715	0.2271	0.0634	0.0924
1	0.0000	-2.4743	0.6255	0.1279	0.1526	0.0540	0.1317	0.1113	0.1715	0.2271	0.0634	0.0924
1	0.0000	1.2382	2.7907	0.1201	0.1458	0.0461	0.1055	0.1023	0.1437	0.2147	0.0411	0.0908
1	0.0000	-1.2382	2.7907	0.1201	0.1458	0.0461	0.1055	0.1023	0.1437	0.2147	0.0411	0.0908
9	0.0000	1.3416	-1.6994	-0.1945	0.2077	-0.0976	-0.1637	-0.1210	-0.1878	-0.2941	-0.6560	-0.1678

Dipole mement (in D) 2.45 (DEN) 2.87 0.47 1.73 2.17 2.57 2.50 4.98 9.12 2.76

File TZVPMol257.out
Molecule PMol257 fluoroacetylene
SP Mol257 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 -0.5417 0.5417
Quadrupole -1.3506 -1.3506 2.7012 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-1.2839	-0.2973	-0.1543	-0.1335	-0.4647	-0.1839	-0.5997	-0.4034	0.2251	-0.1896
6	0.0000	0.0000	-0.0911	0.2385	-0.2792	0.0583	0.2902	0.0780	0.3016	0.4046	0.2573	0.1360
9	0.0000	0.0000	1.1770	-0.1364	0.3051	-0.0148	-0.0605	-0.0385	-0.0467	-0.2403	-0.6597	-0.0828
1	0.0000	0.0000	-2.3434	0.1952	0.1284	0.0901	0.2350	0.1444	0.3448	0.2392	0.1775	0.1364

Dipole mement (in D) 0.54 (DEN) 1.24 1.35 0.30 0.25 0.74 0.58 1.74 7.23 0.89

File TZVPMol258.out
Molecule PMol258 acetyl_fluoride
SP Mol258 B3LYP/Def2TZVP VAC.
0 7
Dipole -2.9202 0.6414 0.0002 2.9898

Quadrupole 0.7118 -2.4661 1.7544 0.9419 0.0002 -0.0006

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.7837	-1.0642	-0.0003	0.1366	0.1377	0.0563	0.1662	0.1115	0.1486	0.2352	0.0557	0.1030
6	-1.3557	-0.0686	-0.0000	-0.3318	-0.2589	-0.0734	-0.6042	-0.2144	-0.4969	-0.7236	0.0194	-0.2464
6	0.1258	-0.1394	0.0000	0.3274	-0.5016	0.2488	0.8869	0.2946	0.7795	0.8506	1.6090	0.4744
8	0.8359	-1.0834	-0.0002	-0.2246	0.1731	-0.2326	-0.5226	-0.2797	-0.4757	-0.5078	-1.1599	-0.3636
1	-1.6987	0.4826	0.8735	0.1410	0.1437	0.0589	0.1647	0.1125	0.1594	0.2427	0.0583	0.1072
1	-1.6986	0.4831	-0.8732	0.1410	0.1437	0.0589	0.1647	0.1125	0.1594	0.2427	0.0583	0.1072
9	0.6525	1.1126	0.0001	-0.1896	0.1622	-0.1167	-0.2556	-0.1371	-0.2744	-0.3397	-0.6418	-0.1819

Dipole mement (in D) 2.99 (DEN) 2.61 1.00 2.16 2.69 2.82 3.00 3.88 7.41 2.85

File TZVPMol259.out
Molecule PMol259 3,3,3-trifluoropropyne
SP Mol259 B3LYP/Def2TZVP VAC.
0 7
Dipole -2.3698 0.0000 0.0000 2.3698
Quadrupole 6.0367 -3.0182 -3.0185 0.0015 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-2.3208	-0.0001	0.0000	0.0147	-0.0199	-0.0386	-0.1079	-0.0894	-0.2889	-0.1238	-0.1020	-0.0967
6	-1.1250	0.0000	0.0000	-0.2427	-0.0644	-0.0589	-0.2887	-0.0564	-0.0983	-0.1380	-0.0789	-0.0654
1	-3.3835	-0.0004	0.0000	0.2097	0.1349	0.1064	0.2123	0.1602	0.2994	0.2386	0.1910	0.1554
6	0.3297	0.0000	0.0000	0.5026	-0.6916	0.2927	1.0197	0.3492	0.6996	0.9166	1.8828	0.5385
9	0.8178	1.2460	0.0000	-0.1614	0.2137	-0.1005	-0.2784	-0.1212	-0.2037	-0.2978	-0.6311	-0.1772
9	0.8178	-0.6230	1.0791	-0.1614	0.2137	-0.1005	-0.2785	-0.1212	-0.2041	-0.2978	-0.6310	-0.1773
9	0.8178	-0.6230	-1.0791	-0.1614	0.2137	-0.1005	-0.2785	-0.1212	-0.2041	-0.2978	-0.6310	-0.1773

Dipole mement (in D) 2.37 (DEN) 3.37 0.20 1.70 2.35 2.18 2.41 3.81 6.00 2.33

File TZVPMol260.out
Molecule PMol260 tetrafluoropropyne
SP Mol260 B3LYP/Def2TZVP VAC.
0 7
Dipole -0.2762 1.9490 0.0000 1.9685
Quadrupole -0.6918 1.4277 -0.7359 -0.3080 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.2506	1.7649	0.0000	0.4752	-0.1936	0.1064	0.3822	0.1296	0.3078	0.4937	0.3465	0.1771
6	-0.0830	0.5854	0.0000	-0.4113	-0.0803	-0.0946	-0.5712	-0.0883	-0.3958	-0.2985	0.3127	-0.1113
9	-0.4270	3.0126	0.0000	-0.1053	0.3355	0.0081	-0.0460	-0.0159	-0.0284	-0.2208	-0.6495	-0.0627
6	0.1206	-0.8499	0.0000	0.5314	-0.6927	0.2905	1.0528	0.3469	0.6995	0.9253	1.8855	0.5366
9	1.4230	-1.1628	0.0000	-0.1633	0.2104	-0.1035	-0.2726	-0.1241	-0.1932	-0.2999	-0.6317	-0.1798
9	-0.4270	-1.4250	1.0787	-0.1634	0.2104	-0.1035	-0.2726	-0.1241	-0.1949	-0.2999	-0.6317	-0.1799
9	-0.4270	-1.4250	-1.0787	-0.1634	0.2104	-0.1035	-0.2726	-0.1241	-0.1949	-0.2999	-0.6317	-0.1799

Dipole mement (in D) 1.97 (DEN) 2.35 1.78 1.58 1.94 1.61 2.00 2.18 1.11 1.57

File TZVPMol261.out
Molecule PMol261 carbonyl_fluoride
SP Mol261 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 -1.0947 1.0947
Quadrupole 2.2313 -0.1001 -2.1312 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.1439	0.4792	-0.6716	0.3431	1.0892	0.4236	0.8270	1.0941	2.4023	0.6287
8	0.0000	0.0000	1.3144	-0.2027	0.1869	-0.2176	-0.5827	-0.2610	-0.4436	-0.5180	-1.1474	-0.3546
9	0.0000	1.0572	-0.6322	-0.1383	0.2424	-0.0627	-0.2532	-0.0813	-0.1917	-0.2881	-0.6274	-0.1371
9	0.0000	-1.0572	-0.6322	-0.1383	0.2424	-0.0627	-0.2532	-0.0813	-0.1917	-0.2881	-0.6274	-0.1371
Dipole mement (in D)	1.09 (DEN)			0.11	0.76	0.76	1.39	0.86	1.06	0.76	1.77	0.97

File TZVPMol262.out
Molecule PMol262 bis(trifluoromethyl)ethe
SP Mol262 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0000 0.0000 0.0393 0.0393
Quadrupole 0.1421 0.0763 -0.2184 -0.1528 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.0000	-0.0001	0.7755	-0.2465	0.2914	-0.1489	-0.7388	-0.2069	-0.3134	-0.5190	-1.0391	-0.2997
6	-1.1856	0.0044	0.0791	0.5723	-0.8377	0.3421	1.2259	0.4262	0.6044	1.1398	2.4144	0.6638
6	1.1856	-0.0044	0.0791	0.5723	-0.8377	0.3421	1.2259	0.4262	0.6291	1.1398	2.4134	0.6638
9	-2.1175	0.3723	0.9322	-0.1440	0.2425	-0.0822	-0.2676	-0.1005	-0.1402	-0.2851	-0.6328	-0.1636
9	-1.1630	0.8479	-0.9450	-0.1542	0.2258	-0.0908	-0.2967	-0.1094	-0.1563	-0.2989	-0.6316	-0.1741
9	-1.4790	-1.2021	-0.3847	-0.1508	0.2238	-0.0946	-0.2922	-0.1129	-0.1548	-0.2964	-0.6301	-0.1763
9	1.1630	-0.8477	-0.9451	-0.1542	0.2258	-0.0908	-0.2967	-0.1094	-0.1611	-0.2989	-0.6316	-0.1741
9	2.1175	-0.3725	0.9322	-0.1440	0.2425	-0.0822	-0.2676	-0.1005	-0.1474	-0.2851	-0.6328	-0.1636
9	1.4790	1.2022	-0.3845	-0.1508	0.2238	-0.0946	-0.2922	-0.1129	-0.1603	-0.2964	-0.6301	-0.1763
Dipole mement (in D)	0.04 (DEN)			0.18	0.26	0.14	0.44	0.06	0.04	0.19	0.36	0.16

File TZVPMol263.out
Molecule PMol263 cyanic_fluoride
SP Mol263 B3LYP/Def2TZVP VAC.
0 3
Dipole 0.0000 0.0000 2.3213 2.3213
Quadrupole 1.3243 1.3243 -2.6485 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	1.1108	-0.0885	0.3403	0.0208	-0.0755	0.0007	-0.0441	-0.2193	-0.6428	-0.0486
6	0.0000	0.0000	-0.1466	0.1565	-0.3750	0.1945	0.5635	0.3355	0.5083	0.6232	1.7176	0.4187
7	0.0000	0.0000	-1.3025	-0.0680	0.0347	-0.2154	-0.4880	-0.3363	-0.4642	-0.4039	-1.0747	-0.3701
Dipole mement (in D)	2.32 (DEN)			0.16	1.86	1.32	2.25	1.87	2.31	0.92	2.08	1.76

File TZVPMol264.out
Molecule PMol264 trifluroacetonitrile
SP Mol264 B3LYP/Def2TZVP VAC.
0 6
Dipole 1.3480 0.0004 0.0000 1.3480
Quadrupole -4.1251 2.0626 2.0626 -0.0016 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1543	-0.0001	0.0000	-0.2466	-0.1367	0.0686	0.0415	0.1931	0.2548	0.1550	0.9729	0.2051
6	0.3215	0.0001	0.0000	0.6221	-0.7084	0.3115	0.9808	0.3725	0.5549	0.9060	1.9677	0.5630
9	0.7828	1.2463	0.0000	-0.1405	0.2393	-0.0798	-0.2666	-0.1005	-0.1599	-0.2802	-0.6233	-0.1581
9	0.7828	-0.6230	1.0793	-0.1405	0.2393	-0.0798	-0.2666	-0.1005	-0.1601	-0.2801	-0.6233	-0.1581
9	0.7828	-0.6230	-1.0793	-0.1405	0.2393	-0.0798	-0.2666	-0.1005	-0.1601	-0.2801	-0.6233	-0.1581
7	-2.3054	-0.0004	0.0000	0.0459	0.1271	-0.1406	-0.2226	-0.2640	-0.3296	-0.2206	-1.0706	-0.2937
Dipole mement (in D)	1.35 (DEN)			0.24	0.96	0.76	0.74	1.29	1.29	0.18	2.47	1.20

File TZVPMol265.out
Molecule PMol265 1-fluoro-4-nitrobenzene
SP Mol265 B3LYP/Def2TZVP VAC.
0 14
Dipole 3.3018 0.0000 0.0001 3.3018
Quadrupole -11.3758 8.4246 2.9512 0.0000 -0.0002 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0030	1.2134	0.0000	-0.1449	-0.0805	-0.0173	-0.0609	-0.0641	-0.1463	-0.1617	0.0195	-0.0619
6	1.3856	1.2153	0.0000	-0.1603	-0.1026	-0.0393	-0.2642	-0.0900	-0.2256	-0.2682	0.0123	-0.0915
6	2.0508	0.0000	0.0000	0.3221	-0.2504	0.1133	0.4085	0.1250	0.3758	0.4099	0.5426	0.2039
6	1.3856	-1.2153	0.0000	-0.1603	-0.1026	-0.0393	-0.2642	-0.0900	-0.2256	-0.2682	0.0122	-0.0915
6	0.0030	-1.2134	0.0000	-0.1449	-0.0805	-0.0173	-0.0609	-0.0641	-0.1463	-0.1617	0.0196	-0.0619
6	-0.6681	0.0000	0.0000	0.0676	-0.1626	0.0201	-0.0220	0.0718	0.0675	0.0054	0.2176	0.1157
1	-0.5659	2.1315	0.0000	0.1669	0.1614	0.0561	0.1347	0.1208	0.1638	0.2494	0.1042	0.0890
1	1.9516	2.1359	0.0000	0.1367	0.1560	0.0597	0.1421	0.1172	0.1683	0.2342	0.0749	0.0991
1	1.9516	-2.1359	0.0000	0.1367	0.1560	0.0597	0.1421	0.1172	0.1683	0.2342	0.0749	0.0991
1	-0.5659	-2.1315	0.0000	0.1669	0.1614	0.0561	0.1347	0.1208	0.1638	0.2494	0.1042	0.0890
9	3.3833	0.0000	-0.0000	-0.1893	0.2117	-0.0910	-0.1695	-0.1158	-0.2026	-0.2970	-0.6604	-0.1576
7	-2.1371	0.0000	0.0000	0.4233	-0.0247	0.2437	0.7315	0.0783	0.6470	0.5033	0.4375	0.2248
8	-2.7013	-1.0848	-0.0000	-0.3103	-0.0213	-0.2022	-0.4260	-0.1634	-0.4041	-0.3645	-0.4798	-0.2280
8	-2.7013	1.0848	-0.0000	-0.3103	-0.0213	-0.2022	-0.4260	-0.1634	-0.4041	-0.3645	-0.4798	-0.2280
Dipole mement (in D)	3.30 (DEN)			3.11	2.98	2.61	3.30	2.90	3.29	2.95	2.88	2.84

File TZVPMol322.out
Molecule PMol322 SiH
SP Mol322 B3LYP/Def2TZVP VAC.
0 2

Dipole 0.0000 0.0000 -0.0864 0.0864
Quadrupole -1.4901 3.1347 -1.6445 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0000	0.0000	0.1013	0.0480	0.0868	0.1224	0.2628	0.0492	0.1257	0.3489	0.7115	0.0523
1	0.0000	0.0000	-1.4176	-0.0480	-0.0868	-0.1224	-0.2628	-0.0492	-0.1257	-0.3489	-0.7115	-0.0523

Dipole mement (in D) 0.09 (DEN) 0.35 0.63 0.89 1.92 0.36 0.92 2.55 5.19 0.38

File TZVPMol323.out
Molecule PMol323 SiS
SP Mol323 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 -1.7688 1.7688
Quadrupole 0.2180 0.2180 -0.4360 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0000	0.0000	-1.0301	0.2320	-0.1217	0.2221	0.3973	0.1805	0.3130	0.6562	1.1758	0.2035
16	0.0000	0.0000	0.9014	-0.2320	0.1217	-0.2221	-0.3973	-0.1805	-0.3130	-0.6562	-1.1758	-0.2035

Dipole mement (in D) 1.77 (DEN) 2.15 1.13 2.06 3.69 1.67 2.90 6.09 10.91 1.89

File TZVPMol324.out
Molecule PMol324 silyl_radical
SP Mol324 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 -0.0001 -0.0927 0.0927
Quadrupole 0.1063 0.1062 -0.2125 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.0000	0.0000	-0.0811	0.0904	0.1570	0.2165	0.6570	-0.0275	0.3371	0.5478	2.0004	-0.0316
1	-1.1446	-0.8107	0.3786	-0.0301	-0.0523	-0.0722	-0.2190	0.0092	-0.1153	-0.1826	-0.6668	0.0105
1	1.2744	-0.5858	0.3786	-0.0301	-0.0523	-0.0722	-0.2190	0.0092	-0.1108	-0.1826	-0.6668	0.0105
1	-0.1298	1.3965	0.3788	-0.0301	-0.0523	-0.0722	-0.2190	0.0092	-0.1109	-0.1826	-0.6668	0.0105

Dipole mement (in D) 0.09 (DEN) 0.20 0.35 0.48 1.45 0.06 0.75 1.21 4.42 0.07

File TZVPMol325.out
Molecule PMol325 silylmethyl_radical
SP Mol325 B3LYP/Def2TZVP VAC.
0 7
Dipole -0.6762 0.0000 0.0395 0.6774
Quadrupole 0.6702 0.4580 -1.1282 0.0000 -0.1096 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2612	-0.0000	-0.0042	-0.3794	-0.3142	-0.1296	-0.5852	-0.1895	-0.5712	-0.7016	-0.8283	-0.1751
1	-1.8535	0.9073	0.0171	0.1319	0.1093	0.0367	0.1411	0.0904	0.1717	0.1867	0.0503	0.0925
1	-1.8535	-0.9073	0.0171	0.1319	0.1093	0.0367	0.1411	0.0904	0.1717	0.1867	0.0503	0.0925
14	0.5712	0.0000	-0.0017	0.2853	0.2207	0.2931	1.1165	0.0006	0.9005	0.8328	2.7407	-0.0133

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   1      1.0854    1.2057   -0.6824   -0.0576   -0.0426   -0.0790   -0.2716    0.0029   -0.2258   -0.1693   -0.6743    0.0014
   1      1.1067   -0.0001    1.3800   -0.0545   -0.0399   -0.0787   -0.2703    0.0022   -0.2211   -0.1660   -0.6646    0.0007
   1      1.0854   -1.2056   -0.6826   -0.0576   -0.0426   -0.0790   -0.2716    0.0029   -0.2258   -0.1693   -0.6743    0.0014

 Dipole mement (in D)   0.68 (DEN)      0.16      0.10      0.31      0.17      0.42      0.66      0.57      1.08      0.60

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File TZVPMol326.out
Molecule PMol326    methylsilane
 SP Mol326 B3LYP/Def2TZVP VAC.
    0    8
Dipole          0.8005    0.0001    0.0000    0.8005
Quadrupole     -0.1849    0.0925    0.0924   -0.0001    0.0000    0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      1.2331    0.0000   -0.0000   -0.4601   -0.4799   -0.1730   -0.8051   -0.2824   -0.3849   -1.0699   -0.7408   -0.2852
   1      1.6292   -1.0127    0.0513    0.1250    0.1254    0.0381    0.1569    0.0928    0.0812    0.2337    0.0204    0.0974
   1      1.6293    0.5508    0.8514    0.1250    0.1254    0.0381    0.1569    0.0928    0.0825    0.2337    0.0204    0.0974
   1      1.6293    0.4619   -0.9027    0.1250    0.1254    0.0381    0.1569    0.0928    0.0812    0.2337    0.0204    0.0974
  14     -0.6308    0.0000    0.0000    0.2728    0.2456    0.3088    1.1830    0.0087    0.7611    0.9010    2.7252    0.0014
   1     -1.1518   -0.6299    1.2311   -0.0625   -0.0473   -0.0833   -0.2829   -0.0016   -0.2061   -0.1774   -0.6816   -0.0029
   1     -1.1518    1.3811   -0.0701   -0.0625   -0.0473   -0.0833   -0.2829   -0.0016   -0.2062   -0.1774   -0.6816   -0.0029
   1     -1.1518   -0.7512   -1.1610   -0.0625   -0.0473   -0.0833   -0.2829   -0.0016   -0.2089   -0.1774   -0.6816   -0.0029

 Dipole mement (in D)   0.80 (DEN)      0.42      0.14      0.32      0.03      0.51      0.77      0.63      0.85      0.64

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File TZVPMol327.out
Molecule PMol327    dimethylsilane
 SP Mol327 B3LYP/Def2TZVP VAC.
    0   11
Dipole          0.0000   -0.7723    0.0000    0.7723
Quadrupole     -0.0886   -0.7179    0.8066    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1      1.1938    1.4252    0.0000   -0.0731   -0.0421   -0.0914   -0.3153   -0.0094   -0.2314   -0.1955   -0.6891   -0.0148
  14      0.0000    0.5492    0.0000    0.3450    0.2582    0.3282    1.3684    0.0539    0.8454    1.1623    2.7612    0.0524
   1     -1.1938    1.4252    0.0000   -0.0731   -0.0421   -0.0914   -0.3153   -0.0094   -0.2328   -0.1955   -0.6891   -0.0148
   6      0.0000   -0.5092    1.5368   -0.4613   -0.4608   -0.1777   -0.8418   -0.2869   -0.5158   -1.0793   -0.7348   -0.2919
   6      0.0000   -0.5092   -1.5368   -0.4613   -0.4608   -0.1777   -0.8418   -0.2869   -0.5158   -1.0793   -0.7344   -0.2919
   1     -0.8780   -1.1534    1.5727    0.1188    0.1243    0.0346    0.1575    0.0894    0.1105    0.2298    0.0130    0.0928
   1     -0.0000    0.0930    2.4438    0.1243    0.1252    0.0359    0.1579    0.0906    0.1054    0.2340    0.0173    0.0949
   1      0.8780   -1.1534    1.5727    0.1188    0.1243    0.0346    0.1575    0.0894    0.1092    0.2298    0.0130    0.0928
   1     -0.8780   -1.1534   -1.5727    0.1188    0.1243    0.0346    0.1575    0.0894    0.1105    0.2298    0.0130    0.0928
   1      0.8780   -1.1534   -1.5727    0.1188    0.1243    0.0346    0.1575    0.0894    0.1092    0.2298    0.0130    0.0928
   1     -0.0000    0.0930   -2.4438    0.1243    0.1252    0.0359    0.1579    0.0906    0.1054    0.2340    0.0173    0.0949

 Dipole mement (in D)   0.77 (DEN)      0.36      0.28      0.25      0.06      0.48      0.77      0.78      1.17      0.61

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File TZVPMol328.out
Molecule PMol328 ethylsilane
 SP Mol328 B3LYP/Def2TZVP VAC.
  0 11
Dipole -0.3389 0.8008 0.0000 0.8696
Quadrupole -0.3847 -0.0791 0.4638 0.4187 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.5237	0.8289	0.0000	-0.3370	-0.3274	-0.0800	-0.2712	-0.2273	-0.0947	-0.5892	0.0185	-0.2379
6	0.0000	0.8673	0.0000	-0.2823	-0.4334	-0.1309	-0.6117	-0.2019	-0.0697	-0.8253	-0.6873	-0.1757
14	0.7978	-0.8264	0.0000	0.2603	0.2713	0.3023	1.1537	0.0029	0.6923	0.8963	2.7115	-0.0073
1	0.3649	1.4210	0.8683	0.1054	0.1379	0.0338	0.1316	0.0920	0.0025	0.2232	0.0042	0.0905
1	0.3649	1.4210	-0.8683	0.1054	0.1379	0.0338	0.1316	0.0920	0.0025	0.2232	0.0042	0.0905
1	2.2721	-0.7207	0.0000	-0.0627	-0.0459	-0.0824	-0.2829	-0.0007	-0.2092	-0.1736	-0.6811	-0.0021
1	-1.9585	1.8284	0.0000	0.1130	0.1148	0.0297	0.1073	0.0810	0.0405	0.2037	-0.0019	0.0829
1	-1.9136	0.3095	0.8758	0.1126	0.1180	0.0303	0.1055	0.0828	0.0162	0.1990	-0.0035	0.0836
1	-1.9136	0.3095	-0.8758	0.1126	0.1180	0.0303	0.1055	0.0828	0.0162	0.1990	-0.0035	0.0836
1	0.3782	-1.5879	-1.1969	-0.0637	-0.0456	-0.0835	-0.2847	-0.0019	-0.1982	-0.1783	-0.6805	-0.0040
1	0.3782	-1.5879	1.1969	-0.0637	-0.0456	-0.0835	-0.2847	-0.0019	-0.1982	-0.1783	-0.6805	-0.0040

 Dipole mement (in D) 0.87 (DEN) 0.46 0.09 0.35 0.26 0.57 0.84 0.72 0.90 0.71

File TZVPMol329.out
Molecule PMol329 trimethylsilane
 SP Mol329 B3LYP/Def2TZVP VAC.
  0 14
Dipole 0.4623 -0.3165 0.0000 0.5603
Quadrupole -0.3644 0.0146 0.3499 0.4883 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.5395	1.0533	0.0000	-0.0811	-0.0366	-0.0977	-0.3458	-0.0154	-0.2506	-0.2107	-0.6947	-0.0252
14	-0.3152	0.2155	0.0000	0.4142	0.2455	0.3494	1.5502	0.1003	0.9078	1.4102	2.7960	0.1081
6	1.1817	1.3334	0.0000	-0.4616	-0.4421	-0.1813	-0.8784	-0.2901	-0.5753	-1.0872	-0.7286	-0.2980
6	-0.3152	-0.8553	1.5309	-0.4616	-0.4421	-0.1813	-0.8784	-0.2901	-0.5648	-1.0872	-0.7285	-0.2980
6	-0.3152	-0.8553	-1.5309	-0.4616	-0.4421	-0.1813	-0.8784	-0.2901	-0.5648	-1.0872	-0.7283	-0.2980
1	2.1049	0.7529	0.0000	0.1136	0.1237	0.0317	0.1589	0.0867	0.1199	0.2266	0.0067	0.0889
1	0.5717	-1.4888	1.5663	0.1136	0.1237	0.0317	0.1589	0.0867	0.1178	0.2266	0.0067	0.0889
1	0.5717	-1.4888	-1.5663	0.1136	0.1237	0.0317	0.1589	0.0867	0.1178	0.2266	0.0067	0.0889
1	1.2046	1.9783	0.8778	0.1185	0.1244	0.0328	0.1590	0.0876	0.1177	0.2304	0.0106	0.0908
1	-1.1839	-1.5119	1.5651	0.1185	0.1244	0.0329	0.1590	0.0876	0.1146	0.2304	0.0107	0.0908
1	-0.3231	-0.2580	-2.4421	0.1185	0.1244	0.0329	0.1591	0.0876	0.1138	0.2304	0.0106	0.0908
1	1.2046	1.9783	-0.8778	0.1185	0.1244	0.0328	0.1590	0.0876	0.1177	0.2304	0.0106	0.0908
1	-0.3231	-0.2580	2.4421	0.1185	0.1244	0.0329	0.1591	0.0876	0.1138	0.2304	0.0106	0.0908
1	-1.1839	-1.5119	-1.5651	0.1185	0.1244	0.0329	0.1590	0.0876	0.1146	0.2304	0.0107	0.0908

 Dipole mement (in D) 0.56 (DEN) 0.22 0.36 0.14 0.12 0.35 0.59 0.71 1.15 0.43

File TZVPMol330.out

Molecule PMol330 vinylsilane
 SP Mol330 B3LYP/Def2TZVP VAC.
    0   9
Dipole   0.3106   0.6590   0.0000   0.7285
Quadrupole   1.0417   0.9227   -1.9644   -0.1294   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.8583	0.0000	-0.2042	-0.3311	-0.1254	-0.5217	-0.1458	-0.2821	-0.6271	-0.7370	-0.1036
6	1.2857	1.2003	0.0000	-0.2375	-0.2050	-0.0586	-0.1324	-0.1565	-0.3543	-0.3287	-0.0628	-0.1561
1	2.0777	0.4581	0.0000	0.1164	0.1199	0.0378	0.1046	0.0918	0.1609	0.1848	0.0299	0.0877
14	-0.5989	-0.8975	0.0000	0.2806	0.2884	0.3035	1.1317	0.0120	0.7274	0.8806	2.7306	-0.0083
1	-0.7349	1.6605	0.0000	0.1089	0.1365	0.0396	0.1389	0.0974	0.1379	0.2132	0.0302	0.0897
1	1.6167	2.2336	0.0000	0.1152	0.1178	0.0396	0.1093	0.0920	0.1703	0.1898	0.0325	0.0885
1	0.5695	-1.8007	0.0000	-0.0630	-0.0398	-0.0770	-0.2766	0.0054	-0.1757	-0.1725	-0.6732	0.0022
1	-1.4294	-1.1688	1.1923	-0.0582	-0.0433	-0.0799	-0.2769	0.0019	-0.1922	-0.1701	-0.6750	-0.0000
1	-1.4294	-1.1688	-1.1923	-0.0582	-0.0433	-0.0799	-0.2769	0.0019	-0.1922	-0.1701	-0.6750	-0.0000

Dipole mement (in D)	0.73 (DEN)	0.14	0.34	0.30	0.43	0.44	0.69	0.74	1.18	0.63	

File TZVPMol331.out
Molecule PMol331 phenylsilane
 SP Mol331 B3LYP/Def2TZVP VAC.
    0   15
Dipole   0.9588   -0.0071   0.0000   0.9588
Quadrupole   1.2562   3.1295   -4.3857   -0.0804   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.4679	0.0021	-0.0000	-0.0000	-0.2517	-0.0928	-0.4386	-0.0659	-0.1131	-0.4487	-0.7025	-0.0150
6	0.2532	-1.1975	-0.0000	-0.1324	-0.1285	-0.0327	-0.0133	-0.0821	-0.1109	-0.1850	-0.0294	-0.0756
6	0.2551	1.1985	-0.0000	-0.1386	-0.1310	-0.0334	-0.0137	-0.0830	-0.0822	-0.1861	-0.0296	-0.0762
6	1.6397	-1.2024	0.0000	-0.1339	-0.1383	-0.0376	-0.0930	-0.0935	-0.1063	-0.2052	-0.0269	-0.0825
6	1.6438	1.1995	0.0000	-0.1347	-0.1383	-0.0382	-0.0940	-0.0940	-0.1241	-0.2068	-0.0277	-0.0831
6	2.3379	-0.0015	0.0000	-0.0787	-0.1334	-0.0337	-0.0764	-0.0896	-0.0730	-0.1957	-0.0262	-0.0778
1	-0.2753	-2.1454	-0.0000	0.1100	0.1443	0.0400	0.0887	0.0978	0.1037	0.2031	0.0211	0.0850
1	-0.2739	2.1452	-0.0000	0.1110	0.1444	0.0379	0.0888	0.0958	0.0885	0.2065	0.0258	0.0829
1	2.1776	-2.1422	0.0000	0.1100	0.1428	0.0417	0.0926	0.0978	0.1031	0.2091	0.0310	0.0859
1	2.1836	2.1382	0.0000	0.1097	0.1428	0.0416	0.0926	0.0976	0.1080	0.2091	0.0309	0.0857
1	3.4207	-0.0034	0.0000	0.1126	0.1427	0.0425	0.0935	0.0985	0.0984	0.2087	0.0318	0.0868
14	-2.3335	0.0011	0.0000	0.2399	0.3260	0.3023	1.1135	0.0121	0.5809	0.8996	2.7271	-0.0154
1	-2.8575	-0.6973	1.1927	-0.0564	-0.0415	-0.0801	-0.2804	0.0018	-0.1608	-0.1688	-0.6755	-0.0012
1	-2.8181	1.3959	-0.0000	-0.0620	-0.0386	-0.0774	-0.2797	0.0050	-0.1513	-0.1709	-0.6750	0.0018
1	-2.8575	-0.6974	-1.1927	-0.0564	-0.0415	-0.0801	-0.2804	0.0018	-0.1608	-0.1688	-0.6755	-0.0012

Dipole mement (in D)	0.96 (DEN)	0.24	0.47	0.48	0.87	0.62	0.91	0.76	1.00	0.85	

File TZVPMol332.out
Molecule PMol332 SiO
 SP Mol332 B3LYP/Def2TZVP VAC.

```
    0    2
Dipole          0.0000    0.0000    3.1043    3.1043
Quadrupole      1.3421    1.3421   -2.6841    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  14      0.0000    0.0000    0.5491    0.3977    0.2191    0.3935    0.7326    0.3959    0.5286    1.1759    1.4295    0.3727
   8      0.0000    0.0000   -0.9609   -0.3977   -0.2191   -0.3935   -0.7327   -0.3959   -0.5286   -1.1759   -1.4295   -0.3727

 Dipole mement (in D)   3.10 (DEN)      2.88      1.59      2.85      5.31      2.87      3.83      8.53     10.37      2.70

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File TZVPMol333.out
Molecule PMol333    disiloxane
 SP Mol333 B3LYP/Def2TZVP VAC.
    0    9
Dipole          0.0000    0.0000   -0.2151    0.2151
Quadrupole     -0.4234    0.9496   -0.5262    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  14      0.0000    1.5821   -0.0539    0.3569    0.1584    0.3919    1.5327    0.1482    0.8943    1.2622    2.8883    0.1408
   1      0.0000    2.3472    1.2038   -0.0614   -0.0525   -0.0786   -0.3151    0.0072   -0.1994   -0.2094   -0.6807    0.0020
   1      1.2018    1.9238   -0.8391   -0.0649   -0.0546   -0.0819   -0.3266    0.0031   -0.2094   -0.2160   -0.6844   -0.0015
   1     -1.2018    1.9238   -0.8391   -0.0649   -0.0546   -0.0819   -0.3266    0.0031   -0.2101   -0.2160   -0.6844   -0.0015
   8      0.0000    0.0000    0.3072   -0.3316    0.0066   -0.2991   -1.1288   -0.3231   -0.5507   -1.2419   -1.6779   -0.2797
  14      0.0000   -1.5821   -0.0539    0.3569    0.1584    0.3919    1.5327    0.1482    0.8943    1.2622    2.8883    0.1408
   1     -1.2018   -1.9238   -0.8391   -0.0649   -0.0546   -0.0819   -0.3266    0.0031   -0.2101   -0.2160   -0.6844   -0.0015
   1      1.2018   -1.9238   -0.8391   -0.0649   -0.0546   -0.0819   -0.3266    0.0031   -0.2094   -0.2160   -0.6844   -0.0015
   1      0.0000   -2.3472    1.2038   -0.0614   -0.0525   -0.0786   -0.3151    0.0072   -0.1994   -0.2094   -0.6807    0.0020

 Dipole mement (in D)   0.22 (DEN)      0.34      0.20      0.23      0.84      0.52      0.20      1.42      0.81      0.44

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File TZVPMol334.out
Molecule PMol334    methyl_silyl_ether
 SP Mol334 B3LYP/Def2TZVP VAC.
    0    9
Dipole          1.0726   -0.2803    0.0000    1.1086
Quadrupole      1.6004   -0.8562   -0.7443    1.6716    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   8      0.0000    0.7275    0.0000   -0.3644    0.0432   -0.2407   -0.6591   -0.3075   -0.4493   -0.8456   -1.3758   -0.2838
   6      1.4026    0.8405    0.0000   -0.1610   -0.3588    0.0055   -0.0050   -0.1102    0.0035   -0.2405    0.5100   -0.0865
   1      1.8486    0.3786    0.8863    0.1073    0.1014    0.0329    0.0708    0.0926    0.0464    0.1624    0.0078    0.0857
   1      1.8486    0.3786   -0.8863    0.1073    0.1014    0.0329    0.0708    0.0926    0.0464    0.1624    0.0078    0.0857
   1      1.6651    1.8971    0.0000    0.1198    0.1080    0.0407    0.0913    0.1008    0.0776    0.1822    0.0265    0.0900
  14     -0.7689   -0.7199    0.0000    0.3987    0.1697    0.3734    1.3903    0.1218    0.8828    1.2193    2.8696    0.1139
   1     -0.4032   -1.5097    1.1965   -0.0746   -0.0578   -0.0858   -0.3301   -0.0018   -0.2072   -0.2215   -0.6858   -0.0060
   1     -2.2070   -0.4190    0.0000   -0.0586   -0.0492   -0.0732   -0.2989    0.0133   -0.1931   -0.1972   -0.6745    0.0069
   1     -0.4032   -1.5097   -1.1965   -0.0746   -0.0578   -0.0858   -0.3301   -0.0018   -0.2072   -0.2215   -0.6858   -0.0060

 Dipole mement (in D)   1.11 (DEN)      1.37      0.55      0.71      1.42      1.32      1.11      2.56      3.19      1.30
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File TZVPMol335.out
Molecule PMol335 hexamethyldisiloxane
 SP Mol335 B3LYP/Def2TZVP VAC.
  0 27
Dipole 0.0001 -0.0002 -0.4668 0.4668
Quadrupole 2.0919 -0.7491 -1.3428 -0.0937 0.0000 0.0009

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-2.6249	0.4782	1.5152	-0.4563	-0.4183	-0.1842	-0.9604	-0.2906	-0.6024	-1.1257	-0.7342	-0.3048
1	-2.5102	-0.2210	2.3433	0.1166	0.1264	0.0339	0.1726	0.0898	0.1254	0.2327	0.0126	0.0899
1	-3.6808	0.4908	1.2432	0.1085	0.1242	0.0311	0.1627	0.0862	0.1058	0.2271	0.0045	0.0880
1	-2.3729	1.4699	1.8905	0.1149	0.1257	0.0333	0.1716	0.0891	0.1199	0.2318	0.0113	0.0893
14	-1.5517	0.0025	0.0738	0.5203	0.0950	0.4218	2.0739	0.2506	1.1888	1.9412	2.9634	0.2762
6	-1.9998	-1.7006	-0.5374	-0.4573	-0.4210	-0.1858	-0.9853	-0.2926	-0.6661	-1.1307	-0.7334	-0.3069
1	-1.4025	-1.9880	-1.4031	0.1188	0.1241	0.0310	0.1753	0.0869	0.1356	0.2296	0.0078	0.0873
1	-1.8407	-2.4558	0.2327	0.1166	0.1260	0.0326	0.1739	0.0884	0.1333	0.2313	0.0099	0.0888
1	-3.0477	-1.7569	-0.8350	0.1133	0.1249	0.0311	0.1663	0.0862	0.1222	0.2286	0.0051	0.0880
6	-1.7351	1.2345	-1.3158	-0.4704	-0.4227	-0.1856	-0.9985	-0.2924	-0.6792	-1.1334	-0.7318	-0.3068
1	-1.1117	0.9698	-2.1715	0.1142	0.1235	0.0305	0.1723	0.0865	0.1347	0.2265	0.0024	0.0873
1	-2.7639	1.2869	-1.6743	0.1194	0.1255	0.0318	0.1693	0.0868	0.1264	0.2305	0.0067	0.0887
1	-1.4488	2.2393	-1.0032	0.1218	0.1258	0.0326	0.1771	0.0884	0.1390	0.2314	0.0100	0.0891
8	0.0000	-0.0004	0.5933	-0.3607	0.0818	-0.3089	-1.3418	-0.3271	-0.7556	-1.2419	-1.6683	-0.3080
14	1.5517	-0.0027	0.0738	0.5203	0.0951	0.4218	2.0739	0.2506	1.1506	1.9412	2.9629	0.2763
6	2.0015	1.7032	-0.5283	-0.4572	-0.4210	-0.1858	-0.9851	-0.2926	-0.6580	-1.1307	-0.7330	-0.3069
1	3.0488	1.7597	-0.8278	0.1132	0.1249	0.0311	0.1663	0.0861	0.1245	0.2286	0.0051	0.0880
1	1.4028	1.9964	-1.3912	0.1188	0.1241	0.0310	0.1753	0.0869	0.1317	0.2296	0.0078	0.0873
1	1.8449	2.4542	0.2463	0.1166	0.1260	0.0327	0.1738	0.0884	0.1340	0.2313	0.0099	0.0888
6	2.6245	-0.4873	1.5125	-0.4564	-0.4183	-0.1842	-0.9605	-0.2906	-0.6059	-1.1257	-0.7345	-0.3048
1	2.5103	0.2073	2.3446	0.1166	0.1264	0.0339	0.1726	0.0898	0.1287	0.2328	0.0127	0.0899
1	2.3716	-1.4809	1.8824	0.1148	0.1257	0.0333	0.1716	0.0891	0.1224	0.2317	0.0113	0.0893
1	3.6804	-0.4992	1.2405	0.1085	0.1242	0.0311	0.1627	0.0862	0.1083	0.2271	0.0045	0.0880
6	1.7339	-1.2275	-1.3223	-0.4705	-0.4227	-0.1856	-0.9986	-0.2924	-0.6225	-1.1334	-0.7319	-0.3068
1	2.7626	-1.2790	-1.6810	0.1195	0.1255	0.0318	0.1693	0.0868	0.1151	0.2305	0.0067	0.0887
1	1.4465	-2.2336	-1.0152	0.1218	0.1258	0.0326	0.1771	0.0884	0.1254	0.2314	0.0100	0.0891
1	1.1109	-0.9575	-2.1767	0.1142	0.1235	0.0305	0.1723	0.0865	0.1179	0.2266	0.0024	0.0873

Dipole mement (in D)	0.47 (DEN)	0.71	0.14	0.28	1.02	0.83	0.48	1.30	0.14	0.75

File TZVPMol336.out
Molecule PMol336 methoxytrimethylsilane
 SP Mol336 B3LYP/Def2TZVP VAC.
  0 18
Dipole -0.1090 0.0002 0.9987 1.0046
Quadrupole 2.6238 -0.6042 -2.0196 -0.0002 -0.7264 -0.0003

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.3767	-0.0000	0.0053	0.5688	0.1061	0.4146	1.9542	0.2355	1.0306	1.9129	2.9505	0.2593

```
   6      0.4653   -1.5198    1.0834   -0.4728   -0.4242   -0.1863   -0.9969   -0.2936   -0.4877   -1.1359   -0.7339   -0.3069
   1     -0.3216   -1.5297    1.8385    0.1147    0.1239    0.0303    0.1630    0.0858    0.0914    0.2281    0.0049    0.0874
   1      0.3684   -2.4346    0.4986    0.1222    0.1264    0.0332    0.1695    0.0888    0.1026    0.2326    0.0122    0.0898
   1      1.4153   -1.5734    1.6163    0.1159    0.1263    0.0323    0.1702    0.0873    0.0811    0.2311    0.0077    0.0893
   6      0.4655    1.5205    1.0824   -0.4728   -0.4242   -0.1863   -0.9969   -0.2936   -0.4876   -1.1359   -0.7339   -0.3069
   1      0.3691    2.4350    0.4970    0.1222    0.1264    0.0332    0.1695    0.0888    0.1025    0.2326    0.0122    0.0898
   1      1.4154    1.5741    1.6156    0.1159    0.1263    0.0323    0.1702    0.0873    0.0811    0.2311    0.0077    0.0893
   1     -0.3216    1.5311    1.8373    0.1147    0.1239    0.0303    0.1630    0.0858    0.0914    0.2281    0.0049    0.0874
   6      1.7153   -0.0005   -1.2788   -0.4481   -0.4144   -0.1817   -0.9735   -0.2878   -0.7268   -1.1232   -0.7375   -0.3026
   1      1.6481   -0.8788   -1.9201    0.1198    0.1280    0.0357    0.1714    0.0918    0.1580    0.2353    0.0168    0.0914
   1      1.6481    0.8773   -1.9207    0.1198    0.1280    0.0357    0.1714    0.0918    0.1580    0.2353    0.0168    0.0914
   1      2.7065   -0.0003   -0.8251    0.1092    0.1247    0.0318    0.1655    0.0870    0.1530    0.2275    0.0055    0.0889
   8     -1.0352   -0.0002   -0.8537   -0.3725    0.0820   -0.2466   -0.7394   -0.3111   -0.4971   -0.8536   -1.3724   -0.2990
   6     -2.3014   -0.0000   -0.2525   -0.1790   -0.3633   -0.0001    0.0165   -0.1153    0.0161   -0.2363    0.5250   -0.0912
   1     -2.4633    0.8858    0.3716    0.1013    0.0991    0.0281    0.0696    0.0879    0.0308    0.1563   -0.0017    0.0793
   1     -3.0619   -0.0000   -1.0331    0.1193    0.1061    0.0356    0.0833    0.0955    0.0719    0.1776    0.0174    0.0840
   1     -2.4634   -0.8858    0.3717    0.1013    0.0991    0.0281    0.0696    0.0879    0.0308    0.1563   -0.0017    0.0793

 Dipole mement (in D)   1.00 (DEN)      1.14      0.04      0.54      1.46      1.23      1.04      2.11      3.28      1.20

-----------------------------------------
File TZVPMol337.out
Molecule PMol337    methylsilanol
 SP Mol337 B3LYP/Def2TZVP VAC.
    0    9
Dipole         -0.8375   -0.9053    1.1833    1.7091
Quadrupole     -0.7963    0.7085    0.0878   -1.3853    2.3880   -1.9241
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14      0.1094    0.4918    0.0191    0.4875    0.1476    0.3845    1.6439    0.1542    0.9612    1.4551    2.9028    0.1552
   1      0.2342    1.3896   -1.1411   -0.0728   -0.0454   -0.0831   -0.3355    0.0038   -0.1962   -0.2212   -0.6827   -0.0066
   1      0.2006    1.2839    1.2672   -0.0902   -0.0570   -0.0950   -0.3666   -0.0107   -0.2503   -0.2392   -0.6965   -0.0179
   6     -1.5175   -0.4040   -0.0141   -0.4635   -0.4668   -0.1817   -0.9161   -0.2891   -0.5458   -1.1231   -0.7514   -0.2955
   1     -1.6295   -0.9944   -0.9224    0.1276    0.1263    0.0381    0.1681    0.0936    0.1259    0.2364    0.0224    0.0961
   1     -1.6257   -1.0797    0.8341    0.1147    0.1230    0.0342    0.1604    0.0895    0.1138    0.2302    0.0121    0.0925
   1     -2.3496    0.2992    0.0268    0.1196    0.1281    0.0382    0.1659    0.0931    0.1079    0.2357    0.0189    0.0971
   8      1.3950   -0.5306   -0.1088   -0.5308   -0.1259   -0.3013   -0.9985   -0.4814   -0.7124   -1.0591   -1.4122   -0.4011
   1      1.5838   -1.1145    0.6227    0.3078    0.1700    0.1660    0.4783    0.3472    0.3958    0.4851    0.5866    0.2802

 Dipole mement (in D)   1.71 (DEN)      1.47      1.22      0.75      1.84      1.58      1.66      2.38      2.28      1.42

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File TZVPMol338.out
Molecule PMol338    silanediol
 SP Mol338 B3LYP/Def2TZVP VAC.
    0    7
Dipole          0.0000    0.0000   -1.1206    1.1206
Quadrupole      1.0669   -2.4857    1.4188    4.8042    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
```

14	0.0000	0.0000	0.4590	0.5745	0.0111	0.4261	1.9066	0.2405	1.1443	1.6686	3.0257	0.2436
1	-1.2187	0.1192	1.2714	-0.0854	-0.0588	-0.0836	-0.3787	0.0064	-0.2299	-0.2528	-0.6877	-0.0065
1	1.2187	-0.1192	1.2714	-0.0854	-0.0588	-0.0836	-0.3787	0.0064	-0.2295	-0.2528	-0.6877	-0.0065
8	0.0000	1.3698	-0.4376	-0.5167	-0.1183	-0.2995	-1.0602	-0.4784	-0.7531	-1.0705	-1.4171	-0.3990
1	0.7618	1.5553	-0.9838	0.3149	0.1716	0.1700	0.4856	0.3517	0.4116	0.4890	0.5918	0.2837
8	0.0000	-1.3698	-0.4376	-0.5167	-0.1183	-0.2995	-1.0602	-0.4784	-0.7588	-1.0705	-1.4172	-0.3990
1	-0.7618	-1.5553	-0.9838	0.3149	0.1716	0.1700	0.4856	0.3517	0.4154	0.4890	0.5918	0.2837

Dipole mement (in D)	1.12 (DEN)	0.58	1.82	0.43	0.55	0.71	1.01	0.47	1.36	0.55	

File TZVPMol339.out
Molecule PMol339 silanone
SP Mol339 B3LYP/Def2TZVP VAC.
0 4
Dipole -0.0001 3.6701 0.0000 3.6701
Quadrupole 2.5330 -2.6712 0.1381 -0.0001 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.0000	0.4355	0.0000	0.5285	0.3247	0.5177	1.5313	0.3575	1.1995	1.5721	2.7672	0.3337
8	-0.0000	-1.0782	0.0000	-0.4800	-0.2135	-0.4176	-0.9184	-0.4251	-0.7554	-1.0993	-1.4586	-0.3941
1	0.0000	1.2641	1.2219	-0.0243	-0.0556	-0.0501	-0.3064	0.0338	-0.2221	-0.2364	-0.6543	0.0302
1	0.0000	1.2641	-1.2219	-0.0243	-0.0556	-0.0501	-0.3064	0.0338	-0.2221	-0.2364	-0.6543	0.0302

Dipole mement (in D)	3.67 (DEN)	3.30	1.11	2.64	4.24	3.36	3.72	6.11	5.40	3.11	

File TZVPMol340.out
Molecule PMol340 silanole
SP Mol340 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.2319 -1.3494 0.0000 1.3692
Quadrupole 0.8350 0.3011 -1.1361 -2.9831 0.0001 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.5302	-0.0092	0.0000	0.4240	0.1440	0.3749	1.4541	0.1203	0.9219	1.2201	2.8762	0.1148
1	-1.0249	-0.7210	1.1970	-0.0768	-0.0635	-0.0870	-0.3313	-0.0031	-0.2276	-0.2232	-0.6890	-0.0059
1	-1.0249	-0.7214	-1.1968	-0.0768	-0.0635	-0.0870	-0.3313	-0.0031	-0.2276	-0.2232	-0.6890	-0.0059
1	-1.0231	1.3746	-0.0002	-0.0608	-0.0510	-0.0744	-0.3001	0.0123	-0.1748	-0.2042	-0.6749	0.0061
8	1.1087	0.1109	-0.0000	-0.5226	-0.1372	-0.2969	-0.9714	-0.4779	-0.6902	-1.0567	-1.4143	-0.3953
1	1.6261	-0.6911	0.0000	0.3129	0.1712	0.1705	0.4800	0.3515	0.3983	0.4873	0.5916	0.2862

Dipole mement (in D)	1.37 (DEN)	1.26	1.24	0.63	1.90	1.33	1.32	2.67	2.53	1.09	

File TZVPMol341.out
Molecule PMol341 fluorosilane
SP Mol341 B3LYP/Def2TZVP VAC.
0 5
Dipole -0.0001 1.2787 0.0000 1.2787

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Quadrupole      0.3614   -0.7228    0.3614    0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14     -0.0000    0.5000    0.0000    0.5061    0.1873    0.4251    1.3686    0.1548    0.9853    1.2994    2.8908    0.1537
   1     -1.3968    0.9590    0.0000   -0.0612   -0.0584   -0.0727   -0.3041    0.0112   -0.2107   -0.2205   -0.6764    0.0095
   1      0.6984    0.9589    1.2097   -0.0612   -0.0584   -0.0727   -0.3041    0.0112   -0.2112   -0.2205   -0.6764    0.0095
   1      0.6984    0.9589   -1.2097   -0.0612   -0.0584   -0.0727   -0.3041    0.0112   -0.2112   -0.2205   -0.6764    0.0095
   9     -0.0000   -1.0974    0.0000   -0.3223   -0.0119   -0.2070   -0.4563   -0.1883   -0.3522   -0.6380   -0.8614   -0.1822

 Dipole mement (in D)   1.28 (DEN)      2.07      0.30      1.11      1.49      1.52      1.31      3.44      2.14      1.46

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File TZVPMol342.out
Molecule PMol342    difluorosilane
 SP Mol342 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0001    1.4733    0.0000    1.4733
Quadrupole      1.0910    0.9323   -2.0233    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14      0.0000    0.4476    0.0000    0.7306    0.0766    0.5207    1.7271    0.3048    0.9967    1.8077    3.0545    0.3180
   9      0.0000   -0.4856    1.2776   -0.3014    0.0227   -0.1943   -0.5053   -0.1735   -0.3210   -0.6412   -0.8539   -0.1735
   9      0.0000   -0.4856   -1.2776   -0.3014    0.0227   -0.1943   -0.5053   -0.1735   -0.3210   -0.6412   -0.8539   -0.1735
   1      1.2303    1.2378    0.0000   -0.0639   -0.0610   -0.0660   -0.3582    0.0211   -0.1777   -0.2627   -0.6733    0.0144
   1     -1.2303    1.2377    0.0000   -0.0639   -0.0610   -0.0660   -0.3582    0.0211   -0.1771   -0.2627   -0.6733    0.0144

 Dipole mement (in D)   1.47 (DEN)      2.22      0.67      1.24      1.81      1.72      1.53      3.75      2.54      1.66

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File TZVPMol343.out
Molecule PMol343    trifluorosilane
 SP Mol343 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000    1.3177    1.3177
Quadrupole     -1.0843   -1.0843    2.1686    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14      0.0000    0.0000    0.3226    0.9028   -0.1043    0.5977    2.0816    0.4369    1.1911    2.2065    3.1992    0.4692
   1      0.0000    0.0000    1.7709   -0.0531   -0.0581   -0.0494   -0.4037    0.0420   -0.1873   -0.2870   -0.6591    0.0297
   9      0.0000    1.4673   -0.2329   -0.2832    0.0541   -0.1828   -0.5593   -0.1596   -0.3344   -0.6398   -0.8466   -0.1663
   9     -1.2707   -0.7336   -0.2329   -0.2832    0.0541   -0.1828   -0.5593   -0.1596   -0.3348   -0.6398   -0.8466   -0.1663
   9      1.2707   -0.7336   -0.2329   -0.2832    0.0541   -0.1828   -0.5593   -0.1596   -0.3346   -0.6398   -0.8466   -0.1663

 Dipole mement (in D)   1.32 (DEN)      1.90      0.84      1.12      1.67      1.57      1.37      3.12      2.19      1.54

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File TZVPMol344.out
Molecule PMol344    fluoromethylsilane
 SP Mol344 B3LYP/Def2TZVP VAC.
    0    8
Dipole          1.6635    0.4707    0.0001    1.7288
```

Quadrupole -0.4926 0.0031 0.4895 -0.9350 -0.0001 -0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.1508	0.4823	0.0000	0.5695	0.1808	0.4241	1.5606	0.1782	0.9739	1.5234	2.9150	0.1841
1	-0.3442	1.3071	-1.2056	-0.0777	-0.0527	-0.0821	-0.3413	0.0020	-0.2212	-0.2355	-0.6846	-0.0037
1	-0.3443	1.3068	1.2058	-0.0777	-0.0527	-0.0821	-0.3413	0.0020	-0.2212	-0.2355	-0.6846	-0.0037
6	1.4964	-0.3526	0.0000	-0.4642	-0.4603	-0.1754	-0.9148	-0.2819	-0.5082	-1.1335	-0.7665	-0.2912
1	1.6246	-0.9805	-0.8800	0.1301	0.1297	0.0434	0.1727	0.0987	0.1228	0.2412	0.0298	0.1020
1	2.3012	0.3821	0.0002	0.1231	0.1311	0.0424	0.1711	0.0975	0.0974	0.2390	0.0247	0.1018
1	1.6245	-0.9808	0.8798	0.1301	0.1297	0.0434	0.1727	0.0987	0.1228	0.2412	0.0298	0.1020
9	-1.3032	-0.6302	-0.0001	-0.3333	-0.0056	-0.2137	-0.4798	-0.1952	-0.3663	-0.6402	-0.8644	-0.1914

Dipole mement (in D) 1.73 (DEN) 2.29 0.49 1.31 1.44 1.84 1.72 3.24 2.00 1.83

File TZVPMol345.out
Molecule PMol345 difluoromethylsilane
SP Mol345 B3LYP/Def2TZVP VAC.
0 8
Dipole -2.0155 0.0000 0.6627 2.1217
Quadrupole 0.9711 -2.0272 1.0560 0.0000 0.5616 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0862	0.0000	0.3403	0.7827	0.0351	0.5099	1.9376	0.3176	1.1588	1.9977	3.0707	0.3409
1	0.3215	-0.0000	1.7863	-0.0825	-0.0544	-0.0743	-0.4017	0.0129	-0.2224	-0.2743	-0.6799	0.0022
6	-1.6766	-0.0000	-0.1630	-0.4672	-0.4394	-0.1744	-1.0234	-0.2783	-0.7037	-1.1788	-0.7856	-0.2943
1	-2.1942	-0.8790	0.2174	0.1305	0.1342	0.0469	0.1842	0.1026	0.1583	0.2446	0.0340	0.1059
1	-2.1939	0.8797	0.2163	0.1306	0.1342	0.0469	0.1842	0.1026	0.1583	0.2446	0.0340	0.1059
1	-1.7721	-0.0007	-1.2476	0.1359	0.1357	0.0497	0.1881	0.1057	0.1890	0.2498	0.0413	0.1076
9	0.8162	1.2730	-0.2644	-0.3149	0.0273	-0.2023	-0.5345	-0.1816	-0.3691	-0.6418	-0.8575	-0.1840
9	0.8162	-1.2730	-0.2644	-0.3149	0.0273	-0.2023	-0.5345	-0.1816	-0.3692	-0.6418	-0.8575	-0.1840

Dipole mement (in D) 2.12 (DEN) 2.70 0.73 1.63 1.69 2.28 2.15 3.46 2.19 2.24

File TZVPMol346.out
Molecule PMol346 trifluoromethylsilane
SP Mol346 B3LYP/Def2TZVP VAC.
0 8
Dipole -2.3601 -0.0011 0.0002 2.3601
Quadrupole 2.4124 -1.2075 -1.2049 0.0025 -0.0011 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0360	0.0000	-0.0000	0.9593	-0.1718	0.5844	2.2231	0.4480	1.2630	2.3730	3.2103	0.4910
6	-1.7850	-0.0009	0.0003	-0.4770	-0.4170	-0.1680	-1.0879	-0.2698	-0.7965	-1.2112	-0.7968	-0.2922
1	-2.1753	0.3223	-0.9624	0.1387	0.1397	0.0531	0.1963	0.1095	0.1994	0.2517	0.0457	0.1119
1	-2.1747	-0.9964	0.2018	0.1387	0.1397	0.0531	0.1963	0.1095	0.1996	0.2517	0.0457	0.1119
1	-2.1752	0.6712	0.7617	0.1387	0.1397	0.0531	0.1963	0.1095	0.2011	0.2517	0.0457	0.1119
9	0.6203	-0.4471	1.3918	-0.2994	0.0566	-0.1919	-0.5747	-0.1689	-0.3555	-0.6390	-0.8503	-0.1782
9	0.6186	1.4298	-0.3087	-0.2995	0.0565	-0.1919	-0.5747	-0.1689	-0.3552	-0.6390	-0.8502	-0.1781
9	0.6200	-0.9817	-1.0834	-0.2995	0.0566	-0.1919	-0.5747	-0.1689	-0.3560	-0.6390	-0.8503	-0.1782

```
 Dipole mement (in D)   2.36 (DEN)      2.77      0.33      1.84      1.57      2.55      2.40      2.80      1.64      2.51

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File TZVPMol347.out
Molecule PMol347    fluorodisilane
 SP Mol347 B3LYP/Def2TZVP VAC.
    0    8
Dipole         -0.9067    0.8905    0.0001    1.2709
Quadrupole     -1.4309    0.3798    1.0511    1.3995    0.0000    0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14      0.7263    0.5148    0.0000    0.4721    0.0828    0.3427    1.0178    0.1540    0.5875    1.1028    2.1126    0.1674
   1      1.0696    1.3038    1.1996   -0.0634   -0.0483   -0.0746   -0.2716    0.0093   -0.1504   -0.2050   -0.6705    0.0041
   1      1.0695    1.3037   -1.1997   -0.0634   -0.0483   -0.0746   -0.2716    0.0093   -0.1504   -0.2050   -0.6705    0.0041
  14     -1.5186   -0.1370    0.0000    0.1015    0.1365    0.2219    0.5119   -0.0239    0.4563    0.3418    2.0720   -0.0260
   1     -2.3642    1.0760   -0.0011   -0.0446   -0.0359   -0.0698   -0.1902    0.0123   -0.1589   -0.1341   -0.6616    0.0110
   1     -1.8268   -0.9367   -1.2029   -0.0377   -0.0369   -0.0677   -0.1870    0.0148   -0.1418   -0.1299   -0.6594    0.0133
   1     -1.8275   -0.9349    1.2039   -0.0377   -0.0369   -0.0677   -0.1870    0.0148   -0.1417   -0.1299   -0.6594    0.0133
   9      1.6636   -0.7889    0.0000   -0.3269   -0.0129   -0.2102   -0.4222   -0.1904   -0.3007   -0.6406   -0.8642   -0.1870

 Dipole mement (in D)   1.27 (DEN)      2.04      0.39      1.20      1.41      1.61      1.27      3.51      2.75      1.53

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File TZVPMol348.out
Molecule PMol348    1,1,1-trifluorodisilane
 SP Mol348 B3LYP/Def2TZVP VAC.
    0    8
Dipole          2.1198   -0.0006    0.0000    2.1198
Quadrupole      1.3404   -0.6697   -0.6707   -0.0013    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  14     -0.4282   -0.0002    0.0000    0.8918   -0.2242    0.4996    1.6694    0.4235    0.7178    2.0274    2.0500    0.4673
  14      1.8936    0.0004    0.0000    0.0635    0.1651    0.2499    0.3602    0.0036    0.4448    0.2635    2.4628   -0.0075
   1      2.3654    0.6990    1.2092   -0.0260   -0.0284   -0.0589   -0.1573    0.0244   -0.1258   -0.1202   -0.6520    0.0223
   1      2.3670   -1.3955    0.0000   -0.0260   -0.0284   -0.0589   -0.1572    0.0244   -0.1228   -0.1202   -0.6520    0.0223
   1      2.3654    0.6990   -1.2092   -0.0260   -0.0284   -0.0589   -0.1573    0.0244   -0.1258   -0.1202   -0.6520    0.0223
   9     -1.0227    1.4624    0.0000   -0.2924    0.0481   -0.1909   -0.5193   -0.1667   -0.2589   -0.6434   -0.8522   -0.1756
   9     -1.0227   -0.7315   -1.2667   -0.2924    0.0481   -0.1909   -0.5193   -0.1667   -0.2647   -0.6434   -0.8522   -0.1756
   9     -1.0227   -0.7315    1.2667   -0.2924    0.0481   -0.1909   -0.5193   -0.1667   -0.2647   -0.6434   -0.8522   -0.1756

 Dipole mement (in D)   2.12 (DEN)      2.16      0.29      2.05      2.13      2.45      2.19      3.61      8.51      2.32

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File TZVPMol349.out
Molecule PMol349    chlorosilane
 SP Mol349 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.0002   -1.2286    0.0000    1.2286
Quadrupole     -0.2818    0.5638   -0.2820    0.0002    0.0000    0.0000
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       Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  14     -0.0000   -0.9820    0.0000    0.3770   -0.0461    0.3406    1.1393    0.0496    0.6065    0.8829    2.7615    0.0686
   1     -1.3939   -1.4498    0.0000   -0.0414   -0.0518   -0.0685   -0.2720    0.0150   -0.1260   -0.1718   -0.6649    0.0127
   1      0.6970   -1.4499    1.2071   -0.0414   -0.0518   -0.0685   -0.2720    0.0150   -0.1264   -0.1718   -0.6649    0.0127
   1      0.6970   -1.4499   -1.2071   -0.0414   -0.0518   -0.0685   -0.2720    0.0150   -0.1264   -0.1718   -0.6649    0.0127
  17     -0.0000    1.0645    0.0000   -0.2529    0.2015   -0.1350   -0.3233   -0.0946   -0.2276   -0.3676   -0.7676   -0.1066

 Dipole mement (in D)   1.23 (DEN)      2.21      2.33      0.86      1.34      1.03      1.39      2.46      3.06      1.13

-----------------------------------------
File TZVPMol350.out
Molecule PMol350    dichlorosilane
 SP Mol350 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000    1.1209    1.1209
Quadrupole      0.1626   -1.5125    1.3499    0.0000    0.0000    0.0000
       Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  14      0.0000    0.0000    0.7595    0.5076   -0.3818    0.3586    1.2538    0.1016    0.4867    1.0608    2.8227    0.1540
   1      1.2183    0.0000    1.5732   -0.0331   -0.0502   -0.0629   -0.2953    0.0228   -0.0742   -0.1771   -0.6556    0.0152
   1     -1.2183    0.0000    1.5732   -0.0331   -0.0502   -0.0629   -0.2953    0.0228   -0.0766   -0.1771   -0.6556    0.0152
  17      0.0000    1.6680   -0.4053   -0.2207    0.2411   -0.1164   -0.3316   -0.0737   -0.1680   -0.3533   -0.7558   -0.0922
  17      0.0000   -1.6680   -0.4053   -0.2207    0.2411   -0.1164   -0.3316   -0.0737   -0.1680   -0.3533   -0.7558   -0.0922

 Dipole mement (in D)   1.12 (DEN)      2.21      3.09      0.81      1.40      1.00      1.29      2.57      3.33      1.15

-----------------------------------------
File TZVPMol351.out
Molecule PMol351    trichlorosilane
 SP Mol351 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.6200    0.4363    0.0000    0.7581
Quadrupole      0.5823   -0.0040   -0.5782    0.8168    0.0000    0.0000
       Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  14      0.4065    0.2861    0.0000    0.6015   -0.7730    0.3611    1.3551    0.1382    0.2816    1.2117    2.8775    0.2272
  17     -1.2419    1.4620    0.0000   -0.1925    0.2735   -0.1017   -0.3455   -0.0568   -0.0943   -0.3453   -0.7449   -0.0821
  17      0.4065   -0.8819    1.6540   -0.1924    0.2736   -0.1017   -0.3455   -0.0568   -0.0938   -0.3453   -0.7449   -0.0821
  17      0.4065   -0.8819   -1.6540   -0.1924    0.2736   -0.1017   -0.3455   -0.0568   -0.0938   -0.3453   -0.7449   -0.0821
   1      1.5992    1.1256    0.0000   -0.0242   -0.0477   -0.0559   -0.3184    0.0323    0.0002   -0.1757   -0.6428    0.0193

 Dipole mement (in D)   0.76 (DEN)      1.69      2.98      0.59      1.11      0.78      0.91      2.11      2.71      0.93

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File TZVPMol352.out
Molecule PMol352    chloro(methyl)silane
 SP Mol352 B3LYP/Def2TZVP VAC.
    0    8
Dipole         -1.8240   -0.0117    0.0000    1.8240
Quadrupole      0.2625   -0.0671   -0.1955    0.2109    0.0000    0.0000
```

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.4402	0.6229	0.0000	0.4371	-0.0322	0.3499	1.3377	0.0843	0.6323	1.1344	2.7894	0.1109
1	-0.5114	1.4705	-1.2024	-0.0530	-0.0453	-0.0771	-0.3086	0.0067	-0.1513	-0.1874	-0.6731	0.0003
17	1.4062	-0.2829	-0.0000	-0.2718	0.2008	-0.1499	-0.3475	-0.1103	-0.2463	-0.3820	-0.7738	-0.1256
1	-0.5113	1.4703	1.2026	-0.0530	-0.0453	-0.0771	-0.3086	0.0067	-0.1513	-0.1875	-0.6731	0.0003
6	-1.7640	-0.6707	0.0000	-0.4465	-0.4681	-0.1739	-0.8846	-0.2812	-0.3276	-1.1004	-0.7604	-0.2883
1	-1.6917	-1.3077	-0.8797	0.1317	0.1301	0.0429	0.1706	0.0982	0.0776	0.2421	0.0325	0.1002
1	-2.7525	-0.2117	0.0001	0.1239	0.1300	0.0424	0.1703	0.0974	0.0891	0.2388	0.0255	0.1018
1	-1.6917	-1.3078	0.8797	0.1317	0.1301	0.0429	0.1706	0.0982	0.0776	0.2421	0.0325	0.1002
Dipole mement (in D)	1.82 (DEN)			2.56	2.19	1.17	1.35	1.46	1.92	2.38	2.94	1.62

File TZVPMol353.out
Molecule PMol353 trichloro(methyl)silane
SP Mol353 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.0013 0.0004 1.9065 1.9065
Quadrupole -1.2897 -1.2907 2.5804 -0.0006 -0.0005 0.0025

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	-0.0002	0.0000	0.2541	0.6519	-0.7822	0.3743	1.5934	0.1777	0.3872	1.4567	2.8906	0.2823
6	-0.0005	0.0014	2.0898	-0.4298	-0.4455	-0.1725	-1.0283	-0.2771	-0.3469	-1.1401	-0.7745	-0.2913
1	1.0188	0.0195	2.4709	0.1372	0.1369	0.0490	0.1904	0.1052	0.1162	0.2511	0.0454	0.1046
1	-0.5255	0.8756	2.4700	0.1372	0.1369	0.0490	0.1904	0.1052	0.1178	0.2511	0.0454	0.1046
1	-0.4948	-0.8899	2.4715	0.1372	0.1369	0.0490	0.1904	0.1051	0.1136	0.2511	0.0454	0.1046
17	0.9155	1.6700	-0.4615	-0.2113	0.2723	-0.1163	-0.3788	-0.0720	-0.1297	-0.3567	-0.7510	-0.1016
17	-1.9043	-0.0428	-0.4612	-0.2112	0.2724	-0.1162	-0.3788	-0.0720	-0.1297	-0.3566	-0.7510	-0.1016
17	0.9892	-1.6280	-0.4602	-0.2112	0.2723	-0.1163	-0.3788	-0.0720	-0.1285	-0.3567	-0.7510	-0.1016
Dipole mement (in D)	1.91 (DEN)			2.77	2.36	1.24	0.92	1.66	1.97	1.64	2.36	1.82

File TZVPMol354.out
Molecule PMol354 (chloromethyl)silane
SP Mol354 B3LYP/Def2TZVP VAC.
0 8
Dipole 1.2406 1.1195 0.0000 1.6710
Quadrupole -2.0271 1.5377 0.4894 0.0846 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	1.4633	-0.3321	0.0000	0.2567	0.2460	0.3098	1.1379	0.0129	0.7343	0.8934	2.7259	0.0029
1	1.4073	-1.1745	1.2070	-0.0415	-0.0388	-0.0725	-0.2714	0.0105	-0.1707	-0.1617	-0.6686	0.0058
1	2.7123	0.4582	0.0000	-0.0575	-0.0427	-0.0778	-0.2715	0.0040	-0.1880	-0.1731	-0.6764	0.0025
1	1.4073	-1.1745	-1.2070	-0.0415	-0.0388	-0.0725	-0.2714	0.0105	-0.1707	-0.1617	-0.6686	0.0058
6	0.0000	0.8473	0.0000	-0.2325	-0.6289	-0.0933	-0.6233	-0.1567	-0.4102	-0.7977	-0.5478	-0.0951
1	-0.0175	1.4902	0.8773	0.1361	0.1227	0.0475	0.1513	0.1057	0.1687	0.2306	0.0574	0.1038
1	-0.0175	1.4902	-0.8773	0.1361	0.1227	0.0475	0.1513	0.1057	0.1687	0.2306	0.0574	0.1038
17	-1.5281	-0.0896	0.0000	-0.1557	0.2577	-0.0887	-0.0031	-0.0928	-0.1322	-0.0605	-0.2788	-0.1297

Dipole mement (in D) 1.67 (DEN) 1.90 1.59 0.96 0.84 1.23 1.77 2.25 3.37 1.53

File TZVPMol355.out
Molecule PMol355 dichloro(ethyl)silane
SP Mol355 B3LYP/Def2TZVP VAC.
0 11
Dipole 1.6389 -1.2442 0.1764 2.0652
Quadrupole -0.2509 -0.4784 0.7293 -1.5662 -0.2872 -0.0030

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.6056	-0.7405	0.0116	-0.3467	-0.3213	-0.0786	-0.2679	-0.2256	-0.0862	-0.5920	0.0152	-0.2378
1	2.8221	0.2786	-0.3070	0.1245	0.1200	0.0305	0.1083	0.0838	0.0238	0.2090	0.0114	0.0781
1	2.7757	-0.7839	1.0876	0.1135	0.1195	0.0326	0.1105	0.0853	0.0282	0.2008	-0.0008	0.0858
1	3.3431	-1.3910	-0.4563	0.1199	0.1184	0.0347	0.1196	0.0862	0.0261	0.2102	0.0072	0.0884
6	1.1846	-1.1516	-0.3549	-0.2698	-0.4189	-0.1337	-0.7564	-0.2013	0.0635	-0.8820	-0.7198	-0.1823
1	0.9906	-2.1877	-0.0656	0.1133	0.1460	0.0404	0.1519	0.0995	0.0071	0.2349	0.0186	0.0949
1	1.0339	-1.1155	-1.4360	0.1165	0.1463	0.0409	0.1524	0.1003	0.0018	0.2383	0.0251	0.0935
14	-0.1254	-0.1088	0.4357	0.5498	-0.3540	0.3618	1.4319	0.1310	0.2996	1.3043	2.8272	0.1938
1	-0.0718	-0.1287	1.9032	-0.0458	-0.0409	-0.0707	-0.3368	0.0153	-0.0526	-0.1908	-0.6612	0.0027
17	0.0996	1.8395	-0.1488	-0.2409	0.2411	-0.1278	-0.3528	-0.0864	-0.1529	-0.3689	-0.7610	-0.1069
17	-1.9748	-0.7687	-0.1316	-0.2344	0.2437	-0.1300	-0.3606	-0.0880	-0.1584	-0.3636	-0.7631	-0.1100

Dipole mement (in D) 2.07 (DEN) 2.85 2.86 1.30 1.55 1.70 2.15 2.29 3.08 1.81

File TZVPMol356.out
Molecule PMol356 chlorotrimethylsilane
SP Mol356 B3LYP/Def2TZVP VAC.
0 14
Dipole 2.1403 -0.0004 -0.0011 2.1403
Quadrupole -1.6668 0.8336 0.8332 0.0003 0.0001 -0.0002

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.8866	1.5945	-0.7730	-0.4442	-0.4296	-0.1812	-0.9665	-0.2882	-0.5624	-1.1192	-0.7457	-0.3004
14	0.3310	-0.0001	-0.0001	0.5259	-0.0743	0.3822	1.7307	0.1672	0.8149	1.6389	2.8451	0.2183
6	0.8859	-1.4667	-0.9946	-0.4440	-0.4296	-0.1811	-0.9665	-0.2881	-0.5521	-1.1193	-0.7459	-0.3004
6	0.8873	-0.1281	1.7670	-0.4442	-0.4296	-0.1812	-0.9664	-0.2881	-0.5213	-1.1192	-0.7457	-0.3004
17	-1.7447	0.0002	0.0005	-0.2946	0.2036	-0.1721	-0.3867	-0.1337	-0.2927	-0.4081	-0.7827	-0.1574
1	0.5228	1.6894	-1.7952	0.1260	0.1294	0.0377	0.1730	0.0931	0.1257	0.2387	0.0233	0.0935
1	0.5238	2.4556	-0.2134	0.1260	0.1294	0.0377	0.1730	0.0931	0.1253	0.2386	0.0233	0.0935
1	1.9754	1.6547	-0.8029	0.1151	0.1277	0.0357	0.1724	0.0908	0.1337	0.2317	0.0122	0.0931
1	0.5227	-2.3993	-0.5649	0.1260	0.1294	0.0377	0.1731	0.0931	0.1233	0.2387	0.0233	0.0935
1	1.9747	-1.5224	-1.0329	0.1150	0.1277	0.0357	0.1724	0.0908	0.1301	0.2317	0.0122	0.0931
1	0.5220	-1.4131	-2.0198	0.1260	0.1294	0.0377	0.1730	0.0931	0.1235	0.2386	0.0233	0.0935
1	0.5243	-1.0429	2.2334	0.1260	0.1294	0.0377	0.1730	0.0931	0.1143	0.2386	0.0232	0.0935
1	0.5243	0.7101	2.3603	0.1260	0.1294	0.0377	0.1730	0.0931	0.1145	0.2386	0.0233	0.0935
1	1.9762	-0.1328	1.8333	0.1150	0.1277	0.0357	0.1724	0.0908	0.1232	0.2317	0.0122	0.0931

Dipole mement (in D) 2.14 (DEN) 2.81 1.73 1.32 1.16 1.69 2.28 1.92 2.25 1.89

File TZVPMol357.out
Molecule PMol357 dichloromethylsilane
 SP Mol357 B3LYP/Def2TZVP VAC.
  0 8
Dipole 0.0000 1.9383 0.2618 1.9559
Quadrupole -2.1531 1.7887 0.3644 0.0000 0.0000 0.0746

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0000	0.3217	0.4525	0.5580	-0.3830	0.3673	1.4697	0.1358	0.4732	1.3027	2.8424	0.2002
1	-0.0000	0.3362	1.9192	-0.0442	-0.0424	-0.0701	-0.3356	0.0161	-0.0893	-0.1893	-0.6621	0.0042
17	1.6631	-0.7036	-0.1495	-0.2395	0.2404	-0.1310	-0.3589	-0.0890	-0.1814	-0.3655	-0.7622	-0.1114
17	-1.6631	-0.7036	-0.1495	-0.2395	0.2404	-0.1310	-0.3589	-0.0890	-0.1817	-0.3655	-0.7622	-0.1114
6	-0.0000	2.0029	-0.2997	-0.4346	-0.4568	-0.1740	-0.9618	-0.2797	-0.2557	-1.1227	-0.7718	-0.2905
1	0.8828	2.5627	0.0056	0.1317	0.1334	0.0460	0.1817	0.1015	0.0834	0.2454	0.0362	0.1034
1	-0.8826	2.5629	0.0061	0.1317	0.1334	0.0460	0.1817	0.1015	0.0810	0.2454	0.0362	0.1034
1	-0.0003	1.9389	-1.3862	0.1365	0.1347	0.0468	0.1821	0.1027	0.0705	0.2495	0.0432	0.1020

Dipole mement (in D)	1.96 (DEN)	2.88	2.80	1.27	1.34	1.63	2.07	2.35	3.08	1.81

File TZVPMol358.out
Molecule PMol358 trichlorofluorosilane
 SP Mol358 B3LYP/Def2TZVP VAC.
  0 5
Dipole -0.2282 -0.5274 0.0000 0.5747
Quadrupole 0.4278 -1.2455 0.8177 -0.8954 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
14	0.0957	0.2203	0.0000	0.7694	-0.9903	0.4304	1.7483	0.2623	0.3730	1.6678	3.0550	0.3699
17	-1.9043	0.4057	0.0000	-0.1694	0.3125	-0.0825	-0.4051	-0.0339	-0.0731	-0.3485	-0.7359	-0.0676
17	0.7217	-0.7336	1.6529	-0.1693	0.3126	-0.0825	-0.4051	-0.0338	-0.0717	-0.3484	-0.7358	-0.0675
17	0.7217	-0.7336	-1.6529	-0.1693	0.3126	-0.0825	-0.4051	-0.0338	-0.0717	-0.3484	-0.7358	-0.0675
9	0.7217	1.6625	0.0000	-0.2614	0.0525	-0.1830	-0.5329	-0.1607	-0.1566	-0.6225	-0.8472	-0.1673

Dipole mement (in D)	0.57 (DEN)	0.45	2.42	0.64	0.37	0.91	0.53	1.56	0.24	0.65

File TZVPMol359.out
Molecule PMol359 iodomethylsilane
 SP Mol359 B3LYP/Def2SVP VAC.
  0 8
Dipole -0.4107 -1.9122 0.0000 1.9558
Quadrupole -1.4120 3.2177 -1.8058 0.4499 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0246	-2.5004	0.0000	-0.2257	-0.2483	-0.1699	-0.8429	-0.2783	-0.1657	-1.1315	-0.7577	-0.2843
1	1.3474	-1.7640	1.2011	-0.0686	-0.0953	-0.0763	-0.3003	0.0068	-0.0992	-0.1653	-0.6673	0.0042
1	1.3474	-1.7640	-1.2011	-0.0686	-0.0953	-0.0763	-0.3003	0.0068	-0.0992	-0.1653	-0.6673	0.0042
1	-0.7914	-3.5656	0.0000	0.0514	0.0405	0.0414	0.1625	0.0963	0.0710	0.2481	0.0273	0.1026

```
   1     -1.6296   -2.2893    0.8796    0.0578    0.0406    0.0400    0.1597    0.0952    0.0383    0.2507    0.0343    0.0998
   1     -1.6296   -2.2893   -0.8796    0.0578    0.0406    0.0400    0.1597    0.0952    0.0383    0.2507    0.0342    0.0998
  53      0.0000    0.8984    0.0000   -0.2175   -0.0927   -0.1376   -0.2866   -0.0747   -0.1899   -0.2332   -0.5916   -0.0679
  14      0.5359   -1.4959    0.0000    0.4133    0.4099    0.3387    1.2483    0.0528    0.4064    0.9457    2.5884    0.0416

 Dipole mement (in D)   1.96 (DEN)      2.20      0.42      1.28      1.34      1.24      2.15      1.54      2.26      1.26

-----------------------------------------
File TZVPMol360.out
Molecule PMol360    phosphine
 SP Mol360 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0001   -0.6168    0.0000    0.6168
Quadrupole      0.7201   -1.4393    0.7192    0.0004    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
  15      0.0000    0.1292    0.0000   -0.1655    0.0154    0.0401    0.1063   -0.2019   -0.1685    0.0248    1.5227   -0.2310
   1      1.1812   -0.6460    0.0000    0.0551   -0.0051   -0.0133   -0.0354    0.0673    0.0549   -0.0082   -0.5075    0.0770
   1     -0.5906   -0.6462    1.0226    0.0552   -0.0051   -0.0134   -0.0354    0.0673    0.0568   -0.0083   -0.5077    0.0770
   1     -0.5906   -0.6462   -1.0226    0.0552   -0.0051   -0.0134   -0.0354    0.0673    0.0568   -0.0083   -0.5077    0.0770

 Dipole mement (in D)   0.62 (DEN)      0.62      0.06      0.15      0.40      0.75      0.63      0.09      5.67      0.86

-----------------------------------------
File TZVPMol361.out
Molecule PMol361    methylphosphine
 SP Mol361 B3LYP/Def2TZVP VAC.
    0    7
Dipole          0.9939    0.0000    0.6150    1.1688
Quadrupole     -0.2044    0.9731   -0.7686    0.0000   -1.3102    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
  15     -0.6615    0.0000   -0.1247   -0.0463    0.1971    0.0535    0.2455   -0.1562   -0.2833    0.2926    1.5136   -0.1935
   1     -0.9219   -1.0222    0.8174    0.0292   -0.0024   -0.0218   -0.0554    0.0601    0.0819   -0.0354   -0.5266    0.0635
   1     -0.9219    1.0222    0.8174    0.0292   -0.0024   -0.0218   -0.0554    0.0601    0.0819   -0.0354   -0.5266    0.0635
   6      1.1784   -0.0000    0.0251   -0.3873   -0.5216   -0.1232   -0.5382   -0.2401    0.0539   -0.8847   -0.5298   -0.2314
   1      1.5782    0.8750   -0.4826    0.1239    0.1119    0.0387    0.1351    0.0933    0.0406    0.2223    0.0226    0.1004
   1      1.5782   -0.8750   -0.4826    0.1239    0.1119    0.0387    0.1351    0.0933    0.0406    0.2223    0.0226    0.1004
   1      1.5386   -0.0000    1.0500    0.1274    0.1054    0.0359    0.1332    0.0896   -0.0156    0.2182    0.0239    0.0971

 Dipole mement (in D)   1.17 (DEN)      0.59      1.10      0.28      0.67      0.88      1.13      0.81      5.73      1.16

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File TZVPMol362.out
Molecule PMol362    dimethyl_methylphosphona
 SP Mol362 B3LYP/Def2TZVP VAC.
    0   16
Dipole          0.5120   -0.2764   -2.1713    2.2479
Quadrupole      5.7983    3.5824   -9.3808    1.4418   -0.8373   -1.1733
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
```

15	-0.0001	0.3493	0.1711	0.8009	0.2311	0.4590	2.1297	0.4041	1.0822	2.3816	3.5678	0.4620
8	0.8642	-0.6962	-0.6803	-0.3574	0.0397	-0.1859	-0.6588	-0.2522	-0.3807	-0.7984	-1.3365	-0.2506
8	-1.4375	0.1566	-0.4715	-0.3403	0.0509	-0.1783	-0.6392	-0.2441	-0.3567	-0.7881	-1.3362	-0.2450
8	0.1144	0.1597	1.6191	-0.5351	-0.2592	-0.4053	-0.9840	-0.4239	-0.6406	-1.0948	-1.5110	-0.4296
6	2.0960	-1.1751	-0.1490	-0.1664	-0.3446	0.0091	-0.0387	-0.1082	0.0514	-0.2505	0.4647	-0.0885
1	2.3615	-2.0680	-0.7081	0.1221	0.1089	0.0435	0.1005	0.1041	0.0644	0.1851	0.0328	0.0944
1	2.8871	-0.4327	-0.2736	0.1050	0.1016	0.0359	0.0844	0.0960	0.0370	0.1659	0.0143	0.0887
1	1.9964	-1.4157	0.9084	0.1453	0.1105	0.0419	0.1063	0.1065	0.0554	0.1973	0.0605	0.0889
6	0.4320	1.9640	-0.4498	-0.3804	-0.4078	-0.1198	-0.9127	-0.2258	-0.7102	-1.0328	-0.6769	-0.2415
1	1.4736	2.1705	-0.2134	0.1288	0.1262	0.0518	0.1814	0.1099	0.2112	0.2397	0.0409	0.1111
1	0.2939	2.0169	-1.5265	0.1360	0.1263	0.0510	0.1889	0.1099	0.1886	0.2438	0.0495	0.1057
1	-0.1836	2.7210	0.0292	0.1375	0.1290	0.0559	0.1917	0.1140	0.2050	0.2486	0.0537	0.1139
6	-2.1909	-1.0058	-0.1293	-0.1845	-0.3383	0.0127	-0.0471	-0.1044	-0.0784	-0.2534	0.4574	-0.0861
1	-1.7441	-1.8962	-0.5722	0.1228	0.1051	0.0392	0.0912	0.1011	0.0760	0.1774	0.0320	0.0876
1	-2.2457	-1.1273	0.9521	0.1401	0.1103	0.0438	0.1018	0.1069	0.0924	0.1907	0.0506	0.0926
1	-3.1894	-0.8664	-0.5321	0.1257	0.1103	0.0457	0.1048	0.1065	0.1031	0.1879	0.0363	0.0965

Dipole mement (in D)	2.25 (DEN)	1.77	1.87	1.99	2.25	2.06	2.23	2.19	3.23	2.06

File TZVPMol363.out
Molecule PMol363 hypophosphorous_acid
SP Mol363 B3LYP/Def2TZVP VAC.
0 6
Dipole -2.3137 1.0137 0.9115 2.6854
Quadrupole -4.5595 3.1096 1.4499 4.2698 -1.2671 -1.3671

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.2764	-0.5366	-0.0327	-0.5030	-0.2914	-0.3935	-0.8621	-0.4131	-0.5963	-1.0502	-1.4886	-0.4062
15	0.1204	0.3598	0.0184	0.6117	0.2984	0.4253	1.6164	0.2637	0.8078	1.7780	3.3709	0.2670
8	-1.3328	-0.3015	-0.0711	-0.4708	-0.1538	-0.2239	-0.8894	-0.4084	-0.6034	-0.9725	-1.3703	-0.3371
1	0.0596	1.1564	1.1780	0.0076	-0.0206	-0.0048	-0.1929	0.0864	-0.0545	-0.1358	-0.5650	0.0811
1	-0.0265	1.2902	-1.0221	0.0218	-0.0091	0.0050	-0.1673	0.0983	0.0001	-0.1226	-0.5584	0.0897
1	-1.3880	-1.1383	0.3992	0.3328	0.1765	0.1919	0.4953	0.3730	0.4462	0.5030	0.6111	0.3054

Dipole mement (in D)	2.69 (DEN)	2.54	1.89	2.31	2.79	2.70	2.71	4.15	3.53	2.70

File TZVPMol364.out
Molecule PMol364 trimethylphosphine
SP Mol364 B3LYP/Def2TZVP VAC.
0 13
Dipole 0.0002 0.0001 1.1888 1.1888
Quadrupole 1.4683 1.4684 -2.9367 -0.0003 -0.0002 0.0004

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.0000	0.0001	-0.6057	0.1754	0.4490	0.0920	0.5597	-0.0577	-0.2293	0.7750	1.5349	-0.0936
6	0.2660	1.5887	0.2786	-0.4069	-0.4785	-0.1308	-0.6004	-0.2449	-0.1494	-0.9124	-0.5520	-0.2455
1	-0.5031	2.3065	-0.0022	0.1216	0.1129	0.0355	0.1385	0.0903	0.0803	0.2237	0.0164	0.0952
1	1.2271	2.0167	-0.0021	0.1216	0.1129	0.0355	0.1385	0.0903	0.0824	0.2237	0.0164	0.0952

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   1      0.2458    1.4688    1.3636    0.1053    0.1030    0.0291    0.1368    0.0837    0.0562    0.2066    0.0075    0.0863
   6     -1.5090   -0.5641    0.2783   -0.4071   -0.4785   -0.1307   -0.6002   -0.2449   -0.1357   -0.9123   -0.5519   -0.2455
   1     -1.7461   -1.5890   -0.0027    0.1216    0.1129    0.0355    0.1385    0.0902    0.0779    0.2237    0.0164    0.0952
   1     -1.3954   -0.5218    1.3634    0.1053    0.1030    0.0291    0.1368    0.0837    0.0543    0.2066    0.0075    0.0863
   1     -2.3602    0.0543   -0.0024    0.1216    0.1129    0.0355    0.1385    0.0903    0.0791    0.2237    0.0164    0.0952
   6      1.2430   -1.0247    0.2782   -0.4069   -0.4785   -0.1308   -0.6004   -0.2449   -0.0835   -0.9123   -0.5517   -0.2455
   1      1.1500   -0.9471    1.3632    0.1052    0.1030    0.0291    0.1368    0.0837    0.0376    0.2066    0.0075    0.0863
   1      1.1328   -2.0711   -0.0023    0.1216    0.1129    0.0355    0.1385    0.0903    0.0633    0.2237    0.0164    0.0952
   1      2.2491   -0.7179   -0.0033    0.1216    0.1129    0.0355    0.1385    0.0903    0.0669    0.2237    0.0164    0.0952

 Dipole mement (in D)   1.19 (DEN)      0.08      1.21      0.22      1.36      0.82      1.14      1.87      6.53      0.98

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File TZVPMol365.out
Molecule PMol365    dimethylphosphine
 SP Mol365 B3LYP/Def2TZVP VAC.
    0   10
Dipole         -0.3871    1.2018    0.0000    1.2626
Quadrupole      0.1678   -1.8061    1.6383    1.3392    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  15      0.0375   -0.6651    0.0000    0.0754    0.3414    0.0715    0.3955   -0.1076   -0.2952    0.5450    1.5208   -0.1470
   1     -1.3539   -0.9272    0.0000    0.0033    0.0020   -0.0281   -0.0743    0.0552    0.1087   -0.0597   -0.5409    0.0516
   6      0.0375    0.5250    1.4050   -0.4012   -0.5004   -0.1278   -0.5678   -0.2433   -0.0756   -0.9001   -0.5425   -0.2389
   6      0.0375    0.5250   -1.4050   -0.4012   -0.5004   -0.1278   -0.5678   -0.2433   -0.0756   -0.9001   -0.5426   -0.2389
   1     -0.7039    1.3156    1.2994    0.1162    0.1039    0.0322    0.1345    0.0863    0.0317    0.2116    0.0143    0.0914
   1     -0.1457   -0.0006    2.3397    0.1265    0.1126    0.0377    0.1362    0.0922    0.0579    0.2261    0.0215    0.0989
   1      1.0204    0.9869    1.4830    0.1192    0.1122    0.0361    0.1365    0.0909    0.0793    0.2198    0.0167    0.0964
   1     -0.7039    1.3156   -1.2994    0.1162    0.1039    0.0322    0.1345    0.0863    0.0317    0.2116    0.0143    0.0914
   1      1.0204    0.9869   -1.4830    0.1192    0.1122    0.0361    0.1365    0.0909    0.0793    0.2198    0.0167    0.0964
   1     -0.1457   -0.0006   -2.3397    0.1265    0.1126    0.0377    0.1362    0.0922    0.0579    0.2261    0.0215    0.0989

 Dipole mement (in D)   1.26 (DEN)      0.32      1.25      0.23      1.00      0.87      1.27      1.38      6.06      1.13

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File TZVPMol366.out
Molecule PMol366    PH
 SP Mol366 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000   -0.4536    0.4536
Quadrupole     -0.1104   -0.1104    0.2208    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  15      0.0000    0.0000    0.0889   -0.0509    0.0381    0.0281    0.0633   -0.0507   -0.0640    0.1159    0.5210   -0.0536
   1      0.0000    0.0000   -1.3330    0.0509   -0.0381   -0.0281   -0.0633    0.0507    0.0640   -0.1159   -0.5210    0.0536

 Dipole mement (in D)   0.45 (DEN)      0.35      0.26      0.19      0.43      0.35      0.44      0.79      3.56      0.37

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File TZVPMol367.out
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Molecule PMol367   CH2PH2
 SP Mol367 B3LYP/Def2TZVP VAC.
    0   6
Dipole   -0.2294   0.0002   0.3620   0.4286
Quadrupole   0.4535   1.6745   -2.1280   0.0003   1.4373   -0.0003

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.5760	-0.0000	-0.1231	0.0059	0.2487	0.0799	0.2820	-0.1304	-0.0943	0.3512	1.6892	-0.1684
6	-1.1728	-0.0000	0.0705	-0.3500	-0.4667	-0.1313	-0.4615	-0.1945	-0.4479	-0.7010	-0.7848	-0.1694
1	0.9313	-1.0482	0.7559	0.0423	0.0087	-0.0096	-0.0415	0.0726	0.0792	-0.0204	-0.5062	0.0757
1	0.9312	1.0488	0.7551	0.0423	0.0087	-0.0096	-0.0415	0.0726	0.0792	-0.0204	-0.5062	0.0757
1	-1.7330	0.9177	-0.0439	0.1297	0.1003	0.0353	0.1313	0.0898	0.1919	0.1953	0.0539	0.0933
1	-1.7331	-0.9177	-0.0442	0.1297	0.1003	0.0353	0.1312	0.0898	0.1920	0.1953	0.0539	0.0933

 Dipole mement (in D)   0.43 (DEN)   0.24   1.75   0.34   1.07   0.51   0.46   1.63   6.17   0.67

File TZVPMol368.out
Molecule PMol368   CH3CH(PH2)CH3
 SP Mol368 B3LYP/Def2TZVP VAC.
    0   13
Dipole   -1.1465   0.4906   -0.0385   1.2477
Quadrupole   -1.4796   0.0334   1.4462   1.7285   0.7529   -0.4907

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1308	-1.2378	0.1049	-0.3402	-0.3151	-0.0838	-0.3592	-0.2294	-0.4634	-0.5989	0.0094	-0.2411
6	-0.4180	0.0100	-0.4006	-0.0659	-0.4847	-0.0454	-0.0834	-0.0863	0.3778	-0.4535	-0.4239	-0.0133
6	-1.0816	1.2750	0.1163	-0.3176	-0.3136	-0.0854	-0.3498	-0.2321	-0.5266	-0.5935	0.0184	-0.2428
15	1.3986	-0.1192	-0.0018	-0.0565	0.2637	0.0480	0.1815	-0.1606	-0.3553	0.2910	1.4542	-0.2108
1	-0.6877	-2.1537	-0.2840	0.1219	0.1189	0.0306	0.1027	0.0837	0.1192	0.2100	0.0038	0.0854
1	-2.1831	-1.2295	-0.1821	0.1084	0.1193	0.0310	0.1089	0.0830	0.0996	0.2052	-0.0011	0.0833
1	-1.0955	-1.2940	1.1946	0.1057	0.1187	0.0293	0.1055	0.0825	0.1455	0.1980	-0.0038	0.0827
1	-0.4620	0.0092	-1.4941	0.0806	0.1409	0.0332	0.0922	0.0949	0.0476	0.2110	0.0004	0.0892
1	-0.6022	2.1755	-0.2647	0.1120	0.1165	0.0288	0.1014	0.0815	0.1124	0.2060	-0.0011	0.0839
1	-1.0387	1.3191	1.2060	0.1019	0.1180	0.0279	0.1036	0.0809	0.1225	0.1992	-0.0030	0.0811
1	-2.1355	1.3136	-0.1692	0.1017	0.1178	0.0279	0.1028	0.0797	0.1329	0.1995	-0.0075	0.0796
1	1.7397	1.2242	-0.2884	0.0254	-0.0009	-0.0209	-0.0545	0.0614	0.0953	-0.0343	-0.5239	0.0622
1	1.2694	0.1401	1.3854	0.0228	0.0006	-0.0214	-0.0517	0.0609	0.0924	-0.0398	-0.5208	0.0606

 Dipole mement (in D)   1.25 (DEN)   0.58   1.45   0.31   0.67   0.94   1.23   0.81   5.63   1.28

File TZVPMol369.out
Molecule PMol369   CH3PH
 SP Mol369 B3LYP/Def2TZVP VAC.
    0   6
Dipole   -1.2072   0.5206   0.0001   1.3147
Quadrupole   -0.3326   0.2124   0.1202   1.0114   0.0001   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1355	0.0121	0.0000	-0.3912	-0.5493	-0.1305	-0.5656	-0.2447	0.1383	-0.9460	-0.5600	-0.2369

15	0.6981	-0.0984	-0.0000	-0.0202	0.2267	0.0422	0.2099	-0.0870	-0.2166	0.3462	1.0082	-0.1156
1	-1.5698	-0.9846	-0.0000	0.1267	0.1096	0.0377	0.1371	0.0922	0.0157	0.2221	0.0238	0.0993
1	-1.5041	0.5425	-0.8779	0.1306	0.1132	0.0404	0.1435	0.0943	-0.0057	0.2295	0.0318	0.1011
1	-1.5040	0.5424	0.8780	0.1306	0.1132	0.0404	0.1435	0.0943	-0.0057	0.2295	0.0318	0.1011
1	0.9195	1.3035	0.0001	0.0235	-0.0135	-0.0302	-0.0683	0.0509	0.0740	-0.0814	-0.5350	0.0510

Dipole mement (in D) 1.31 (DEN) 0.71 1.24 0.24 0.60 0.89 1.28 1.13 5.13 1.16

File TZVPMol370.out
Molecule PMol370 (CH3)3PH2
SP Mol370 B3LYP/Def2TZVP VAC.
0 16
Dipole -1.0898 0.0000 0.5503 1.2209
Quadrupole -1.2394 1.4465 -0.2071 0.0000 1.9022 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.8234	-0.0000	1.4542	-0.3223	-0.2890	-0.0865	-0.3893	-0.2314	-0.5115	-0.5964	0.0158	-0.2464
6	-0.3502	0.0000	0.0059	0.0348	-0.5119	-0.0117	0.1315	-0.0158	0.5955	-0.2601	-0.3792	0.0938
6	-0.8662	1.2484	-0.7070	-0.3435	-0.2906	-0.0850	-0.3995	-0.2286	-0.4512	-0.6041	0.0048	-0.2447
15	1.5216	-0.0000	-0.1366	-0.0626	0.2953	0.0487	0.1812	-0.1595	-0.3710	0.2939	1.4262	-0.2170
6	-0.8662	-1.2484	-0.7070	-0.3435	-0.2906	-0.0850	-0.3995	-0.2286	-0.4512	-0.6041	0.0045	-0.2447
1	-1.9161	-0.0000	1.5016	0.0980	0.1200	0.0267	0.1075	0.0792	0.1308	0.1977	-0.0099	0.0772
1	-0.4720	0.8797	1.9933	0.1088	0.1188	0.0279	0.1062	0.0813	0.1020	0.2048	-0.0032	0.0818
1	-0.4720	-0.8798	1.9933	0.1088	0.1188	0.0279	0.1062	0.0813	0.1020	0.2048	-0.0032	0.0818
1	-1.9580	1.2705	-0.6906	0.1046	0.1219	0.0301	0.1142	0.0828	0.0967	0.2038	-0.0030	0.0810
1	-0.5521	1.2799	-1.7505	0.1196	0.1211	0.0298	0.1079	0.0836	0.1167	0.2087	0.0015	0.0835
1	-0.5151	2.1626	-0.2267	0.1117	0.1203	0.0298	0.1087	0.0833	0.1228	0.2045	-0.0035	0.0836
1	1.7616	-1.0255	0.8099	0.0249	0.0013	-0.0211	-0.0529	0.0615	0.0911	-0.0352	-0.5232	0.0609
1	1.7617	1.0255	0.8098	0.0249	0.0013	-0.0211	-0.0529	0.0615	0.0911	-0.0352	-0.5232	0.0609
1	-0.5521	-1.2799	-1.7505	0.1196	0.1211	0.0298	0.1079	0.0836	0.1167	0.2087	0.0015	0.0835
1	-1.9580	-1.2704	-0.6906	0.1046	0.1219	0.0301	0.1142	0.0828	0.0967	0.2038	-0.0030	0.0810
1	-0.5151	-2.1626	-0.2268	0.1117	0.1203	0.0298	0.1087	0.0833	0.1228	0.2045	-0.0035	0.0836

Dipole mement (in D) 1.22 (DEN) 0.54 1.45 0.31 0.63 0.94 1.21 0.84 5.56 1.29

File TZVPMol371.out
Molecule PMol371 CH3CH(PH)CH3
SP Mol371 B3LYP/Def2TZVP VAC.
0 12
Dipole -1.4067 0.0000 0.0785 1.4089
Quadrupole -2.0631 0.6400 1.4231 -0.0001 1.1618 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0571	-1.2582	0.1143	-0.3264	-0.3138	-0.0841	-0.3515	-0.2300	-0.4486	-0.5949	0.0117	-0.2409
6	-0.3773	0.0000	-0.4108	-0.0655	-0.5108	-0.0534	-0.1031	-0.0924	0.4726	-0.5088	-0.4454	-0.0217
6	-1.0571	1.2582	0.1143	-0.3264	-0.3138	-0.0841	-0.3515	-0.2300	-0.4485	-0.5949	0.0119	-0.2409
15	1.4382	0.0000	-0.0218	-0.0406	0.2967	0.0417	0.1502	-0.0866	-0.2849	0.3500	0.9496	-0.1292
1	-0.5855	-2.1675	-0.2567	0.1186	0.1179	0.0292	0.1009	0.0821	0.1158	0.2083	0.0017	0.0835

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   1     -2.1083   -1.2862   -0.1802    0.1069    0.1197    0.0307    0.1080    0.0825    0.0963    0.2038   -0.0016    0.0826
   1     -1.0221   -1.2915    1.2043    0.1040    0.1185    0.0287    0.1056    0.0819    0.1060    0.2001   -0.0006    0.0822
   1     -0.4398    0.0000   -1.5027    0.0821    0.1392    0.0321    0.0926    0.0937   -0.0117    0.2109    0.0014    0.0881
   1     -0.5855    2.1675   -0.2567    0.1186    0.1179    0.0292    0.1009    0.0821    0.1158    0.2083    0.0017    0.0835
   1     -1.0221    1.2915    1.2043    0.1040    0.1185    0.0287    0.1056    0.0819    0.1060    0.2001   -0.0006    0.0822
   1     -2.1083    1.2862   -0.1801    0.1069    0.1197    0.0307    0.1080    0.0825    0.0963    0.2038   -0.0017    0.0826
   1      1.2472   -0.0001    1.3876    0.0180   -0.0096   -0.0292   -0.0656    0.0524    0.0850   -0.0869   -0.5286    0.0482

 Dipole mement (in D)   1.41 (DEN)      0.77      1.62      0.22      0.66      0.94      1.38      1.20      4.94      1.26

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File TZVPMol372.out
Molecule PMol372    phosphorus_mononitride
 SP Mol372 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000    2.8788    2.8788
Quadrupole      0.8727    0.8727   -1.7454    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  15      0.0000    0.0000    0.4732    0.2531    0.3736    0.2542    0.5129    0.3227    0.4050    0.8388    1.3964    0.3451
   7      0.0000    0.0000   -1.0140   -0.2531   -0.3736   -0.2542   -0.5129   -0.3227   -0.4050   -0.8388   -1.3964   -0.3451

 Dipole mement (in D)   2.88 (DEN)      1.81      2.67      1.82      3.66      2.31      2.89      5.99      9.98      2.47

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File TZVPMol373.out
Molecule PMol373    phosphorus_oxychloride
 SP Mol373 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.0010   -0.0009   -2.4969    2.4969
Quadrupole      2.6836    2.6795   -5.3632    0.0004   -0.0010    0.0025
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  15      0.0000   -0.0003    0.4209    0.7746   -0.3992    0.3823    1.5512    0.2734    0.2853    1.6578    3.1051    0.3648
  17     -1.5015   -1.0137   -0.4174   -0.1111    0.2074   -0.0142   -0.2419    0.0266    0.0158   -0.2209   -0.5626    0.0003
  17     -0.1276    1.8071   -0.4170   -0.1113    0.2071   -0.0144   -0.2421    0.0265    0.0155   -0.2211   -0.5625    0.0001
  17      1.6289   -0.7929   -0.4176   -0.1112    0.2073   -0.0142   -0.2419    0.0267    0.0155   -0.2210   -0.5626    0.0003
   8      0.0003   -0.0006    1.8714   -0.4411   -0.2226   -0.3395   -0.8253   -0.3532   -0.3320   -0.9948   -1.4175   -0.3655

 Dipole mement (in D)   2.50 (DEN)      1.73      4.05      2.19      2.83      2.78      2.50      4.26      3.08      2.55

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File TZVPMol374.out
Molecule PMol374    thiophosphoryl_fluorid
 SP Mol374 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.5542    0.0007   -0.0013    0.5542
Quadrupole      0.0340   -0.0182   -0.0157   -0.0014    0.0022    0.0004
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  15     -0.1691    0.0002   -0.0003    0.9089   -0.1311    0.4852    1.8394    0.3928    0.2531    2.1065    3.3279    0.4595
```

16	1.6885	-0.0001	-0.0005	-0.2619	0.0470	-0.1706	-0.6268	-0.1323	-0.1237	-0.5041	-0.9219	-0.1582
9	-0.9067	1.3513	-0.1003	-0.2157	0.0279	-0.1049	-0.4042	-0.0868	-0.0441	-0.5341	-0.8021	-0.1004
9	-0.9055	-0.5883	1.2205	-0.2157	0.0281	-0.1049	-0.4042	-0.0869	-0.0438	-0.5342	-0.8022	-0.1004
9	-0.9079	-0.7631	-1.1187	-0.2156	0.0281	-0.1049	-0.4042	-0.0868	-0.0416	-0.5341	-0.8022	-0.1004

Dipole mement (in D) 0.55 (DEN) 0.04 0.12 0.41 1.30 0.26 0.65 1.18 0.30 0.34

File TZVPMol375.out
Molecule PMol375 hypophosphorous_acid(=Mo
SP Mol375 B3LYP/Def2TZVP VAC.
0 6
Dipole -2.3137 1.0137 0.9115 2.6854
Quadrupole -4.5595 3.1096 1.4499 4.2698 -1.2671 -1.3670

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.1204	0.3598	0.0184	0.6117	0.2984	0.4253	1.6164	0.2637	0.8078	1.7780	3.3709	0.2670
1	-0.0265	1.2902	-1.0221	0.0218	-0.0091	0.0050	-0.1673	0.0983	0.0001	-0.1226	-0.5584	0.0897
1	0.0596	1.1564	1.1780	0.0076	-0.0206	-0.0048	-0.1929	0.0864	-0.0545	-0.1358	-0.5650	0.0811
8	-1.3328	-0.3015	-0.0711	-0.4708	-0.1538	-0.2239	-0.8894	-0.4084	-0.6034	-0.9725	-1.3703	-0.3371
1	-1.3880	-1.1383	0.3992	0.3328	0.1765	0.1919	0.4953	0.3730	0.4462	0.5030	0.6111	0.3054
8	1.2764	-0.5366	-0.0327	-0.5030	-0.2914	-0.3935	-0.8621	-0.4131	-0.5963	-1.0502	-1.4886	-0.4062

Dipole mement (in D) 2.69 (DEN) 2.54 1.89 2.31 2.79 2.70 2.71 4.15 3.53 2.70

File TZVPMol376.out
Molecule PMol376 methylphosphonic_acid
SP Mol376 B3LYP/Def2TZVP VAC.
0 10
Dipole -0.4811 0.0000 -1.3777 1.4593
Quadrupole 4.4392 3.2075 -7.6467 0.0000 -4.5672 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.8721	-0.0000	1.3473	-0.5304	-0.2729	-0.4180	-0.9906	-0.4353	-0.6797	-1.0916	-1.5215	-0.4394
15	0.0886	0.0000	0.1097	0.7661	0.1808	0.4617	2.2120	0.3985	1.0829	2.3491	3.5733	0.4555
6	-1.6870	-0.0000	0.2131	-0.3697	-0.4074	-0.1170	-0.8866	-0.2227	-0.4538	-1.0348	-0.6847	-0.2390
8	0.3538	1.2696	-0.8288	-0.4704	-0.1222	-0.2325	-0.9538	-0.4111	-0.6095	-0.9868	-1.3751	-0.3543
8	0.3538	-1.2696	-0.8288	-0.4704	-0.1222	-0.2325	-0.9538	-0.4111	-0.6095	-0.9868	-1.3753	-0.3543
1	1.1618	1.7239	-0.5764	0.3341	0.1783	0.1852	0.4979	0.3691	0.4129	0.5052	0.6108	0.2956
1	1.1618	-1.7239	-0.5764	0.3341	0.1783	0.1852	0.4979	0.3691	0.4129	0.5052	0.6108	0.2956
1	-2.1250	-0.0000	-0.7822	0.1403	0.1303	0.0557	0.1987	0.1149	0.1758	0.2480	0.0555	0.1107
1	-2.0217	-0.8853	0.7466	0.1331	0.1285	0.0561	0.1891	0.1143	0.1340	0.2462	0.0525	0.1148
1	-2.0217	0.8853	0.7466	0.1331	0.1285	0.0561	0.1891	0.1143	0.1340	0.2462	0.0525	0.1148

Dipole mement (in D) 1.46 (DEN) 1.34 1.67 1.85 0.92 1.32 1.53 1.02 1.56 1.59

File TZVPMol377.out
Molecule PMol377 phosphine_oxide

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 SP Mol377 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0001    3.5989    0.0000    3.5989
Quadrupole      1.1706   -2.3414    1.1707    0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      0.0000   -1.0931    0.0000   -0.5150   -0.3228   -0.3928   -0.7855   -0.4137   -0.5781   -1.0361   -1.4749   -0.4006
  15      0.0000    0.3784    0.0000    0.4349    0.3717    0.3849    1.2136    0.1506    0.7232    1.3288    3.1273    0.1239
   1     -1.2551    1.0229    0.0000    0.0267   -0.0163    0.0026   -0.1427    0.0877   -0.0482   -0.0976   -0.5508    0.0922
   1      0.6276    1.0230    1.0870    0.0267   -0.0163    0.0026   -0.1427    0.0877   -0.0484   -0.0976   -0.5508    0.0922
   1      0.6276    1.0230   -1.0870    0.0267   -0.0163    0.0026   -0.1427    0.0877   -0.0484   -0.0976   -0.5508    0.0922

 Dipole mement (in D)   3.60 (DEN)      3.89      2.13      2.80      4.23      3.74      3.64      6.42      5.31      3.69

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File TZVPMol378.out
Molecule PMol378    OPH
 SP Mol378 B3LYP/Def2TZVP VAC.
    0    3
Dipole         -0.3237   -2.3461    0.0000    2.3683
Quadrupole     -0.4022   -1.6912    2.0934    0.4625    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      0.0591    1.0019    0.0000   -0.3807   -0.2556   -0.2960   -0.5667   -0.3102   -0.3335   -0.9088   -1.3112   -0.3028
  15      0.0591   -0.4784    0.0000    0.3886    0.3079    0.3389    0.7354    0.2762    0.3046    1.0923    1.8437    0.2691
   1     -1.3586   -0.8385    0.0000   -0.0079   -0.0523   -0.0429   -0.1687    0.0341    0.0289   -0.1835   -0.5321    0.0337

 Dipole mement (in D)   2.37 (DEN)      2.69      1.76      2.05      3.91      2.28      2.43      6.27      9.15      2.22

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File TZVPMol379.out
Molecule PMol379    hydroxyphosphane
 SP Mol379 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.8386   -0.0265    0.0000    0.8390
Quadrupole      0.4772   -0.2938   -0.1835    3.8051    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   8      0.0399    1.0862    0.0000   -0.4948   -0.2471   -0.2540   -0.7276   -0.4390   -0.4741   -0.9456   -1.3267   -0.3530
  15      0.0399   -0.5704    0.0000    0.1066    0.1282    0.1341    0.4478   -0.0317   -0.1589    0.6144    1.8053   -0.0516
   1      0.9420    1.4069    0.0000    0.3171    0.1517    0.1663    0.4424    0.3468    0.4183    0.4819    0.5850    0.2845
   1     -0.9300   -0.7701    1.0155    0.0356   -0.0164   -0.0233   -0.0813    0.0619    0.1074   -0.0753   -0.5317    0.0601
   1     -0.9300   -0.7701   -1.0155    0.0356   -0.0164   -0.0233   -0.0813    0.0619    0.1074   -0.0753   -0.5317    0.0601

 Dipole mement (in D)   0.84 (DEN)      1.44      0.95      1.02      3.03      0.98      0.81      3.95      8.48      0.71

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File TZVPMol380.out
Molecule PMol380    trimethylphosphine_oxide
 SP Mol380 B3LYP/Def2TZVP VAC.
    0   14
```

Dipole 0.0002 0.0011 -4.2886 4.2886
Quadrupole 3.3303 3.3285 -6.6589 0.0006 0.0002 0.0042

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.0000	-0.0001	0.1876	0.6157	0.4315	0.3798	1.7948	0.2259	1.0992	1.9633	3.1549	0.2293
6	-0.7825	1.4512	-0.5499	-0.3993	-0.4172	-0.1241	-0.8261	-0.2351	-0.5529	-1.0021	-0.6501	-0.2440
6	1.6479	-0.0476	-0.5503	-0.3992	-0.4172	-0.1241	-0.8260	-0.2350	-0.5739	-1.0021	-0.6498	-0.2439
6	-0.8654	-1.4028	-0.5509	-0.3992	-0.4172	-0.1241	-0.8262	-0.2350	-0.5562	-1.0021	-0.6503	-0.2440
8	-0.0001	-0.0007	1.6643	-0.5641	-0.2847	-0.4287	-0.8978	-0.4463	-0.7171	-1.0815	-1.5105	-0.4471
1	-1.8162	1.5149	-0.2161	0.1340	0.1252	0.0498	0.1788	0.1062	0.1486	0.2413	0.0406	0.1085
1	-0.7661	1.4189	-1.6385	0.1140	0.1179	0.0408	0.1694	0.0960	0.1297	0.2256	0.0208	0.0995
1	-0.2668	2.3499	-0.2175	0.1340	0.1252	0.0498	0.1788	0.1062	0.1489	0.2413	0.0406	0.1085
1	2.1689	-0.9431	-0.2175	0.1340	0.1252	0.0498	0.1788	0.1062	0.1549	0.2413	0.0406	0.1085
1	2.2197	0.8163	-0.2173	0.1340	0.1252	0.0498	0.1788	0.1062	0.1547	0.2413	0.0407	0.1085
1	1.6113	-0.0465	-1.6389	0.1140	0.1179	0.0408	0.1694	0.0961	0.1345	0.2256	0.0208	0.0995
1	-1.9011	-1.4067	-0.2170	0.1341	0.1252	0.0498	0.1789	0.1063	0.1496	0.2413	0.0407	0.1086
1	-0.4026	-2.3300	-0.2192	0.1340	0.1252	0.0498	0.1788	0.1062	0.1496	0.2413	0.0406	0.1085
1	-0.8472	-1.3707	-1.6395	0.1140	0.1179	0.0408	0.1694	0.0961	0.1306	0.2256	0.0208	0.0995

Dipole mement (in D) 4.29 (DEN) 4.32 2.15 3.38 4.13 4.43 4.35 5.77 4.82 4.46

File TZVPMol381.out
Molecule PMol381 PO
SP Mol381 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 2.1072 2.1072
Quadrupole 2.0326 -0.7648 -1.2678 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.0000	0.0000	0.5140	0.3293	0.2460	0.2708	0.5014	0.2794	0.3011	0.9047	1.2786	0.2797
8	0.0000	0.0000	-0.9637	-0.3293	-0.2460	-0.2709	-0.5014	-0.2795	-0.3011	-0.9047	-1.2786	-0.2797

Dipole mement (in D) 2.11 (DEN) 2.34 1.75 1.92 3.56 1.98 2.14 6.42 9.08 1.99

File TZVPMol382.out
Molecule PMol382 phosphorus_trichloride
SP Mol382 B3LYP/Def2TZVP VAC.
0 4
Dipole -0.0001 0.0003 0.5648 0.5648
Quadrupole -0.1627 -0.1617 0.3245 0.0003 0.0000 -0.0004

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	-0.0000	-0.0002	0.7273	0.4738	-0.2802	0.2410	0.5692	0.1369	0.1383	0.7648	1.5754	0.1841
17	1.7341	-0.5456	-0.2138	-0.1580	0.0933	-0.0804	-0.1898	-0.0457	-0.0457	-0.2549	-0.5252	-0.0614
17	-1.3397	-1.2286	-0.2142	-0.1580	0.0934	-0.0803	-0.1897	-0.0456	-0.0468	-0.2549	-0.5253	-0.0614
17	-0.3944	1.7743	-0.2137	-0.1579	0.0935	-0.0803	-0.1897	-0.0456	-0.0458	-0.2549	-0.5254	-0.0613

Dipole mement (in D) 0.56 (DEN) 2.14 1.27 1.09 2.57 0.62 0.63 3.46 7.12 0.83

File TZVPMol383.out
Molecule PMol383 phosphorus_trifluoride
 SP Mol383 B3LYP/Def2TZVP VAC.
    0   4
Dipole   -0.7136   0.8223   0.0000   1.0888
Quadrupole   0.0866   0.2122   -0.2988   -0.4416   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	-0.3308	0.3811	0.0000	0.7190	0.1452	0.4278	1.0399	0.3769	0.2912	1.6894	2.4209	0.4023
9	1.2131	0.6817	0.0000	-0.2396	-0.0483	-0.1426	-0.3466	-0.1256	-0.0973	-0.5631	-0.8069	-0.1341
9	-0.3308	-0.6584	1.1807	-0.2397	-0.0484	-0.1426	-0.3467	-0.1257	-0.0970	-0.5631	-0.8069	-0.1341
9	-0.3308	-0.6584	-1.1807	-0.2397	-0.0484	-0.1426	-0.3467	-0.1257	-0.0970	-0.5631	-0.8069	-0.1341

Dipole mement (in D)	1.09 (DEN)	2.71	0.55	1.61	3.92	1.42	1.10	6.37	9.13	1.52		

File TZVPMol384.out
Molecule PMol384 phosphoryl_fluoride
 SP Mol384 B3LYP/Def2TZVP VAC.
    0   5
Dipole   -1.8542   0.0026   0.0000   1.8542
Quadrupole   -3.1725   1.5861   1.5864   0.0075   0.0019   0.0002

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	1.5831	-0.0026	-0.0006	-0.4333	-0.1914	-0.3418	-0.9565	-0.3535	-0.5292	-1.0294	-1.4620	-0.3748
15	0.1471	-0.0003	-0.0001	1.0681	0.0366	0.6155	2.2656	0.5684	1.0633	2.6239	3.8626	0.6515
9	-0.5506	-0.2149	1.3445	-0.2116	0.0516	-0.0912	-0.4364	-0.0717	-0.1781	-0.5315	-0.8003	-0.0923
9	-0.5486	1.2731	-0.4850	-0.2116	0.0516	-0.0912	-0.4364	-0.0717	-0.1780	-0.5315	-0.8003	-0.0922
9	-0.5532	-1.0554	-0.8588	-0.2116	0.0516	-0.0912	-0.4364	-0.0717	-0.1780	-0.5315	-0.8003	-0.0922

Dipole mement (in D)	1.85 (DEN)	0.86	1.84	1.44	2.21	1.72	1.86	1.76	2.04	1.66		

File TZVPMol385.out
Molecule PMol385 FCP
 SP Mol385 B3LYP/Def2TZVP VAC.
    0   3
Dipole   0.0000   0.0000   0.0617   0.0617
Quadrupole   -0.5373   -0.5373   1.0746   0.0000   0.0000   0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	-1.6587	-0.1012	0.2940	-0.0112	-0.0155	-0.0328	0.0601	-0.2573	-0.6581	-0.0741
6	0.0000	0.0000	-0.3898	0.2483	-0.6360	0.0001	0.0018	0.0874	-0.1080	-0.0936	-0.3832	0.1634
15	0.0000	0.0000	1.1512	-0.1470	0.3420	0.0111	0.0138	-0.0547	0.0478	0.3509	1.0412	-0.0894

Dipole mement (in D)	0.06 (DEN)	0.47	0.74	0.15	0.20	0.20	0.01	4.17	11.72	0.21		

File TZVPMol386.out
Molecule PMol386 CH3P(O)(OCH3)(SCH3)

SP Mol386 B3LYP/Def2TZVP VAC.
0 16
Dipole 0.1220 -0.2199 -1.5622 1.5823
Quadrupole 4.4390 4.2915 -8.7305 1.5272 1.8063 -2.8975

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.1766	0.4449	1.6425	-0.5317	-0.2635	-0.3868	-0.9032	-0.4074	-0.5883	-1.0808	-1.4867	-0.4060
15	-0.3561	0.4509	0.1843	0.7106	0.1636	0.3929	1.8027	0.3161	0.9615	2.0202	3.0645	0.3676
6	-0.6080	2.0548	-0.5653	-0.3596	-0.4250	-0.1190	-0.8799	-0.2258	-0.7859	-1.0133	-0.6601	-0.2359
8	-1.6376	-0.3084	-0.3908	-0.3416	0.0364	-0.1761	-0.5987	-0.2431	-0.3262	-0.7892	-1.3298	-0.2371
16	1.2260	-0.4983	-0.8166	-0.1983	0.3243	-0.0504	-0.2233	-0.0560	-0.2487	-0.1383	-0.3878	-0.1112
6	2.4956	-0.4032	0.4736	-0.3108	-0.5178	-0.0781	-0.3993	-0.2094	-0.1492	-0.7153	-0.0917	-0.1947
6	-1.9033	-1.6388	0.0539	-0.1812	-0.3462	0.0089	-0.0571	-0.1085	0.0124	-0.2560	0.4502	-0.0879
1	0.2529	2.6848	-0.3572	0.1320	0.1260	0.0529	0.1819	0.1102	0.2293	0.2430	0.0477	0.1126
1	-1.4957	2.5151	-0.1358	0.1349	0.1279	0.0558	0.1907	0.1139	0.2380	0.2475	0.0541	0.1131
1	-0.7324	1.9642	-1.6413	0.1351	0.1252	0.0502	0.1826	0.1082	0.2035	0.2447	0.0506	0.1065
1	3.1704	-1.2405	0.3218	0.1296	0.1086	0.0435	0.1349	0.0971	0.1215	0.2191	0.0392	0.1041
1	2.0236	-0.4803	1.4482	0.1688	0.1155	0.0444	0.1562	0.1046	0.0758	0.2483	0.0935	0.0941
1	3.0552	0.5254	0.4049	0.1251	0.1032	0.0388	0.1271	0.0924	0.0832	0.2083	0.0334	0.0980
1	-2.8247	-1.9529	-0.4267	0.1264	0.1106	0.0461	0.1063	0.1069	0.0797	0.1896	0.0377	0.0969
1	-2.0239	-1.6655	1.1361	0.1385	0.1097	0.0439	0.1020	0.1062	0.0625	0.1890	0.0477	0.0932
1	-1.0930	-2.3092	-0.2357	0.1222	0.1015	0.0327	0.0769	0.0944	0.0308	0.1832	0.0374	0.0866

Dipole mement (in D)	1.58 (DEN)	1.34	3.36	2.01	2.47	2.01	1.56	3.56	4.55	1.74

File TZVPMol387.out
Molecule PMol387 CH3P(O)(SCH3)2
SP Mol387 B3LYP/Def2TZVP VAC.
0 16
Dipole 0.6054 -0.0056 -1.4570 1.5778
Quadrupole 5.3059 4.3600 -9.6659 2.4229 -0.4587 -3.2612

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.1980	0.4279	1.7131	-0.5345	-0.2747	-0.3825	-0.8298	-0.4027	-0.5293	-1.0719	-1.4674	-0.3970
15	0.0068	0.5449	0.2553	0.6066	0.0736	0.3180	1.4623	0.2190	0.7056	1.6096	2.5532	0.2616
6	0.2607	2.1984	-0.4068	-0.3685	-0.4495	-0.1192	-0.8549	-0.2274	-0.6543	-1.0061	-0.6457	-0.2307
16	-1.8822	0.0708	-0.4873	-0.1641	0.3377	-0.0354	-0.1529	-0.0410	-0.1789	-0.0794	-0.3756	-0.0877
16	1.2429	-0.7648	-0.8200	-0.1729	0.3181	-0.0455	-0.1717	-0.0518	-0.2339	-0.0995	-0.3588	-0.0999
6	2.6730	-0.7623	0.2951	-0.3192	-0.5208	-0.0791	-0.4098	-0.2103	-0.0988	-0.7249	-0.0971	-0.1955
6	-2.0817	-1.4954	0.4006	-0.3238	-0.5179	-0.0753	-0.4254	-0.2062	-0.2008	-0.7219	-0.0939	-0.1905
1	0.0847	2.2220	-1.4796	0.1387	0.1239	0.0488	0.1754	0.1053	0.1799	0.2447	0.0500	0.1080
1	1.2883	2.4978	-0.2093	0.1357	0.1267	0.0544	0.1856	0.1114	0.2228	0.2462	0.0506	0.1141
1	-0.4110	2.8931	0.0937	0.1421	0.1271	0.0547	0.1862	0.1116	0.2103	0.2482	0.0558	0.1136
1	3.2646	-1.6405	0.0527	0.1333	0.1104	0.0453	0.1378	0.0989	0.1087	0.2235	0.0420	0.1059
1	2.3306	-0.8234	1.3239	0.1669	0.1145	0.0452	0.1540	0.1039	0.0781	0.2429	0.0853	0.0957
1	3.2835	0.1267	0.1583	0.1239	0.1022	0.0382	0.1263	0.0918	0.0638	0.2069	0.0308	0.0974
1	-3.0894	-1.8448	0.1974	0.1363	0.1115	0.0475	0.1430	0.1012	0.1489	0.2260	0.0450	0.1083
1	-1.9571	-1.3378	1.4678	0.1589	0.1131	0.0475	0.1495	0.1039	0.0961	0.2332	0.0709	0.1008
1	-1.3637	-2.2298	0.0451	0.1405	0.1042	0.0372	0.1244	0.0923	0.0819	0.2225	0.0530	0.0960

Dipole mement (in D) 1.58 (DEN) 1.74 4.58 2.18 2.77 2.23 1.53 4.96 5.10 1.91

File TZVPMol388.out
Molecule PMol388 OP(OCH3)(SCH3)2
SP Mol388 B3LYP/Def2TZVP VAC.
0 17
Dipole 0.4050 0.1873 -2.8505 2.8852
Quadrupole 5.5256 5.5157 -11.0413 1.9455 0.2226 -0.8133

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.1723	-0.5052	1.8196	-0.5079	-0.2525	-0.3712	-0.8556	-0.3881	-0.4965	-1.0631	-1.4615	-0.3899
15	0.0030	0.1541	0.5237	0.7302	-0.0427	0.3529	1.6085	0.3072	0.6107	1.8321	2.7737	0.3608
8	0.3011	1.7138	0.6111	-0.3155	0.0445	-0.1671	-0.5822	-0.2307	-0.2684	-0.7826	-1.3237	-0.2240
16	1.2083	-0.6633	-0.9747	-0.1768	0.3229	-0.0328	-0.2036	-0.0383	-0.1738	-0.1173	-0.3557	-0.0885
16	-1.8881	0.1015	-0.3394	-0.1657	0.3420	-0.0281	-0.1979	-0.0321	-0.1596	-0.0961	-0.3621	-0.0832
6	-2.1580	-1.6848	-0.1958	-0.3213	-0.5161	-0.0734	-0.4179	-0.2044	-0.2248	-0.7184	-0.0913	-0.1890
6	2.6274	-1.1382	0.0512	-0.3148	-0.5154	-0.0755	-0.4084	-0.2067	-0.0958	-0.7204	-0.0935	-0.1926
6	0.2452	2.5659	-0.5291	-0.1868	-0.3591	0.0070	-0.0568	-0.1103	0.0699	-0.2559	0.4543	-0.0880
1	-3.1485	-1.8823	-0.5950	0.1356	0.1119	0.0485	0.1448	0.1021	0.1566	0.2257	0.0464	0.1094
1	-2.1160	-1.9881	0.8456	0.1590	0.1134	0.0491	0.1498	0.1050	0.1230	0.2320	0.0693	0.1036
1	-1.4186	-2.2306	-0.7760	0.1419	0.1041	0.0375	0.1241	0.0928	0.0729	0.2237	0.0551	0.0966
1	3.2265	-0.2728	0.3193	0.1331	0.1061	0.0429	0.1320	0.0971	0.0812	0.2138	0.0419	0.1014
1	3.2277	-1.8213	-0.5428	0.1326	0.1104	0.0458	0.1390	0.0994	0.0941	0.2225	0.0421	0.1065
1	2.2776	-1.6384	0.9489	0.1655	0.1149	0.0473	0.1552	0.1056	0.0809	0.2420	0.0843	0.0984
1	0.6798	3.5157	-0.2318	0.1326	0.1131	0.0500	0.1122	0.1108	0.0776	0.1947	0.0452	0.1009
1	-0.7867	2.7251	-0.8436	0.1290	0.1025	0.0367	0.0847	0.0980	0.0480	0.1798	0.0326	0.0912
1	0.8165	2.1450	-1.3580	0.1292	0.1000	0.0307	0.0721	0.0929	0.0040	0.1874	0.0435	0.0863

Dipole mement (in D) 2.89 (DEN) 2.94 4.63 2.98 4.21 3.61 2.82 7.14 8.86 3.24

File TZVPMol389.out
Molecule PMol389 trimethylphosphine_sulfi
SP Mol389 B3LYP/Def2TZVP VAC.
0 14
Dipole 4.6906 -0.0003 -0.0003 4.6906
Quadrupole -4.3221 2.1614 2.1607 0.0000 0.0006 0.0002

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.1554	0.0000	-0.0001	0.3893	0.3036	0.2927	1.4265	0.1001	0.5182	1.3740	2.5519	0.1062
6	0.9164	-1.2205	-1.1004	-0.3609	-0.4245	-0.1207	-0.7771	-0.2326	-0.4684	-0.9681	-0.6241	-0.2363
6	0.9166	1.5632	-0.5068	-0.3609	-0.4245	-0.1207	-0.7770	-0.2325	-0.4260	-0.9680	-0.6240	-0.2362
6	0.9168	-0.3428	1.6070	-0.3610	-0.4245	-0.1207	-0.7771	-0.2326	-0.4650	-0.9680	-0.6243	-0.2363
16	-1.7737	0.0000	0.0002	-0.4625	-0.1323	-0.3514	-0.6528	-0.3242	-0.4515	-0.6040	-1.0209	-0.3513
1	0.5897	-2.2174	-0.8138	0.1353	0.1252	0.0495	0.1761	0.1054	0.1450	0.2435	0.0459	0.1089
1	2.0045	-1.1745	-1.0600	0.1147	0.1170	0.0413	0.1671	0.0965	0.1506	0.2244	0.0219	0.1001
1	0.5884	-1.0391	-2.1214	0.1354	0.1252	0.0495	0.1760	0.1054	0.1482	0.2435	0.0460	0.1089
1	0.5895	2.3565	0.1614	0.1353	0.1252	0.0495	0.1760	0.1054	0.1348	0.2435	0.0459	0.1089

1	0.5891	1.8139	-1.5131	0.1353	0.1252	0.0495	0.1760	0.1054	0.1341	0.2435	0.0459	0.1089
1	2.0048	1.5049	-0.4882	0.1147	0.1170	0.0414	0.1671	0.0965	0.1391	0.2244	0.0219	0.1001
1	0.5890	-1.3177	1.9604	0.1353	0.1252	0.0495	0.1760	0.1054	0.1447	0.2435	0.0460	0.1089
1	0.5905	0.4040	2.3272	0.1353	0.1252	0.0495	0.1760	0.1054	0.1464	0.2435	0.0459	0.1089
1	2.0050	-0.3308	1.5467	0.1147	0.1170	0.0413	0.1671	0.0965	0.1498	0.2244	0.0219	0.1001

Dipole mement (in D) 4.69 (DEN) 5.07 1.25 3.65 4.18 4.34 4.90 4.00 3.77 4.69

File TZVPMol390.out
Molecule PMol390 PS
SP Mol390 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 -0.6643 0.6643
Quadrupole -1.7218 1.1618 0.5599 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.0000	0.0000	-0.9776	0.1354	-0.0495	0.0829	0.1451	0.0486	0.0761	0.2738	0.8007	0.0577
16	0.0000	0.0000	0.9165	-0.1354	0.0495	-0.0829	-0.1451	-0.0487	-0.0761	-0.2738	-0.8007	-0.0577

Dipole mement (in D) 0.66 (DEN) 1.23 0.45 0.75 1.32 0.44 0.69 2.49 7.29 0.52

File TZVPMol391.out
Molecule PMol391 SP(CH3)(OCH3)2
SP Mol391 B3LYP/Def2TZVP VAC.
0 16
Dipole 0.0004 -1.4149 -2.0374 2.4805
Quadrupole 2.6552 4.2444 -6.8996 0.0003 0.0059 -3.5256

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
15	0.0002	0.3958	-0.1741	0.6455	0.1136	0.3773	1.7485	0.2827	0.4607	1.8583	3.0571	0.3212
16	-0.0013	0.5677	1.7316	-0.4405	-0.0828	-0.2936	-0.7087	-0.2646	-0.3406	-0.6258	-1.0372	-0.2972
8	-1.2742	-0.3529	-0.7966	-0.3310	0.0403	-0.1793	-0.5919	-0.2471	-0.2094	-0.7909	-1.3313	-0.2399
8	1.2760	-0.3522	-0.7947	-0.3309	0.0403	-0.1792	-0.5919	-0.2471	-0.2088	-0.7909	-1.3315	-0.2399
6	0.0007	1.8634	-1.1898	-0.3431	-0.4117	-0.1180	-0.8601	-0.2242	-0.6940	-0.9949	-0.6568	-0.2360
6	-1.9327	-1.4120	-0.1136	-0.1709	-0.3542	0.0050	-0.0455	-0.1126	-0.0747	-0.2489	0.4641	-0.0898
6	1.9324	-1.4125	-0.1116	-0.1710	-0.3542	0.0050	-0.0456	-0.1126	-0.0653	-0.2489	0.4641	-0.0897
1	0.0015	1.5851	-2.2414	0.1346	0.1271	0.0530	0.1901	0.1125	0.2162	0.2466	0.0543	0.1062
1	0.8857	2.4541	-0.9716	0.1336	0.1267	0.0535	0.1841	0.1114	0.2268	0.2458	0.0525	0.1117
1	-0.8847	2.4539	-0.9727	0.1336	0.1267	0.0535	0.1841	0.1114	0.2265	0.2458	0.0525	0.1117
1	-2.9005	-1.5417	-0.5897	0.1242	0.1100	0.0446	0.1026	0.1053	0.0923	0.1875	0.0351	0.0952
1	-2.0672	-1.1693	0.9407	0.1373	0.1030	0.0314	0.0861	0.0941	0.0636	0.1968	0.0559	0.0879
1	-1.3669	-2.3409	-0.1979	0.1086	0.1011	0.0353	0.0796	0.0956	0.0799	0.1675	0.0158	0.0879
1	2.9011	-1.5424	-0.5859	0.1242	0.1100	0.0446	0.1026	0.1053	0.0890	0.1875	0.0351	0.0952
1	1.3661	-2.3410	-0.1982	0.1086	0.1011	0.0353	0.0796	0.0956	0.0770	0.1675	0.0158	0.0879
1	2.0648	-1.1712	0.9432	0.1373	0.1030	0.0315	0.0861	0.0941	0.0606	0.1968	0.0559	0.0879

Dipole mement (in D) 2.48 (DEN) 2.27 0.80 1.97 2.69 1.73 2.55 2.22 4.76 1.97

File TZVPMol392.out
Molecule PMol392 SH
 SP Mol392 B3LYP/Def2TZVP VAC.
  0 2
Dipole 0.0000 0.0000 -0.8635 0.8635
Quadrupole -2.1678 0.6020 1.5658 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.0788	-0.1495	-0.0060	-0.0484	-0.0958	-0.1137	-0.1491	-0.0887	0.0073	-0.1204
1	0.0000	0.0000	-1.2613	0.1495	0.0060	0.0484	0.0958	0.1137	0.1491	0.0887	-0.0073	0.1204
Dipole mement (in D)	0.86 (DEN)			0.96	0.04	0.31	0.62	0.73	0.96	0.57	0.05	0.77

File TZVPMol393.out
Molecule PMol393 CH2SH
 SP Mol393 B3LYP/Def2TZVP VAC.
  0 5
Dipole -0.2074 0.8546 0.0000 0.8794
Quadrupole 0.6412 2.2048 -2.8460 1.2272 -0.0001 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1266	0.0217	-0.0000	-0.3344	-0.5671	-0.1264	-0.4179	-0.2129	-0.5656	-0.6297	-0.2951	-0.1775
16	0.5770	-0.0885	0.0000	-0.0694	0.3359	-0.0031	0.0531	-0.0922	-0.0936	0.1170	0.1797	-0.1384
1	-1.6400	0.9676	0.0000	0.1370	0.0923	0.0366	0.1313	0.0901	0.2087	0.1978	0.0698	0.0930
1	-1.6794	-0.9026	0.0000	0.1359	0.0961	0.0362	0.1313	0.0903	0.2657	0.1988	0.0674	0.0922
1	0.8470	1.2218	-0.0000	0.1310	0.0429	0.0568	0.1023	0.1247	0.1847	0.1161	-0.0216	0.1307
Dipole mement (in D)	0.88 (DEN)			0.81	2.67	0.47	0.93	0.78	0.91	1.22	0.94	0.92

File TZVPMol394.out
Molecule PMol394 ethenethiol
 SP Mol394 B3LYP/Def2TZVP VAC.
  0 7
Dipole 0.7179 0.2279 0.0000 0.7532
Quadrupole 0.8579 2.5703 -3.4283 -1.9869 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.2818	1.1006	0.0000	-0.3047	-0.2664	-0.1034	-0.3200	-0.2047	-0.4696	-0.4280	-0.0432	-0.2022
6	0.0000	0.7509	0.0000	-0.0511	-0.4805	-0.0498	-0.0970	-0.0949	-0.1652	-0.3517	-0.1792	-0.0277
16	-0.6894	-0.8505	0.0000	-0.1231	0.3345	-0.0264	-0.0468	-0.1125	-0.1975	0.0583	0.1166	-0.1709
1	2.0841	0.3745	0.0000	0.1130	0.1156	0.0355	0.1148	0.0889	0.2090	0.1891	0.0287	0.0854
1	1.5644	2.1435	0.0000	0.1164	0.1235	0.0393	0.1228	0.0924	0.1814	0.2045	0.0411	0.0882
1	-0.7765	1.5070	0.0000	0.1253	0.1316	0.0499	0.1176	0.1076	0.2413	0.2144	0.0593	0.1019
1	0.4674	-1.5264	0.0000	0.1243	0.0418	0.0548	0.1085	0.1231	0.2006	0.1134	-0.0230	0.1252
Dipole mement (in D)	0.75 (DEN)			0.36	2.61	0.19	0.33	0.57	0.81	0.61	0.43	0.85

File TZVPMol395.out
Molecule PMol395 methanethiol
 SP Mol395 B3LYP/Def2TZVP VAC.
  0 6
Dipole 0.7286 1.3668 0.0000 1.5489
Quadrupole 1.5098 0.3206 -1.8304 -1.2385 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	-0.0475	-0.6618	0.0000	-0.1929	0.1979	-0.0793	-0.0715	-0.1705	-0.2999	-0.0323	0.0256	-0.2196
6	-0.0475	1.1437	0.0000	-0.3159	-0.5416	-0.0837	-0.3952	-0.2189	-0.1963	-0.7135	-0.0838	-0.1980
1	1.2798	-0.8228	0.0000	0.1199	0.0290	0.0423	0.0944	0.1100	0.1816	0.1090	-0.0456	0.1156
1	-1.0885	1.4530	0.0000	0.1289	0.1111	0.0450	0.1324	0.0985	0.1530	0.2196	0.0387	0.1060
1	0.4274	1.5484	0.8893	0.1300	0.1018	0.0379	0.1199	0.0905	0.0808	0.2086	0.0326	0.0980
1	0.4274	1.5484	-0.8893	0.1300	0.1018	0.0379	0.1199	0.0905	0.0808	0.2086	0.0326	0.0980

Dipole mement (in D)	1.55 (DEN)	1.43	1.43	0.55	0.62	1.13	1.62	0.67	0.52	1.50	

File TZVPMol396.out
Molecule PMol396 ethanethiol_(gauche)
 SP Mol396 B3LYP/Def2TZVP VAC.
  0 9
Dipole 1.4914 0.1263 0.6528 1.6329
Quadrupole -1.4210 0.6585 0.7625 1.2772 -0.6095 -1.6732

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.0549	-0.9416	0.9565	0.1156	0.0294	0.0409	0.0946	0.1089	0.1771	0.1060	-0.0483	0.1126
16	-1.1586	-0.0991	-0.0784	-0.2029	0.2287	-0.0797	-0.1050	-0.1697	-0.3403	-0.0395	0.0035	-0.2272
6	0.4929	0.6396	0.0901	-0.1619	-0.5153	-0.0442	-0.1655	-0.1409	0.0499	-0.4964	-0.0427	-0.0879
6	1.6299	-0.3458	-0.0532	-0.3013	-0.3399	-0.0863	-0.3505	-0.2361	-0.1383	-0.6016	0.0254	-0.2416
1	0.5472	1.1784	1.0351	0.1188	0.1189	0.0339	0.0956	0.0898	0.0143	0.2048	0.0229	0.0908
1	0.5273	1.3935	-0.6956	0.1128	0.1258	0.0409	0.1085	0.0977	0.1100	0.2132	0.0265	0.0991
1	2.5937	0.1605	0.0135	0.1046	0.1185	0.0329	0.1089	0.0842	0.0382	0.2051	0.0009	0.0861
1	1.5857	-0.8665	-1.0079	0.1144	0.1184	0.0313	0.1089	0.0837	0.0343	0.2089	0.0127	0.0839
1	1.6012	-1.1006	0.7320	0.0999	0.1153	0.0302	0.1045	0.0824	0.0548	0.1995	-0.0008	0.0842

Dipole mement (in D)	1.63 (DEN)	1.49	1.60	0.57	0.66	1.17	1.68	0.73	0.69	1.59	

File TZVPMol397.out
Molecule PMol397 ethanethiol_(trans)
 SP Mol397 B3LYP/Def2TZVP VAC.
  0 9
Dipole 0.0341 1.6342 0.0000 1.6346
Quadrupole 2.3428 -0.8162 -1.5266 -0.2689 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-2.0276	-0.4353	0.0000	0.1189	0.0287	0.0417	0.0914	0.1095	0.1698	0.1137	-0.0465	0.1146
16	-0.7518	-0.8348	0.0000	-0.2040	0.2215	-0.0832	-0.1057	-0.1732	-0.3291	-0.0498	-0.0027	-0.2313
6	0.0000	0.8243	0.0000	-0.1551	-0.5029	-0.0454	-0.1590	-0.1423	-0.0343	-0.4884	-0.0401	-0.0896
6	1.5063	0.6892	0.0000	-0.3248	-0.3407	-0.0832	-0.3530	-0.2326	-0.0894	-0.6037	0.0213	-0.2388

1	-0.3383	1.3689	0.8802	0.1115	0.1174	0.0339	0.0952	0.0899	0.0640	0.2024	0.0208	0.0912
1	-0.3383	1.3689	-0.8802	0.1115	0.1174	0.0339	0.0952	0.0899	0.0640	0.2024	0.0208	0.0912
1	1.9781	1.6706	0.0000	0.1108	0.1207	0.0360	0.1138	0.0876	0.0231	0.2107	0.0067	0.0898
1	1.8585	0.1513	-0.8790	0.1156	0.1190	0.0331	0.1110	0.0856	0.0660	0.2064	0.0101	0.0864
1	1.8585	0.1513	0.8790	0.1156	0.1190	0.0331	0.1110	0.0856	0.0660	0.2064	0.0101	0.0864

Dipole mement (in D)	1.63 (DEN)	1.40	1.53	0.59	0.82	1.14	1.66	0.73	0.87	1.59		

File TZVPMol398.out
Molecule PMol398 1-propane_thiol
SP Mol398 B3LYP/Def2TZVP VAC.
0 12
Dipole 1.5714 -0.0580 0.6320 1.6947
Quadrupole -2.4990 0.9252 1.5738 0.9615 -1.2175 -1.6583

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.3995	0.0735	0.0097	-0.3322	-0.3087	-0.0828	-0.3268	-0.2345	-0.2849	-0.5882	0.0095	-0.2471
1	3.1610	-0.6982	-0.0886	0.1150	0.1188	0.0326	0.1048	0.0840	0.0713	0.2079	0.0016	0.0863
1	2.5721	0.8048	-0.7805	0.1047	0.1175	0.0292	0.1006	0.0810	0.0476	0.1967	-0.0059	0.0815
1	2.5691	0.5800	0.9604	0.1031	0.1168	0.0285	0.0995	0.0803	0.0604	0.1961	-0.0067	0.0808
6	0.9994	-0.5070	-0.0696	-0.1393	-0.3275	-0.0490	-0.1367	-0.1603	0.3065	-0.3988	0.0652	-0.1327
1	0.8620	-1.2606	0.7099	0.0808	0.1295	0.0272	0.0842	0.0827	-0.0466	0.1921	-0.0119	0.0777
6	-0.0672	0.5611	0.0757	-0.1706	-0.4919	-0.0470	-0.2037	-0.1419	-0.1029	-0.4949	-0.0536	-0.0935
1	0.0260	1.3057	-0.7160	0.1102	0.1277	0.0394	0.1087	0.0968	0.1345	0.2118	0.0235	0.0961
1	0.0444	1.1011	1.0168	0.1161	0.1206	0.0327	0.0965	0.0892	0.0359	0.2034	0.0200	0.0882
16	-1.7716	-0.0438	-0.0728	-0.2006	0.2352	-0.0796	-0.1077	-0.1698	-0.3315	-0.0348	0.0043	-0.2269
1	-1.7346	-0.8657	0.9827	0.1151	0.0296	0.0406	0.0924	0.1086	0.1729	0.1061	-0.0485	0.1124
1	0.8550	-1.0321	-1.0155	0.0977	0.1326	0.0282	0.0881	0.0839	-0.0632	0.2024	0.0023	0.0774

Dipole mement (in D)	1.69 (DEN)	1.52	1.47	0.65	0.74	1.24	1.74	0.75	0.74	1.65		

File TZVPMol399.out
Molecule PMol399 2-methyl-2-propane_thiol
SP Mol399 B3LYP/Def2TZVP VAC.
0 15
Dipole -1.5093 -0.6830 0.0000 1.6566
Quadrupole -1.1625 2.0394 -0.8768 -2.0048 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.8301	-0.7279	1.2507	-0.3132	-0.2890	-0.0896	-0.4345	-0.2357	-0.4848	-0.6039	0.0203	-0.2497
6	-0.3493	-0.0082	0.0000	0.0995	-0.5432	0.0267	0.2753	0.0051	0.4446	-0.1050	0.0018	0.1308
1	-0.4743	-1.7577	1.2811	0.1015	0.1185	0.0290	0.1114	0.0821	0.1214	0.2036	-0.0030	0.0822
1	-0.4861	-0.2292	2.1551	0.1189	0.1220	0.0302	0.1163	0.0836	0.1100	0.2135	0.0109	0.0824
1	-1.9223	-0.7566	1.2734	0.0996	0.1220	0.0298	0.1170	0.0824	0.1390	0.2008	-0.0054	0.0807
6	-0.8301	1.4366	0.0000	-0.3445	-0.2905	-0.0863	-0.4357	-0.2318	-0.3660	-0.6095	0.0118	-0.2466
6	-0.8301	-0.7279	-1.2507	-0.3132	-0.2890	-0.0896	-0.4345	-0.2357	-0.4848	-0.6039	0.0202	-0.2497
1	-0.4842	1.9747	-0.8820	0.1208	0.1227	0.0325	0.1193	0.0860	0.1276	0.2118	0.0087	0.0855
1	-1.9207	1.4630	0.0000	0.1059	0.1246	0.0336	0.1232	0.0865	0.0854	0.2076	0.0020	0.0849

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   1     -0.4842    1.9747    0.8820    0.1208    0.1227    0.0325    0.1193    0.0860    0.1276    0.2118    0.0087    0.0855
   1     -1.9223   -0.7566   -1.2734    0.0996    0.1220    0.0298    0.1170    0.0824    0.1390    0.2008   -0.0054    0.0807
   1     -0.4861   -0.2292   -2.1551    0.1189    0.1220    0.0302    0.1163    0.0836    0.1100    0.2135    0.0109    0.0824
   1     -0.4743   -1.7577   -1.2811    0.1015    0.1185    0.0290    0.1114    0.0821    0.1214    0.2036   -0.0030    0.0822
  16      1.4983    0.0917    0.0000   -0.2314    0.2862   -0.0778   -0.1179   -0.1650   -0.3743   -0.0530   -0.0276   -0.2409
   1      1.7179   -1.2290    0.0000    0.1154    0.0303    0.0398    0.0960    0.1083    0.1838    0.1085   -0.0507    0.1095

 Dipole mement (in D)   1.66 (DEN)      1.54      1.60      0.53      0.51      1.15      1.75      0.80      0.95      1.64

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File TZVPMol400.out
Molecule PMol400    HSSH
 SP Mol400 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0000    1.2184    1.2184
Quadrupole     -0.1666    0.5798   -0.4132   -2.0794    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
  16      0.0000    1.0211   -0.0548   -0.1435   -0.0140   -0.0465   -0.0940   -0.1139   -0.1435   -0.1151    0.0163   -0.1237
  16      0.0000   -1.0211   -0.0548   -0.1435   -0.0140   -0.0465   -0.0940   -0.1139   -0.1437   -0.1151    0.0165   -0.1237
   1     -0.9461    1.2291    0.8762    0.1435    0.0140    0.0465    0.0940    0.1139    0.1436    0.1151   -0.0164    0.1237
   1      0.9461   -1.2291    0.8762    0.1435    0.0140    0.0465    0.0940    0.1139    0.1437    0.1151   -0.0164    0.1237

 Dipole mement (in D)   1.22 (DEN)      1.28      0.12      0.42      0.84      1.02      1.28      1.03      0.15      1.11

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File TZVPMol401.out
Molecule PMol401    CH3SSH
 SP Mol401 B3LYP/Def2TZVP VAC.
    0    7
Dipole          1.0147    1.1836    0.7880    1.7468
Quadrupole      2.0683   -1.9468   -0.1215    0.1570   -1.6257    0.5903
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
  16     -1.3397    0.2443   -0.0881   -0.1672    0.0120   -0.0526   -0.1102   -0.1190   -0.1541   -0.1363   -0.0064   -0.1396
  16      0.4625   -0.6958    0.0157   -0.0489    0.2091   -0.0226    0.0834   -0.0511   -0.1312    0.1163    0.0115   -0.0769
   6      1.6463    0.6666   -0.0052   -0.3018   -0.5487   -0.0903   -0.4579   -0.2227   -0.1008   -0.7400   -0.0989   -0.2035
   1     -1.5597    0.4515    1.2230    0.1360    0.0130    0.0433    0.0907    0.1106    0.1528    0.1115   -0.0238    0.1201
   1      2.6344    0.2108   -0.0481    0.1252    0.1111    0.0459    0.1386    0.0992    0.1126    0.2225    0.0395    0.1059
   1      1.5751    1.2698    0.8963    0.1231    0.1005    0.0371    0.1253    0.0902    0.0476    0.2097    0.0344    0.0961
   1      1.5080    1.2927   -0.8823    0.1336    0.1030    0.0393    0.1300    0.0928    0.0732    0.2163    0.0433    0.0978

 Dipole mement (in D)   1.75 (DEN)      1.66      1.55      0.58      0.60      1.23      1.76      0.81      0.58      1.59

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File TZVPMol402.out
Molecule PMol402    2-propanethiol
 SP Mol402 B3LYP/Def2TZVP VAC.
    0   12
Dipole         -0.2367    1.6303    0.0000    1.6474
```

Quadrupole 2.8011 -1.8070 -0.9940 1.2432 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.0541	1.0895	1.2584	-0.3035	-0.3138	-0.0884	-0.3941	-0.2364	-0.4904	-0.5997	0.0213	-0.2462
6	0.4123	0.3833	0.0000	-0.0186	-0.5188	-0.0067	0.0703	-0.0655	0.2018	-0.3013	-0.0146	0.0225
6	-0.0541	1.0895	-1.2584	-0.3035	-0.3138	-0.0884	-0.3941	-0.2364	-0.4904	-0.5997	0.0218	-0.2462
16	-0.0541	-1.3869	0.0000	-0.2170	0.2606	-0.0779	-0.1238	-0.1665	-0.3410	-0.0447	-0.0133	-0.2326
1	0.3021	0.5928	2.1578	0.1219	0.1197	0.0311	0.1092	0.0838	0.1120	0.2150	0.0134	0.0842
1	-1.1437	1.1178	1.3054	0.0947	0.1176	0.0291	0.1076	0.0819	0.1458	0.1979	-0.0029	0.0818
1	0.2993	2.1221	1.2745	0.1031	0.1200	0.0312	0.1106	0.0831	0.1365	0.2024	-0.0029	0.0832
1	1.5037	0.3339	0.0000	0.0893	0.1410	0.0386	0.0903	0.0990	0.1505	0.2112	0.0184	0.0940
1	0.3021	0.5928	-2.1578	0.1219	0.1197	0.0311	0.1092	0.0838	0.1120	0.2150	0.0134	0.0842
1	-1.1437	1.1178	-1.3054	0.0947	0.1176	0.0291	0.1076	0.0819	0.1458	0.1979	-0.0029	0.0818
1	0.2993	2.1221	-1.2745	0.1031	0.1200	0.0312	0.1106	0.0831	0.1365	0.2024	-0.0029	0.0832
1	-1.3782	-1.1826	0.0000	0.1138	0.0305	0.0401	0.0967	0.1084	0.1809	0.1036	-0.0491	0.1102

Dipole mement (in D) 1.65 (DEN) 1.58 1.69 0.55 0.48 1.17 1.73 0.80 0.76 1.61

File TZVPMol403.out
Molecule PMol403 thioacetone
SP Mol403 B3LYP/Def2TZVP VAC.
0 10
Dipole -2.8523 0.0000 0.0003 2.8523
Quadrupole -0.6066 0.2169 0.3897 0.0000 0.0000 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0588	1.2552	0.0001	-0.3004	-0.2866	-0.0830	-0.4751	-0.2268	-0.3374	-0.6666	0.0085	-0.2420
6	-0.2511	0.0000	0.0001	0.0875	-0.5309	0.0612	0.3273	0.0578	0.3330	-0.0522	-0.4458	0.1505
6	-1.0588	-1.2552	0.0001	-0.3004	-0.2866	-0.0830	-0.4751	-0.2268	-0.3374	-0.6666	0.0087	-0.2420
16	1.3728	0.0000	-0.0002	-0.2291	0.3185	-0.1515	-0.2009	-0.1766	-0.2776	0.0330	0.2506	-0.2314
1	-0.4387	2.1452	-0.0002	0.1314	0.1249	0.0391	0.1326	0.0928	0.0784	0.2308	0.0400	0.0922
1	-1.7188	1.2794	0.8709	0.1199	0.1339	0.0446	0.1397	0.0967	0.1156	0.2228	0.0244	0.0952
1	-1.7193	1.2792	-0.8704	0.1199	0.1339	0.0445	0.1397	0.0967	0.1156	0.2227	0.0244	0.0952
1	-0.4387	-2.1452	0.0001	0.1314	0.1249	0.0391	0.1326	0.0928	0.0784	0.2308	0.0400	0.0922
1	-1.7190	-1.2793	0.8708	0.1199	0.1339	0.0445	0.1397	0.0967	0.1156	0.2228	0.0244	0.0952
1	-1.7191	-1.2793	-0.8705	0.1199	0.1339	0.0446	0.1397	0.0967	0.1156	0.2228	0.0244	0.0952

Dipole mement (in D) 2.85 (DEN) 3.07 0.71 1.86 2.06 2.51 2.95 1.27 1.13 2.78

File TZVPMol404.out
Molecule PMol404 CH3S_radical
SP Mol404 B3LYP/Def2TZVP VAC.
0 5
Dipole -1.7060 -0.0002 0.0827 1.7080
Quadrupole 0.5635 -1.5071 0.9436 0.0003 -0.1684 -0.0018

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0919	0.0000	-0.0095	-0.3177	-0.5833	-0.0893	-0.4558	-0.2205	-0.0730	-0.7906	-0.1203	-0.2065
16	0.6857	0.0000	-0.0021	-0.0975	0.2494	-0.0485	0.0395	-0.0755	-0.1554	0.1149	-0.0214	-0.1087

```
   1     -1.5042    0.8947   -0.4716    0.1364    0.1051    0.0416    0.1318    0.0942    0.0670    0.2169    0.0417    0.1007
   1     -1.4118   -0.0013    1.0353    0.1424    0.1237    0.0545    0.1527    0.1075    0.0947    0.2419    0.0582    0.1138
   1     -1.5041   -0.8936   -0.4737    0.1364    0.1051    0.0416    0.1318    0.0942    0.0667    0.2170    0.0418    0.1007

 Dipole mement (in D)   1.71 (DEN)      1.60      1.53      0.67      0.46      1.19      1.75      0.36      0.45      1.51

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File TZVPMol405.out
Molecule PMol405    1,3-dithiane
 SP Mol405 B3LYP/Def2TZVP VAC.
    0   14
Dipole          0.7488    1.9878    0.0000    2.1242
Quadrupole      0.0034    3.8835   -3.8869   -2.0854    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
  16     -0.0348   -0.6947    1.5252   -0.0849    0.4711   -0.0391    0.0784   -0.0849   -0.1564    0.2181    0.0179   -0.1610
   6      0.8053   -1.1641    0.0000   -0.2144   -0.6933   -0.0638   -0.3641   -0.1379   -0.3999   -0.6959   -0.1706   -0.0748
   6     -0.0348    1.0970   -1.2697   -0.2196   -0.4680   -0.0516   -0.2397   -0.1439   -0.2175   -0.5207   -0.0635   -0.1049
   6     -0.7346    1.5489    0.0000   -0.0976   -0.3172   -0.0517   -0.1735   -0.1584    0.2240   -0.4143    0.0591   -0.1341
   6     -0.0348    1.0970    1.2697   -0.2196   -0.4680   -0.0516   -0.2397   -0.1439   -0.2175   -0.5207   -0.0643   -0.1049
  16     -0.0348   -0.6947   -1.5252   -0.0849    0.4711   -0.0391    0.0784   -0.0849   -0.1564    0.2181    0.0180   -0.1610
   1      1.8187   -0.7593    0.0000    0.1246    0.1086    0.0350    0.1141    0.0933    0.1736    0.2078    0.0430    0.0944
   1      0.8807   -2.2483    0.0000    0.1444    0.1190    0.0502    0.1353    0.1089    0.2854    0.2418    0.0610    0.1135
   1      0.9980    1.4562   -1.2863    0.1082    0.1218    0.0307    0.0971    0.0877    0.1102    0.1988    0.0134    0.0844
   1     -0.5252    1.5081   -2.1503    0.1247    0.1289    0.0424    0.1111    0.0995    0.1351    0.2264    0.0298    0.1002
   1     -0.7701    2.6425    0.0000    0.0924    0.1388    0.0341    0.0981    0.0890   -0.0433    0.2067   -0.0033    0.0838
   1     -1.7670    1.1954    0.0000    0.0938    0.1364    0.0314    0.0960    0.0884    0.0172    0.2088    0.0164    0.0797
   1      0.9980    1.4562    1.2863    0.1082    0.1218    0.0307    0.0971    0.0877    0.1102    0.1988    0.0134    0.0844
   1     -0.5252    1.5081    2.1503    0.1247    0.1289    0.0424    0.1111    0.0995    0.1351    0.2264    0.0298    0.1002

 Dipole mement (in D)   2.12 (DEN)      1.84      2.47      0.70      0.58      1.57      2.18      0.38      0.59      2.17

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File TZVPMol406.out
Molecule PMol406    (CH3)3CS_radical
 SP Mol406 B3LYP/Def2TZVP VAC.
    0   14
Dipole         -1.8400    0.0000    0.2020    1.8511
Quadrupole     -1.5872   -0.4387    2.0259    0.0000   -0.0366   -0.0003
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM        ACP
   6     -0.8617   -1.2537   -0.6698   -0.3129   -0.2894   -0.0899   -0.4359   -0.2355   -0.5029   -0.6000    0.0192   -0.2497
   6     -0.3055   -0.0000   -0.0065    0.1126   -0.5808    0.0184    0.2417   -0.0005    0.5928   -0.1828   -0.0174    0.1159
   6     -0.6371   -0.0001    1.4871   -0.3533   -0.2868   -0.0829   -0.4318   -0.2281   -0.3664   -0.6015    0.0078   -0.2422
   6     -0.8616    1.2538   -0.6696   -0.3129   -0.2894   -0.0899   -0.4359   -0.2355   -0.5029   -0.6000    0.0193   -0.2497
  16      1.5168   -0.0000   -0.0869   -0.1419    0.3439   -0.0408    0.0021   -0.0637   -0.2429    0.1020   -0.0828   -0.1269
   1     -0.5970   -1.2965   -1.7257    0.1105    0.1207    0.0306    0.1146    0.0837    0.1427    0.2081    0.0033    0.0827
   1     -0.4828   -2.1561   -0.1938    0.1151    0.1218    0.0304    0.1153    0.0839    0.0941    0.2136    0.0117    0.0825
   1     -1.9522   -1.2629   -0.6025    0.1001    0.1221    0.0303    0.1180    0.0829    0.1211    0.2004   -0.0046    0.0813
   1     -0.2436    0.8833    1.9879    0.1241    0.1227    0.0328    0.1176    0.0863    0.1074    0.2132    0.0122    0.0858
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1	-1.7226	-0.0001	1.6104	0.1086	0.1281	0.0370	0.1288	0.0898	0.0917	0.2118	0.0092	0.0880
1	-0.2436	-0.8835	1.9878	0.1241	0.1227	0.0328	0.1176	0.0863	0.1074	0.2132	0.0122	0.0858
1	-1.9522	1.2630	-0.6024	0.1001	0.1221	0.0303	0.1180	0.0829	0.1211	0.2004	-0.0046	0.0813
1	-0.4828	2.1562	-0.1934	0.1151	0.1218	0.0304	0.1153	0.0839	0.0941	0.2136	0.0117	0.0825
1	-0.5970	1.2968	-1.7255	0.1105	0.1207	0.0306	0.1146	0.0837	0.1427	0.2081	0.0033	0.0827

Dipole mement (in D) 1.85 (DEN) 1.77 1.74 0.62 0.22 1.21 1.90 0.44 0.88 1.62

File TZVPMol407.out
Molecule PMol407 ethyl_methyl_sulfide
SP Mol407 B3LYP/Def2TZVP VAC.
0 12
Dipole -0.7365 1.2269 0.6805 1.5845
Quadrupole 1.5093 -0.4819 -1.0274 2.6198 -0.2779 -0.0564

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.9430	-0.4607	0.4687	-0.1688	-0.4984	-0.0491	-0.1943	-0.1442	0.0639	-0.5184	-0.0523	-0.0976
6	-1.7990	0.5589	-0.2500	-0.3145	-0.3363	-0.0871	-0.3470	-0.2370	-0.0025	-0.6031	0.0225	-0.2441
1	-1.3744	1.5599	-0.1844	0.1058	0.1146	0.0293	0.1073	0.0820	0.0291	0.1980	-0.0032	0.0829
1	-2.7972	0.6049	0.1865	0.1064	0.1183	0.0318	0.1078	0.0831	-0.0141	0.2055	-0.0004	0.0849
1	-0.8527	-0.2226	1.5305	0.1074	0.1192	0.0314	0.0965	0.0877	0.0230	0.1995	0.0145	0.0866
1	-1.9031	0.3145	-1.3057	0.1100	0.1183	0.0305	0.1075	0.0830	0.0098	0.2073	0.0095	0.0828
16	0.7189	-0.6775	-0.2145	-0.0930	0.4478	-0.0465	0.0787	-0.0972	-0.2716	0.2011	0.0019	-0.1694
1	-1.3911	-1.4526	0.4129	0.1162	0.1263	0.0393	0.1053	0.0961	0.0646	0.2173	0.0245	0.0967
6	1.4179	0.9396	0.1413	-0.3499	-0.5236	-0.0897	-0.4304	-0.2233	-0.2073	-0.7386	-0.0982	-0.2095
1	2.4658	0.9077	-0.1441	0.1348	0.1116	0.0430	0.1314	0.0965	0.1390	0.2251	0.0366	0.1032
1	0.9357	1.7325	-0.4274	0.1254	0.0996	0.0330	0.1183	0.0862	0.0794	0.2031	0.0221	0.0914
1	1.3595	1.1697	1.2045	0.1202	0.1026	0.0344	0.1193	0.0874	0.0867	0.2032	0.0227	0.0923

Dipole mement (in D) 1.58 (DEN) 1.22 1.79 0.44 0.26 1.08 1.61 0.12 0.23 1.48

File TZVPMol408.out
Molecule PMol408 ethyl_methyl_sulfide*
SP Mol408 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.9490 -1.2344 0.0000 1.5570
Quadrupole 1.5636 -0.0880 -1.4756 1.9814 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.2274	-0.9844	0.0000	-0.1792	-0.4867	-0.0500	-0.1854	-0.1450	-0.0006	-0.5103	-0.0512	-0.0989
6	-1.7003	-1.3274	0.0000	-0.3148	-0.3385	-0.0844	-0.3539	-0.2338	-0.2050	-0.5992	0.0216	-0.2397
1	-2.2024	-0.9254	0.8787	0.1137	0.1187	0.0320	0.1084	0.0845	0.0799	0.2061	0.0088	0.0850
1	-1.8448	-2.4067	0.0000	0.1103	0.1197	0.0342	0.1121	0.0857	0.0495	0.2085	0.0039	0.0878
1	0.2689	-1.4003	0.8790	0.1030	0.1169	0.0308	0.0956	0.0872	0.0751	0.1971	0.0121	0.0860
1	-2.2024	-0.9254	-0.8787	0.1137	0.1187	0.0320	0.1084	0.0845	0.0799	0.2061	0.0088	0.0850
16	0.0000	0.8121	0.0000	-0.0874	0.4443	-0.0469	0.0849	-0.0976	-0.2247	0.1973	-0.0005	-0.1706
1	0.2689	-1.4003	-0.8790	0.1030	0.1169	0.0308	0.0956	0.0872	0.0751	0.1971	0.0121	0.0860
6	1.7948	0.8711	0.0000	-0.3378	-0.5241	-0.0893	-0.4310	-0.2227	-0.2872	-0.7327	-0.0966	-0.2080

1	2.0908	1.9164	0.0000	0.1327	0.1112	0.0430	0.1312	0.0964	0.1605	0.2240	0.0364	0.1031
1	2.2090	0.3960	0.8882	0.1214	0.1015	0.0338	0.1170	0.0868	0.0987	0.2029	0.0229	0.0920
1	2.2090	0.3960	-0.8882	0.1214	0.1015	0.0338	0.1170	0.0868	0.0987	0.2029	0.0229	0.0920

Dipole mement (in D) 1.56 (DEN) 1.10 1.86 0.42 0.27 1.05 1.55 0.12 0.33 1.48

File TZVPMol409.out
Molecule PMol409 dimethyl_sulfide
SP Mol409 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0000 0.0000 -1.5378 1.5378
Quadrupole -1.5308 2.8596 -1.3288 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.6584	-0.0780	0.4191	-0.0453	0.1115	-0.0972	-0.1722	0.2093	0.0260	-0.1608
6	0.0000	1.3654	-0.5088	-0.3355	-0.5236	-0.0891	-0.4263	-0.2224	-0.2860	-0.7345	-0.0962	-0.2078
1	0.8881	1.3507	-1.1390	0.1212	0.1015	0.0343	0.1199	0.0872	0.1159	0.2031	0.0234	0.0924
1	-0.8881	1.3507	-1.1390	0.1212	0.1015	0.0343	0.1199	0.0872	0.1125	0.2031	0.0234	0.0924
1	0.0000	2.2888	0.0637	0.1320	0.1111	0.0432	0.1308	0.0967	0.1436	0.2236	0.0364	0.1034
6	0.0000	-1.3654	-0.5088	-0.3355	-0.5236	-0.0891	-0.4263	-0.2224	-0.2860	-0.7345	-0.0964	-0.2078
1	0.8881	-1.3507	-1.1390	0.1212	0.1015	0.0343	0.1199	0.0872	0.1159	0.2031	0.0234	0.0924
1	0.0000	-2.2888	0.0637	0.1320	0.1111	0.0432	0.1308	0.0967	0.1436	0.2236	0.0364	0.1034
1	-0.8881	-1.3507	-1.1390	0.1212	0.1015	0.0343	0.1199	0.0872	0.1125	0.2031	0.0234	0.0924

Dipole mement (in D) 1.54 (DEN) 1.18 1.73 0.43 0.11 1.07 1.56 0.06 0.06 1.45

File TZVPMol410.out
Molecule PMol410 diethyl_sulfide
SP Mol410 B3LYP/Def2TZVP VAC.
0 15
Dipole 0.0000 0.0000 -1.5694 1.5694
Quadrupole -1.4748 2.8745 -1.3997 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.5610	-0.0974	0.4695	-0.0478	0.0573	-0.0973	-0.3119	0.1854	-0.0272	-0.1796
6	0.0000	1.3790	-0.6121	-0.1761	-0.4865	-0.0499	-0.1876	-0.1450	0.0544	-0.5081	-0.0521	-0.0989
6	0.0000	2.6999	0.1247	-0.3177	-0.3385	-0.0845	-0.3524	-0.2338	-0.0958	-0.5983	0.0220	-0.2396
1	-0.8792	1.2922	-1.2537	0.1027	0.1169	0.0305	0.0921	0.0868	0.0348	0.1970	0.0116	0.0858
1	0.8792	1.2922	-1.2537	0.1027	0.1169	0.0305	0.0921	0.0868	0.0385	0.1970	0.0116	0.0858
1	0.0000	3.5332	-0.5767	0.1103	0.1194	0.0338	0.1113	0.0853	0.0189	0.2080	0.0033	0.0874
1	-0.8787	2.8008	0.7602	0.1133	0.1186	0.0318	0.1079	0.0843	0.0535	0.2058	0.0085	0.0847
1	0.8787	2.8008	0.7602	0.1133	0.1186	0.0318	0.1079	0.0843	0.0517	0.2058	0.0085	0.0847
6	0.0000	-1.3790	-0.6121	-0.1761	-0.4865	-0.0499	-0.1876	-0.1450	0.0544	-0.5081	-0.0521	-0.0989
6	0.0000	-2.6999	0.1247	-0.3177	-0.3385	-0.0845	-0.3524	-0.2338	-0.0958	-0.5983	0.0219	-0.2396
1	0.8792	-1.2922	-1.2537	0.1027	0.1169	0.0305	0.0921	0.0868	0.0385	0.1970	0.0116	0.0858
1	-0.8792	-1.2922	-1.2537	0.1027	0.1169	0.0305	0.0921	0.0868	0.0348	0.1970	0.0116	0.0858
1	0.0000	-3.5332	-0.5767	0.1103	0.1194	0.0338	0.1113	0.0853	0.0189	0.2080	0.0033	0.0874
1	0.8787	-2.8008	0.7602	0.1133	0.1186	0.0318	0.1079	0.0843	0.0517	0.2058	0.0085	0.0847

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   1     -0.8787   -2.8008    0.7602    0.1133    0.1186    0.0318    0.1079    0.0843    0.0535    0.2058    0.0085    0.0847

 Dipole mement (in D)   1.57 (DEN)      1.04      1.98      0.39      0.42      1.02      1.49      0.12      0.09      1.50

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File TZVPMol411.out
Molecule PMol411    hydrogen_sulfide
 SP Mol411 B3LYP/Def2TZVP VAC.
    0    3
Dipole          0.0000    0.0000   -1.1113    1.1113
Quadrupole     -2.4816    1.8464    0.6352    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  16      0.0000    0.0000    0.1032   -0.2955   -0.0501   -0.1023   -0.2357   -0.2340   -0.2837   -0.2725    0.0398   -0.2626
   1      0.0000    0.9609   -0.8253    0.1477    0.0250    0.0511    0.1178    0.1170    0.1419    0.1362   -0.0199    0.1313
   1      0.0000   -0.9609   -0.8253    0.1477    0.0250    0.0511    0.1178    0.1170    0.1419    0.1362   -0.0199    0.1313

 Dipole mement (in D)   1.11 (DEN)      1.32      0.22      0.46      1.05      1.04      1.27      1.22      0.18      1.17

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File TZVPMol412.out
Molecule PMol412    thietane
 SP Mol412 B3LYP/Def2TZVP VAC.
    0   10
Dipole         -0.0001   -1.9406    0.0000    1.9406
Quadrupole     -0.3714   -1.9234    2.2949   -0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -0.0000   -0.3305    1.1535   -0.1626   -0.4196   -0.0485   -0.1998   -0.1405    0.2791   -0.4850   -0.0554   -0.1078
   1      0.8822   -0.3557    1.7900    0.1057    0.1120    0.0322    0.0896    0.0875    0.0002    0.2018    0.0197    0.0876
   1     -0.8823   -0.3556    1.7900    0.1057    0.1120    0.0322    0.0896    0.0875   -0.0013    0.2018    0.0197    0.0876
   6     -0.0000   -1.3384    0.0000   -0.1896   -0.2906   -0.0432   -0.1566   -0.1481   -0.5204   -0.4079    0.0623   -0.1298
   1     -0.8753   -1.9860    0.0000    0.1012    0.1283    0.0346    0.0929    0.0894    0.1447    0.2047    0.0053    0.0858
   1      0.8752   -1.9860    0.0000    0.1012    0.1283    0.0346    0.0929    0.0894    0.1450    0.2047    0.0053    0.0858
   6     -0.0000   -0.3305   -1.1535   -0.1626   -0.4196   -0.0485   -0.1998   -0.1405    0.2791   -0.4850   -0.0553   -0.1078
   1      0.8822   -0.3557   -1.7900    0.1057    0.1120    0.0322    0.0896    0.0875    0.0002    0.2018    0.0197    0.0876
   1     -0.8823   -0.3556   -1.7900    0.1057    0.1120    0.0322    0.0896    0.0875   -0.0013    0.2018    0.0197    0.0876
  16      0.0001    1.0869    0.0000   -0.1102    0.4251   -0.0577    0.0119   -0.0994   -0.3254    0.1610   -0.0412   -0.1765

 Dipole mement (in D)   1.94 (DEN)      1.49      2.21      0.75      0.68      1.42      2.00      0.28      0.68      1.98

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File TZVPMol413.out
Molecule PMol413    thiacyclohexane
 SP Mol413 B3LYP/Def2TZVP VAC.
    0   16
Dipole         -1.6833    0.0000    0.5844    1.7819
Quadrupole     -3.2372    3.6037   -0.3664    0.0000    0.3271    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -0.9799   -1.2700   -0.2558   -0.1299   -0.2910   -0.0509   -0.1647   -0.1593    0.0522   -0.4002    0.0514   -0.1400
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6	0.4184	-1.3616	0.3273	-0.2014	-0.4620	-0.0526	-0.2316	-0.1452	-0.1590	-0.5177	-0.0648	-0.1071
6	0.4184	1.3616	0.3273	-0.2014	-0.4620	-0.0526	-0.2316	-0.1452	-0.1590	-0.5177	-0.0647	-0.1071
6	-0.9799	1.2700	-0.2558	-0.1299	-0.2910	-0.0509	-0.1647	-0.1593	0.0522	-0.4002	0.0512	-0.1400
6	-1.7059	0.0000	0.1661	-0.1843	-0.2679	-0.0483	-0.1525	-0.1581	0.0014	-0.3852	0.0421	-0.1435
1	0.3794	-1.3803	1.4200	0.1016	0.1213	0.0292	0.0920	0.0861	0.0813	0.1968	0.0104	0.0826
1	0.9242	-2.2727	0.0117	0.1195	0.1261	0.0391	0.1049	0.0959	0.1320	0.2221	0.0240	0.0964
1	-0.9170	-1.3142	-1.3463	0.0827	0.1347	0.0275	0.0863	0.0838	0.0186	0.1989	-0.0034	0.0753
1	-1.5546	-2.1449	0.0595	0.0902	0.1344	0.0298	0.0869	0.0845	-0.0113	0.2027	-0.0107	0.0795
1	0.3794	1.3803	1.4200	0.1016	0.1213	0.0292	0.0920	0.0861	0.0813	0.1968	0.0104	0.0826
1	0.9242	2.2727	0.0117	0.1195	0.1261	0.0391	0.1049	0.0959	0.1320	0.2221	0.0240	0.0964
1	-1.5546	2.1449	0.0595	0.0902	0.1344	0.0298	0.0869	0.0845	-0.0113	0.2027	-0.0107	0.0795
1	-0.9170	1.3142	-1.3463	0.0827	0.1347	0.0275	0.0863	0.0838	0.0186	0.1989	-0.0034	0.0753
1	-1.8232	0.0000	1.2556	0.0814	0.1333	0.0247	0.0802	0.0805	0.0260	0.1862	-0.0208	0.0719
1	-2.7174	0.0000	-0.2430	0.0957	0.1341	0.0301	0.0845	0.0850	-0.0050	0.2050	-0.0100	0.0805
16	1.4906	-0.0000	-0.1973	-0.1182	0.4735	-0.0512	0.0396	-0.0993	-0.2498	0.1888	-0.0266	-0.1825

Dipole mement (in D) 1.78 (DEN) 1.58 2.06 0.57 0.46 1.23 1.75 0.20 0.56 1.73

File TZVPMol414.out
Molecule PMol414 dimethyl_disulfide
SP Mol414 B3LYP/Def2TZVP VAC.
0 10
Dipole 0.0000 0.0000 2.0066 2.0066
Quadrupole -2.0950 3.7149 -1.6199 -1.4753 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.4425	0.9120	-0.4967	-0.0667	0.2343	-0.0268	0.0672	-0.0543	-0.0944	0.0970	-0.0082	-0.0905
16	-0.4425	-0.9120	-0.4967	-0.0667	0.2343	-0.0268	0.0672	-0.0543	-0.0957	0.0970	-0.0083	-0.0905
6	0.4425	-1.8123	0.7974	-0.3124	-0.5462	-0.0915	-0.4553	-0.2239	-0.2697	-0.7408	-0.1001	-0.2049
1	0.0360	-2.8224	0.8066	0.1244	0.1100	0.0443	0.1363	0.0975	0.1482	0.2215	0.0377	0.1042
1	0.2831	-1.3641	1.7751	0.1220	0.0995	0.0359	0.1249	0.0892	0.1124	0.2069	0.0291	0.0950
1	1.5061	-1.8593	0.5806	0.1328	0.1024	0.0380	0.1269	0.0915	0.1053	0.2154	0.0416	0.0962
6	-0.4425	1.8123	0.7974	-0.3124	-0.5462	-0.0915	-0.4553	-0.2239	-0.2819	-0.7408	-0.1002	-0.2049
1	-1.5061	1.8593	0.5806	0.1328	0.1024	0.0380	0.1269	0.0915	0.1094	0.2154	0.0416	0.0962
1	-0.2831	1.3641	1.7751	0.1220	0.0995	0.0359	0.1249	0.0892	0.1166	0.2069	0.0291	0.0950
1	-0.0360	2.8224	0.8066	0.1244	0.1100	0.0443	0.1363	0.0975	0.1499	0.2215	0.0377	0.1042

Dipole mement (in D) 2.01 (DEN) 1.71 2.18 0.59 0.09 1.33 2.05 0.31 0.29 1.83

File TZVPMol415.out
Molecule PMol415 thiophene
SP Mol415 B3LYP/Def2TZVP VAC.
0 9
Dipole 0.0000 0.0000 -0.4522 0.4522
Quadrupole -4.5632 3.8277 0.7355 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	1.1831	0.0654	0.7117	0.0788	0.2604	0.0367	0.0423	0.4675	0.2514	-0.0429

6	0.0000	1.2286	-0.0026	-0.1457	-0.4097	-0.0740	-0.2712	-0.1124	-0.2081	-0.4328	-0.2370	-0.0745
6	0.0000	0.7069	-1.2640	-0.1405	-0.2110	-0.0616	-0.1050	-0.1149	-0.1322	-0.2534	-0.0099	-0.0943
1	0.0000	1.3142	-2.1577	0.1154	0.1399	0.0457	0.1129	0.1014	0.1356	0.2202	0.0465	0.0894
6	0.0000	-1.2286	-0.0026	-0.1457	-0.4097	-0.0740	-0.2712	-0.1124	-0.2081	-0.4328	-0.2371	-0.0745
6	0.0000	-0.7069	-1.2640	-0.1405	-0.2110	-0.0616	-0.1050	-0.1149	-0.1322	-0.2534	-0.0099	-0.0943
1	0.0000	2.2649	0.2918	0.1381	0.1249	0.0505	0.1331	0.1076	0.1836	0.2322	0.0747	0.1008
1	0.0000	-1.3142	-2.1577	0.1154	0.1399	0.0457	0.1129	0.1014	0.1356	0.2202	0.0465	0.0894
1	0.0000	-2.2649	0.2918	0.1381	0.1249	0.0505	0.1331	0.1076	0.1836	0.2322	0.0747	0.1008

Dipole mement (in D) 0.45 (DEN) 0.08 4.07 0.39 0.79 0.19 0.45 1.83 0.80 0.67

File TZVPMol416.out
Molecule PMol416 2-methylthiophene
SP Mol416 B3LYP/Def2TZVP VAC.
0 12
Dipole -0.4231 0.4690 0.0000 0.6316
Quadrupole 4.0355 0.2901 -4.3256 -0.4788 0.0002 -0.0005

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.6626	-0.2404	0.0001	-0.1657	-0.4104	-0.0783	-0.2769	-0.1168	-0.2775	-0.4299	-0.2352	-0.0786
6	1.3784	1.0920	-0.0001	-0.1327	-0.2112	-0.0646	-0.1059	-0.1177	-0.1338	-0.2480	-0.0105	-0.0966
6	-0.0127	1.3492	-0.0002	-0.1850	-0.1901	-0.0698	-0.1865	-0.1211	-0.2280	-0.2577	-0.0175	-0.1081
6	-0.7779	0.2163	-0.0001	0.0704	-0.4099	-0.0221	0.0551	-0.0225	0.1647	-0.2104	-0.1941	0.0512
16	0.2325	-1.1793	0.0001	0.0386	0.7226	0.0668	0.2032	0.0269	-0.0130	0.4467	0.2109	-0.0629
1	2.6264	-0.7216	0.0001	0.1359	0.1239	0.0489	0.1320	0.1059	0.2107	0.2308	0.0723	0.0989
1	2.1377	1.8610	-0.0001	0.1125	0.1392	0.0440	0.1124	0.0997	0.1412	0.2187	0.0435	0.0874
1	-0.4456	2.3407	-0.0003	0.1075	0.1401	0.0412	0.1123	0.0974	0.1509	0.2154	0.0364	0.0840
6	-2.2601	0.1061	0.0000	-0.3501	-0.2891	-0.0820	-0.4070	-0.2250	-0.3629	-0.6177	0.0387	-0.2423
1	-2.6354	-0.4233	0.8764	0.1243	0.1268	0.0372	0.1172	0.0894	0.1216	0.2164	0.0183	0.0873
1	-2.7084	1.0974	-0.0011	0.1202	0.1312	0.0413	0.1267	0.0942	0.1043	0.2194	0.0193	0.0924
1	-2.6354	-0.4251	-0.8752	0.1243	0.1268	0.0372	0.1172	0.0894	0.1217	0.2164	0.0183	0.0873

Dipole mement (in D) 0.63 (DEN) 0.70 4.21 0.63 0.90 0.52 0.65 1.83 1.09 0.76

File TZVPMol417.out
Molecule PMol417 2,5-dihydrothiophene
SP Mol417 B3LYP/Def2TZVP VAC.
0 11
Dipole 0.0000 0.0000 -1.7548 1.7548
Quadrupole -2.3647 4.3767 -2.0121 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	1.2393	-0.1204	0.4655	-0.0505	0.0360	-0.0933	-0.3226	0.1767	-0.0224	-0.1802
6	0.0000	1.3381	0.0002	-0.1363	-0.4268	-0.0514	-0.2408	-0.1387	0.1933	-0.5400	-0.0553	-0.1053
1	-0.8771	1.9748	0.1347	0.1138	0.1251	0.0365	0.1003	0.0923	0.0329	0.2147	0.0295	0.0891
1	0.8771	1.9748	0.1347	0.1138	0.1251	0.0365	0.1003	0.0923	0.0348	0.2147	0.0295	0.0891
6	0.0000	0.6623	-1.3255	-0.1466	-0.1957	-0.0408	-0.0800	-0.0992	-0.2374	-0.1892	-0.0326	-0.0732
1	0.0000	1.2564	-2.2314	0.1155	0.1397	0.0445	0.1022	0.1000	0.1377	0.2115	0.0392	0.0904

6	0.0000	-0.6623	-1.3255	-0.1466	-0.1957	-0.0408	-0.0800	-0.0992	-0.2374	-0.1892	-0.0325	-0.0732
1	0.0000	-1.2564	-2.2314	0.1155	0.1397	0.0445	0.1022	0.1000	0.1377	0.2115	0.0392	0.0904
6	0.0000	-1.3381	0.0002	-0.1363	-0.4268	-0.0514	-0.2408	-0.1387	0.1933	-0.5400	-0.0547	-0.1053
1	-0.8771	-1.9748	0.1347	0.1138	0.1251	0.0365	0.1003	0.0923	0.0329	0.2147	0.0295	0.0891
1	0.8771	-1.9748	0.1347	0.1138	0.1251	0.0365	0.1003	0.0923	0.0348	0.2147	0.0295	0.0891

Dipole mement (in D) 1.75 (DEN) 1.03 2.59 0.64 0.70 1.20 1.76 0.52 0.48 1.85

File TZVPMol418.out
Molecule PMol418 3-methylthiophene
SP Mol418 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.8082 0.2544 0.0000 0.8473
Quadrupole 1.1691 2.9946 -4.1637 -1.3645 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.0365	1.1367	0.0000	-0.1333	-0.4065	-0.0744	-0.2609	-0.1127	-0.2295	-0.4221	-0.2364	-0.0744
6	0.3229	1.2364	0.0000	-0.1969	-0.1848	-0.0650	-0.1598	-0.1164	-0.2865	-0.2494	-0.0189	-0.1032
6	0.9772	-0.0246	0.0000	0.0899	-0.2390	-0.0133	0.1618	-0.0283	0.3347	-0.0656	0.0173	0.0297
6	0.0723	-1.0505	0.0000	-0.1834	-0.3908	-0.0823	-0.3419	-0.1186	-0.3862	-0.4314	-0.2412	-0.0886
16	-1.5436	-0.4935	-0.0000	0.0550	0.7055	0.0683	0.2552	0.0265	0.0476	0.4603	0.2420	-0.0540
1	-1.7645	1.9310	0.0000	0.1360	0.1245	0.0497	0.1320	0.1067	0.2026	0.2309	0.0727	0.0998
1	0.8482	2.1822	0.0000	0.1101	0.1411	0.0433	0.1172	0.0995	0.1656	0.2164	0.0393	0.0865
1	0.2791	-2.1088	0.0000	0.1295	0.1256	0.0462	0.1360	0.1036	0.2233	0.2282	0.0658	0.0957
6	2.4582	-0.1973	0.0000	-0.3603	-0.2564	-0.0805	-0.3877	-0.2251	-0.3874	-0.6049	0.0260	-0.2478
1	2.9149	0.2674	-0.8747	0.1198	0.1274	0.0358	0.1149	0.0878	0.1095	0.2129	0.0120	0.0847
1	2.9149	0.2674	0.8747	0.1198	0.1274	0.0358	0.1149	0.0878	0.1095	0.2129	0.0120	0.0847
1	2.7420	-1.2472	0.0000	0.1138	0.1261	0.0362	0.1179	0.0889	0.0968	0.2117	0.0089	0.0869

Dipole mement (in D) 0.85 (DEN) 0.38 3.39 0.14 0.53 0.63 0.85 1.51 0.47 1.01

File TZVPMol419.out
Molecule PMol419 carbon_monosulfide
SP Mol419 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 1.9317 1.9317
Quadrupole 0.8313 0.8313 -1.6627 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.4186	0.0815	0.5534	0.0871	0.1659	0.0647	0.2519	0.1740	0.7155	0.0411
6	0.0000	0.0000	-1.1163	-0.0815	-0.5534	-0.0871	-0.1660	-0.0647	-0.2519	-0.1740	-0.7155	-0.0411

Dipole mement (in D) 1.93 (DEN) 0.60 4.08 0.64 1.22 0.48 1.86 1.28 5.27 0.30

File TZVPMol420.out
Molecule PMol420 methyl_isothiocyanate
SP Mol420 B3LYP/Def2TZVP VAC.

```
    0    7
Dipole          3.8737    0.0071    0.0005    3.8737
Quadrupole      3.4562   -1.7282   -1.7280    0.0088    0.0000    0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6     -0.1930   -0.0023   -0.0005    0.0916   -0.5697    0.0733    0.3040    0.2043   -0.1961    0.2176    0.4799    0.2690
  16     -1.7705    0.0011    0.0002   -0.2485    0.2948   -0.1704   -0.2764   -0.1864   -0.1284   -0.0629    0.3590   -0.2366
   7      0.9847   -0.0044   -0.0003   -0.0546    0.1935   -0.0674   -0.2212   -0.2900    0.2785   -0.3913   -1.4627   -0.3011
   6      2.3813    0.0023    0.0003   -0.2175   -0.3030    0.0020   -0.1650   -0.0759   -0.3950   -0.4031    0.4678   -0.0734
   1      2.7640    1.0162   -0.1257    0.1430    0.1281    0.0542    0.1195    0.1160    0.1477    0.2132    0.0520    0.1140
   1      2.7701   -0.3928    0.9400    0.1430    0.1281    0.0542    0.1195    0.1160    0.1466    0.2133    0.0520    0.1141
   1      2.7718   -0.6111   -0.8131    0.1430    0.1282    0.0542    0.1195    0.1160    0.1468    0.2133    0.0520    0.1141

 Dipole mement (in D)   3.87 (DEN)      4.99      0.58      3.25      3.90      3.78      3.94      2.38      2.99      4.05

-----------------------------------------
File TZVPMol421.out
Molecule PMol421    carbon_oxide_sulfide
 SP Mol421 B3LYP/Def2TZVP VAC.
    0    3
Dipole          0.0000    0.0000    0.8119    0.8119
Quadrupole      0.4508    0.4508   -0.9015    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6      0.0000    0.0000   -0.5199    0.2690   -0.6421    0.1744    0.4931    0.2372    0.2402    0.3899    0.5709    0.3700
   8      0.0000    0.0000   -1.6779   -0.1260    0.2264   -0.1377   -0.3244   -0.1811   -0.1894   -0.4275   -1.1104   -0.2678
  16      0.0000    0.0000    1.0339   -0.1429    0.4157   -0.0366   -0.1687   -0.0561   -0.0508    0.0376    0.5396   -0.1022

 Dipole mement (in D)   0.81 (DEN)      0.37      1.84      0.49      0.55      0.59      0.67      2.66     10.20      0.73

-----------------------------------------
File TZVPMol422.out
Molecule PMol422    thioformaldehyde
 SP Mol422 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0000   -1.6882    1.6882
Quadrupole     -0.5809   -1.2632    1.8441    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
  16      0.0000    0.0000    0.5824   -0.1246    0.3236   -0.0857   -0.0642   -0.1149   -0.1383    0.0986    0.4070   -0.1443
   6      0.0000    0.0000   -1.0171   -0.1527   -0.5175   -0.0135   -0.1545   -0.0897   -0.1016   -0.4640   -0.5452   -0.0656
   1      0.0000    0.9174   -1.6078    0.1386    0.0969    0.0496    0.1094    0.1023    0.1199    0.1827    0.0691    0.1049
   1      0.0000   -0.9174   -1.6078    0.1386    0.0969    0.0496    0.1094    0.1023    0.1199    0.1827    0.0691    0.1049

 Dipole mement (in D)   1.69 (DEN)      1.74      1.94      0.94      1.11      1.46      1.74      0.28      2.74      1.70

-----------------------------------------
File TZVPMol423.out
Molecule PMol423    propanethial_S-oxide
 SP Mol423 B3LYP/Def2TZVP VAC.
    0   11
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Dipole -3.8715 -0.7988 0.3171 3.9657
Quadrupole -4.7765 2.1176 2.6589 -2.3342 -0.7596 0.5435

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-2.5551	0.3632	-0.3605	-0.3106	-0.2971	-0.0785	-0.3289	-0.2295	-0.1508	-0.5797	0.0163	-0.2446
1	-3.5002	-0.1740	-0.4165	0.1159	0.1206	0.0364	0.1110	0.0878	0.0440	0.2093	0.0080	0.0903
1	-2.2532	0.6190	-1.3749	0.1124	0.1204	0.0328	0.1096	0.0849	0.0527	0.2049	0.0086	0.0825
1	-2.7357	1.2962	0.1725	0.1083	0.1197	0.0335	0.1101	0.0855	0.0376	0.2014	0.0030	0.0858
6	-1.4904	-0.4757	0.3352	-0.1633	-0.3208	-0.0421	-0.1372	-0.1482	0.1739	-0.4324	0.0736	-0.1247
1	-1.3334	-1.4131	-0.2043	0.0956	0.1368	0.0356	0.0911	0.0924	-0.0185	0.2069	0.0119	0.0863
1	-1.8450	-0.7593	1.3309	0.1091	0.1447	0.0411	0.1122	0.0960	0.0123	0.2149	0.0183	0.0891
6	-0.1972	0.2455	0.4768	-0.1546	-0.4455	-0.0423	-0.3371	-0.0803	-0.2245	-0.5007	-0.6334	-0.0394
1	-0.1566	1.1831	1.0245	0.1383	0.1263	0.0591	0.1569	0.1178	0.1756	0.2279	0.0860	0.1068
16	1.1510	-0.3362	-0.2038	0.4268	0.6655	0.2501	0.7046	0.2621	0.2731	1.1226	1.6614	0.2390
8	2.3579	0.4786	0.0024	-0.4776	-0.3706	-0.3256	-0.5925	-0.3684	-0.3754	-0.8751	-1.2537	-0.3710

Dipole mement (in D)	3.97 (DEN)	4.45	2.66	3.21	4.41	3.96	3.94	6.16	8.71	4.05	

File TZVPMol424.out
Molecule PMol424 thioacetaldehyde
SP Mol424 B3LYP/Def2TZVP VAC.
0 7
Dipole -1.6388 1.8313 0.0000 2.4575
Quadrupole -0.6212 0.6607 -0.0395 -0.6134 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.9596	-0.2557	0.0000	0.1189	0.1234	0.0408	0.1308	0.0941	0.0111	0.2239	0.0392	0.0930
6	-1.4762	0.7170	0.0000	-0.2659	-0.3165	-0.0795	-0.4379	-0.2249	-0.0171	-0.6705	0.0094	-0.2350
6	0.0000	0.6131	0.0000	-0.0451	-0.5121	0.0238	0.1062	-0.0159	0.0645	-0.2480	-0.4904	0.0417
16	0.8703	-0.7426	0.0000	-0.1795	0.3153	-0.1269	-0.1572	-0.1540	-0.2149	0.0518	0.3214	-0.1960
1	-1.8110	1.2884	0.8694	0.1233	0.1353	0.0488	0.1385	0.1004	0.0503	0.2297	0.0329	0.1002
1	-1.8110	1.2884	-0.8694	0.1233	0.1353	0.0488	0.1385	0.1004	0.0503	0.2297	0.0329	0.1002
1	0.5143	1.5796	0.0000	0.1250	0.1192	0.0441	0.0810	0.1000	0.0559	0.1833	0.0549	0.0959

Dipole mement (in D)	2.46 (DEN)	2.65	1.34	1.58	1.83	2.16	2.52	1.00	1.84	2.42	

File TZVPMol425.out
Molecule PMol425 methylthiocyanate
SP Mol425 B3LYP/Def2TZVP VAC.
0 7
Dipole 3.6737 2.1956 0.0000 4.2798
Quadrupole 1.6970 -2.6671 0.9701 -3.5930 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.8881	-0.5835	0.0000	-0.1377	-0.5243	0.0235	0.1747	0.1541	0.3591	0.0023	0.5695	0.2306
7	-1.5367	-1.5485	0.0000	-0.0270	0.0329	-0.2153	-0.3589	-0.3355	-0.4453	-0.3060	-1.1370	-0.3685
16	0.0000	0.8352	0.0000	0.0469	0.6068	0.0928	0.1920	0.0547	-0.0517	0.3265	0.4681	-0.0129
6	1.6749	0.1453	0.0000	-0.3263	-0.4628	-0.0638	-0.4521	-0.1972	-0.3340	-0.7037	-0.0826	-0.1891
1	1.8458	-0.4476	0.8925	0.1514	0.1150	0.0535	0.1474	0.1073	0.1429	0.2263	0.0632	0.1113

1	1.8458	-0.4476	-0.8925	0.1514	0.1150	0.0535	0.1474	0.1073	0.1429	0.2263	0.0632	0.1113
1	2.3443	1.0007	0.0000	0.1414	0.1174	0.0558	0.1497	0.1095	0.1860	0.2282	0.0561	0.1174

Dipole mement (in D) 4.28 (DEN) 2.51 3.78 3.18 3.74 4.03 4.27 4.51 11.18 4.04

File TZVPMol426.out
Molecule PMol426 thiazole
SP Mol426 B3LYP/Def2TZVP VAC.
0 8
Dipole 1.0079 1.2957 0.0000 1.6416
Quadrupole 4.4261 -1.9939 -2.4322 -3.3503 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	1.1766	0.0000	0.0575	0.7016	0.0897	0.2205	0.0572	0.0379	0.4318	0.2429	-0.0191
6	1.2109	-0.0249	0.0000	-0.1312	-0.4228	-0.0762	-0.3330	-0.1076	-0.3073	-0.4646	-0.2414	-0.0703
6	0.6344	-1.2593	0.0000	-0.0779	-0.2807	-0.0107	0.0796	0.0096	0.1607	-0.0541	0.4331	0.0540
6	-1.1931	-0.0647	0.0000	-0.0487	-0.4771	0.0002	0.0056	0.0477	0.1167	-0.1686	0.4201	0.1054
7	-0.7292	-1.2786	0.0000	-0.2148	0.0951	-0.1695	-0.3377	-0.3610	-0.4384	-0.4073	-1.0958	-0.3945
1	-2.2452	0.1807	0.0000	0.1469	0.1207	0.0582	0.1122	0.1239	0.1274	0.2139	0.0895	0.1149
1	2.2574	0.2292	0.0000	0.1419	0.1278	0.0568	0.1478	0.1141	0.2093	0.2394	0.0878	0.1076
1	1.1789	-2.1928	0.0000	0.1262	0.1355	0.0515	0.1048	0.1161	0.0937	0.2096	0.0638	0.1021

Dipole mement (in D) 1.64 (DEN) 1.30 4.10 1.26 2.08 1.77 1.63 3.75 5.17 1.52

File TZVPMol427.out
Molecule PMol427 methanesulfonic_acid
SP Mol427 B3LYP/Def2TZVP VAC.
0 9
Dipole -2.1133 -3.1543 -0.2083 3.8025
Quadrupole 4.9658 0.3042 -5.2700 -2.4606 -0.4979 0.8764

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.6001	-0.3509	-0.0207	-0.3248	-0.4102	-0.0778	-0.7586	-0.2068	-0.5493	-0.8854	-0.1252	-0.2104
16	0.0916	0.1393	0.0670	0.8103	0.5490	0.5047	2.0541	0.5837	1.0649	2.3800	3.2274	0.6559
8	0.2370	1.3749	-0.6207	-0.4042	-0.2494	-0.2955	-0.7464	-0.3460	-0.4692	-0.9077	-1.3493	-0.3742
8	0.7779	-0.9823	-0.8518	-0.4136	-0.1616	-0.1935	-0.8287	-0.3924	-0.5271	-0.8835	-1.2180	-0.3274
8	0.5706	-0.0459	1.4011	-0.4384	-0.2779	-0.3104	-0.7842	-0.3639	-0.5152	-0.9350	-1.3649	-0.3837
1	-1.7185	-1.3349	0.4214	0.1331	0.1211	0.0578	0.1859	0.1151	0.1741	0.2367	0.0645	0.1131
1	-1.9128	-0.3537	-1.0600	0.1505	0.1262	0.0625	0.1953	0.1202	0.2043	0.2453	0.0763	0.1158
1	-2.1763	0.3809	0.5382	0.1475	0.1283	0.0656	0.1922	0.1226	0.2018	0.2474	0.0761	0.1215
1	1.2580	-1.5886	-0.2756	0.3396	0.1745	0.1866	0.4903	0.3675	0.4157	0.5021	0.6142	0.2894

Dipole mement (in D) 3.80 (DEN) 3.78 2.05 2.89 3.57 3.79 3.79 4.76 8.02 3.77

File TZVPMol428.out
Molecule PMol428 methyl_methanesulfenate
SP Mol428 B3LYP/Def2TZVP VAC.

```
    0   10
Dipole         -0.1005    1.7972   -0.8001    1.9698
Quadrupole      3.7232   -1.1730   -2.5502   -0.2126   -0.7084    0.4796
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6     -1.5285    0.8143    0.0630   -0.3306   -0.5389   -0.0948   -0.4960   -0.2261   -0.4345   -0.7762   -0.1155   -0.2168
  16     -0.5649   -0.6751   -0.1661    0.0831    0.4080    0.0494    0.2641    0.0429   -0.0469    0.4803    0.5532   -0.0145
   8      0.8537   -0.2638    0.5830   -0.3141   -0.0941   -0.1706   -0.3190   -0.2540   -0.2221   -0.6180   -1.0785   -0.2212
   6      1.7666    0.4598   -0.2321   -0.1440   -0.3930   -0.0095   -0.0967   -0.1297    0.1012   -0.2521    0.4718   -0.1005
   1     -2.5104    0.6001   -0.3575    0.1251    0.1158    0.0480    0.1433    0.1017    0.1933    0.2285    0.0421    0.1078
   1     -1.1121    1.6687   -0.4682    0.1223    0.0993    0.0348    0.1237    0.0887    0.1477    0.2059    0.0250    0.0930
   1     -1.6470    1.0505    1.1186    0.1326    0.1041    0.0398    0.1351    0.0940    0.1619    0.2155    0.0401    0.0952
   1      2.6616    0.6074    0.3693    0.1170    0.1084    0.0427    0.0979    0.1032    0.0413    0.1861    0.0315    0.0914
   1      1.3667    1.4362   -0.5172    0.0968    0.0945    0.0296    0.0758    0.0891    0.0321    0.1600    0.0080    0.0826
   1      2.0216   -0.0954   -1.1364    0.1118    0.0958    0.0305    0.0718    0.0902    0.0259    0.1701    0.0221    0.0829

 Dipole mement (in D)   1.97 (DEN)      2.00      1.89      0.92      1.39      1.75      2.01      2.92      4.32      1.86

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File TZVPMol429.out
Molecule PMol429    methyl_methanesulfinate
 SP Mol429 B3LYP/Def2TZVP VAC.
    0   11
Dipole         -0.5136   -2.3971   -1.0171    2.6541
Quadrupole      6.3111   -4.9498   -1.3613   -3.1040   -0.4879   -1.0335
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   8      0.5751    1.4503    0.3720   -0.4963   -0.3600   -0.3422   -0.6811   -0.3898   -0.3840   -0.9284   -1.3134   -0.3991
  16      0.4010    0.2342   -0.4176    0.5670    0.6281    0.3383    1.0956    0.3718    0.2893    1.4567    1.8478    0.3673
   8     -0.8101   -0.6787    0.2504   -0.3106   -0.0632   -0.1702   -0.4253   -0.2571   -0.1944   -0.6756   -1.1057   -0.2279
   6      1.6363   -0.9331    0.1556   -0.3294   -0.4697   -0.0940   -0.6544   -0.2240   -0.2887   -0.8309   -0.1545   -0.2232
   6     -2.1075   -0.1388    0.0133   -0.1949   -0.3874   -0.0052   -0.1106   -0.1253   -0.0957   -0.2683    0.4509   -0.1002
   1      1.4823   -1.8987   -0.3174    0.1239    0.1112    0.0486    0.1591    0.1045    0.1051    0.2286    0.0511    0.1031
   1      1.5467   -1.0123    1.2359    0.1361    0.1135    0.0533    0.1779    0.1116    0.1362    0.2400    0.0708    0.1022
   1      2.6098   -0.5327   -0.1130    0.1299    0.1128    0.0509    0.1597    0.1062    0.1616    0.2285    0.0491    0.1081
   1     -2.8160   -0.8529    0.4219    0.1276    0.1123    0.0474    0.1110    0.1082    0.0939    0.1947    0.0412    0.0976
   1     -2.2992   -0.0140   -1.0549    0.1104    0.0971    0.0330    0.0697    0.0929    0.0646    0.1700    0.0209    0.0859
   1     -2.2313    0.8207    0.5167    0.1364    0.1052    0.0399    0.0983    0.1010    0.1120    0.1849    0.0417    0.0860

 Dipole mement (in D)   2.65 (DEN)      3.16      2.23      2.34      4.18      2.70      2.59      5.85      8.23      2.86

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File TZVPMol430.out
Molecule PMol430    methane_sulfonamide
 SP Mol430 B3LYP/Def2TZVP VAC.
    0   10
Dipole          0.1016    3.4038    0.0000    3.4053
Quadrupole      7.4194   -3.1920   -4.2274   -1.9465   -0.0020    0.0034
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   7     -1.1016    1.1108   -0.0002   -0.4992   -0.2790   -0.1865   -1.0972   -0.6278   -0.8745   -1.0772   -1.2597   -0.5273
```

16	-0.0439	-0.1685	0.0001	0.8000	0.5793	0.4804	2.0391	0.5882	1.0968	2.3150	3.1039	0.6553
8	-0.1810	-0.8492	-1.2521	-0.4482	-0.2813	-0.3186	-0.7715	-0.3696	-0.5260	-0.9380	-1.3672	-0.3859
8	-0.1804	-0.8485	1.2527	-0.4482	-0.2813	-0.3186	-0.7715	-0.3696	-0.5261	-0.9380	-1.3672	-0.3859
6	1.5226	0.6481	-0.0005	-0.3116	-0.4102	-0.0840	-0.7433	-0.2113	-0.4084	-0.8739	-0.1268	-0.2090
1	-1.6694	1.1096	0.8352	0.2500	0.1530	0.1278	0.3928	0.3231	0.3900	0.3983	0.4111	0.2565
1	-1.6706	1.1081	-0.8347	0.2500	0.1530	0.1279	0.3929	0.3232	0.3900	0.3983	0.4112	0.2565
1	2.2872	-0.1240	-0.0003	0.1419	0.1246	0.0608	0.1846	0.1179	0.1482	0.2422	0.0679	0.1157
1	1.6112	1.2601	0.8917	0.1327	0.1208	0.0554	0.1870	0.1129	0.1550	0.2366	0.0633	0.1121
1	1.6109	1.2594	-0.8930	0.1327	0.1208	0.0554	0.1870	0.1129	0.1550	0.2367	0.0633	0.1121

Dipole mement (in D)	3.41 (DEN)	3.60	2.11	2.96	2.81	3.27	3.41	4.29	7.11	3.25

File TZVPMol431.out
Molecule PMol431 dicyanogen_sulfide
SP Mol431 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.0000 0.0000 3.0833 3.0833
Quadrupole 3.8341 -7.0980 3.2638 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.8975	0.1841	0.7649	0.2271	0.2781	0.2032	0.1393	0.4516	0.8269	0.1303
6	0.0000	1.2889	-0.1903	-0.1154	-0.4663	0.0466	0.1366	0.1791	0.2749	0.0062	0.6512	0.2458
6	0.0000	-1.2889	-0.1903	-0.1154	-0.4663	0.0466	0.1366	0.1791	0.2749	0.0062	0.6512	0.2458
7	0.0000	2.2340	-0.8626	0.0233	0.0839	-0.1602	-0.2756	-0.2807	-0.3446	-0.2320	-1.0647	-0.3110
7	0.0000	-2.2340	-0.8626	0.0233	0.0839	-0.1602	-0.2756	-0.2807	-0.3446	-0.2320	-1.0647	-0.3110

Dipole mement (in D)	3.08 (DEN)	0.81	3.46	2.22	3.23	2.87	2.95	3.86	11.20	2.69

File TZVPMol432.out
Molecule PMol432 dimethyl_sulfone
SP Mol432 B3LYP/Def2TZVP VAC.
0 11
Dipole 0.0000 0.0000 -4.4640 4.4640
Quadrupole -5.2813 5.8373 -0.5560 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.1941	0.7537	0.6495	0.4641	1.8708	0.4946	1.0877	2.2013	2.6576	0.5365
8	-1.2468	0.0000	0.9066	-0.4552	-0.2828	-0.3227	-0.7516	-0.3754	-0.5346	-0.9369	-1.3619	-0.3941
8	1.2468	0.0000	0.9066	-0.4552	-0.2828	-0.3227	-0.7516	-0.3754	-0.5354	-0.9369	-1.3619	-0.3941
6	0.0000	1.3885	-0.9114	-0.3418	-0.4102	-0.0834	-0.7386	-0.2143	-0.5797	-0.8808	-0.1554	-0.2151
1	0.0000	2.2776	-0.2868	0.1496	0.1283	0.0645	0.1925	0.1214	0.2062	0.2516	0.0768	0.1191
1	0.8959	1.3731	-1.5255	0.1353	0.1200	0.0548	0.1811	0.1105	0.1829	0.2327	0.0559	0.1109
1	-0.8959	1.3731	-1.5255	0.1353	0.1200	0.0548	0.1811	0.1105	0.1818	0.2327	0.0559	0.1109
6	0.0000	-1.3885	-0.9114	-0.3418	-0.4102	-0.0834	-0.7386	-0.2143	-0.5797	-0.8808	-0.1557	-0.2151
1	0.8959	-1.3731	-1.5255	0.1353	0.1200	0.0548	0.1811	0.1105	0.1829	0.2327	0.0559	0.1109
1	0.0000	-2.2776	-0.2868	0.1496	0.1283	0.0645	0.1925	0.1214	0.2062	0.2516	0.0768	0.1191
1	-0.8959	-1.3731	-1.5255	0.1353	0.1200	0.0548	0.1811	0.1105	0.1818	0.2327	0.0559	0.1109

Dipole mement (in D) 4.46 (DEN) 4.65 2.14 3.43 4.17 4.51 4.48 5.91 9.87 4.63

File TZVPMol433.out
Molecule PMol433 dimethyl_sulfoxide
SP Mol433 B3LYP/Def2TZVP VAC.
0 10
Dipole -2.4374 -3.0604 0.0000 3.9124
Quadrupole -2.5785 -1.3816 3.9602 -2.1600 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	-0.2542	0.4308	0.0000	0.4819	0.6788	0.2825	0.9872	0.2698	0.2582	1.2566	1.3628	0.2447
8	1.0779	1.0706	0.0000	-0.5534	-0.4052	-0.3768	-0.6900	-0.4245	-0.4157	-0.9567	-1.3165	-0.4263
6	-0.2542	-0.7831	1.3384	-0.3487	-0.4691	-0.0933	-0.6157	-0.2264	-0.4045	-0.8216	-0.1549	-0.2199
1	0.6202	-1.4242	1.2443	0.1280	0.1087	0.0462	0.1619	0.1013	0.1660	0.2215	0.0474	0.1006
1	-0.2050	-0.2336	2.2742	0.1415	0.1139	0.0502	0.1563	0.1049	0.1756	0.2318	0.0503	0.1074
6	-0.2542	-0.7831	-1.3384	-0.3487	-0.4691	-0.0933	-0.6157	-0.2264	-0.4045	-0.8216	-0.1550	-0.2199
1	-0.2050	-0.2336	-2.2742	0.1415	0.1139	0.0502	0.1563	0.1049	0.1756	0.2318	0.0503	0.1074
1	0.6202	-1.4242	-1.2443	0.1280	0.1087	0.0462	0.1619	0.1013	0.1660	0.2215	0.0474	0.1006
1	-1.1685	-1.3722	-1.3101	0.1149	0.1097	0.0441	0.1490	0.0976	0.1417	0.2183	0.0345	0.1027
1	-1.1685	-1.3722	1.3101	0.1149	0.1097	0.0441	0.1490	0.0976	0.1417	0.2183	0.0345	0.1027

Dipole mement (in D) 3.91 (DEN) 4.42 2.61 3.10 4.51 3.89 3.93 6.59 9.22 4.06

File TZVPMol434.out
Molecule PMol434 HCl
SP Mol434 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 -1.2324 1.2324
Quadrupole -1.2025 -1.2025 2.4050 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	0.0708	-0.2317	-0.0450	-0.1218	-0.2510	-0.1778	-0.2251	-0.2578	-0.2803	-0.1972
1	0.0000	0.0000	-1.2033	0.2317	0.0450	0.1218	0.2510	0.1778	0.2251	0.2578	0.2803	0.1972

Dipole mement (in D) 1.23 (DEN) 1.42 0.28 0.75 1.54 1.09 1.38 1.58 1.72 1.21

File TZVPMol435.out
Molecule PMol435 chloromethane
SP Mol435 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.0000 -1.8977 0.0000 1.8977
Quadrupole -0.5731 1.1463 -0.5732 0.0001 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.6545	0.0000	-0.1587	0.2287	-0.1058	-0.0719	-0.1170	-0.1396	-0.0600	-0.2754	-0.1495
6	0.0000	-1.1191	0.0000	-0.2486	-0.5374	-0.0361	-0.2904	-0.1817	-0.3212	-0.5623	0.1178	-0.1550
1	1.0256	-1.4706	0.0000	0.1357	0.1029	0.0473	0.1208	0.0996	0.1538	0.2074	0.0526	0.1015
1	-0.5128	-1.4707	0.8882	0.1357	0.1029	0.0473	0.1208	0.0996	0.1535	0.2074	0.0526	0.1015

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   1     -0.5128   -1.4707   -0.8882    0.1357    0.1029    0.0473    0.1208    0.0996    0.1535    0.2074    0.0526    0.1015

 Dipole mement (in D)   1.90 (DEN)      2.04      1.43      1.14      1.22      1.50      1.97      1.56      2.61      1.79

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File TZVPMol436.out
Molecule PMol436    dichloromethane
 SP Mol436 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.0001    1.6423    0.0000    1.6423
Quadrupole     -2.1344    1.8355    0.2989    0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  17      1.4746   -0.2143    0.0000   -0.1043    0.2859   -0.0703   -0.0735   -0.0781   -0.0528   -0.0184   -0.2191   -0.1216
   6      0.0000    0.7573    0.0000   -0.0932   -0.7835    0.0278   -0.0736   -0.0697   -0.3396   -0.3959    0.2486    0.0296
  17     -1.4746   -0.2142    0.0000   -0.1043    0.2859   -0.0703   -0.0735   -0.0781   -0.0531   -0.0184   -0.2191   -0.1216
   1      0.0000    1.3707    0.8929    0.1509    0.1059    0.0564    0.1103    0.1129    0.2227    0.2163    0.0948    0.1068
   1      0.0000    1.3707   -0.8929    0.1509    0.1059    0.0564    0.1103    0.1129    0.2227    0.2163    0.0948    0.1068

 Dipole mement (in D)   1.64 (DEN)      1.86      2.04      0.99      1.34      1.39      1.81      1.45      2.60      1.76

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File TZVPMol437.out
Molecule PMol437    trichloromethane
 SP Mol437 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.9099    0.5777    0.0000    1.0778
Quadrupole      0.8037   -0.0983   -0.7054   -0.9585    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   1     -1.2944    0.8214    0.0000    0.1596    0.1078    0.0603    0.0902    0.1212    0.3198    0.2253    0.1325    0.1065
   6     -0.3805    0.2414    0.0000    0.0213   -1.0854    0.0791    0.1485    0.0298   -0.4769   -0.2902    0.3674    0.2056
  17      0.9715    1.3759    0.0000   -0.0603    0.3259   -0.0465   -0.0795   -0.0503    0.0532    0.0216   -0.1666   -0.1041
  17     -0.3805   -0.7547    1.4571   -0.0603    0.3258   -0.0465   -0.0796   -0.0504    0.0520    0.0216   -0.1665   -0.1040
  17     -0.3805   -0.7547   -1.4571   -0.0603    0.3258   -0.0465   -0.0796   -0.0504    0.0520    0.0216   -0.1665   -0.1040

 Dipole mement (in D)   1.08 (DEN)      1.29      1.95      0.67      1.08      1.02      1.26      1.01      1.97      1.35

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File TZVPMol438.out
Molecule PMol438    chloroethane
 SP Mol438 B3LYP/Def2TZVP VAC.
    0    8
Dipole          1.0996    1.7575    0.0000    2.0731
Quadrupole     -0.6560    0.5804    0.0756   -0.2976    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  17     -0.8176   -0.7877    0.0000   -0.1739    0.2426   -0.1122   -0.1098   -0.1219   -0.1974   -0.0816   -0.2973   -0.1594
   6      0.0000    0.8092    0.0000   -0.1048   -0.5100   -0.0001   -0.0436   -0.1070   -0.0229   -0.3477    0.1376   -0.0459
   6      1.4959    0.6621    0.0000   -0.3003   -0.3363   -0.0837   -0.3853   -0.2342   -0.0943   -0.6096    0.0313   -0.2448
   1     -0.3616    1.3345    0.8803    0.1216    0.1195    0.0426    0.0945    0.0981    0.0851    0.2035    0.0421    0.0935
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1	-0.3616	1.3345	-0.8803	0.1216	0.1195	0.0426	0.0945	0.0981	0.0851	0.2035	0.0421	0.0935
1	1.9645	1.6466	0.0000	0.1056	0.1234	0.0383	0.1172	0.0898	0.0410	0.2100	0.0085	0.0916
1	1.8416	0.1239	-0.8800	0.1152	0.1207	0.0362	0.1162	0.0886	0.0517	0.2110	0.0178	0.0858
1	1.8416	0.1239	0.8800	0.1152	0.1207	0.0362	0.1162	0.0886	0.0517	0.2110	0.0178	0.0858

Dipole mement (in D)	2.07 (DEN)	2.15	1.40	1.26	1.39	1.63	2.14	1.81	2.90	1.91

File TZVPMol439.out
Molecule PMol439 1,1-dichloroethane
SP Mol439 B3LYP/Def2TZVP VAC.
0 8
Dipole 0.2763 2.0335 0.0000 2.0522
Quadrupole 0.7093 1.5332 -2.2425 -0.1134 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.9640	1.4343	0.0000	-0.2959	-0.3378	-0.0872	-0.4929	-0.2347	-0.1751	-0.6244	0.0456	-0.2480
1	1.8992	0.8802	0.0000	0.1233	0.1262	0.0419	0.1365	0.0955	0.1108	0.2229	0.0386	0.0874
1	0.9346	2.0661	0.8854	0.1193	0.1272	0.0428	0.1356	0.0956	0.0935	0.2219	0.0294	0.0924
1	0.9346	2.0661	-0.8854	0.1193	0.1272	0.0428	0.1356	0.0956	0.0935	0.2219	0.0294	0.0924
6	-0.2097	0.4995	0.0000	0.0385	-0.7675	0.0626	0.1871	0.0031	-0.1653	-0.1889	0.2433	0.1391
1	-1.1634	1.0173	0.0000	0.1362	0.1243	0.0514	0.0840	0.1113	0.2051	0.2167	0.0879	0.0991
17	-0.2097	-0.5186	-1.4667	-0.1204	0.3003	-0.0772	-0.0931	-0.0832	-0.0813	-0.0351	-0.2372	-0.1312
17	-0.2097	-0.5186	1.4667	-0.1204	0.3003	-0.0772	-0.0931	-0.0832	-0.0813	-0.0351	-0.2372	-0.1312

Dipole mement (in D)	2.05 (DEN)	2.23	2.01	1.22	1.23	1.66	2.14	1.83	3.31	1.97

File TZVPMol440.out
Molecule PMol440 1,1,1-trichloroethane
SP Mol440 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.6629 1.6748 0.0000 1.8012
Quadrupole -0.5982 1.6066 -1.0084 -1.0338 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	1.6913	0.2811	0.0000	-0.0789	0.3399	-0.0533	-0.0858	-0.0554	0.0194	0.0097	-0.1813	-0.1129
6	-0.0926	0.2341	0.0000	0.1654	-1.0641	0.1167	0.4061	0.1053	-0.2107	-0.0799	0.3445	0.3181
6	-0.6463	1.6333	0.0000	-0.3118	-0.3443	-0.0922	-0.6036	-0.2367	-0.3996	-0.6407	0.0637	-0.2522
17	-0.6463	-0.6443	1.4514	-0.0789	0.3399	-0.0534	-0.0859	-0.0554	0.0211	0.0097	-0.1813	-0.1129
17	-0.6463	-0.6443	-1.4514	-0.0789	0.3399	-0.0534	-0.0859	-0.0554	0.0211	0.0097	-0.1813	-0.1129
1	-1.7328	1.5977	0.0000	0.1277	0.1296	0.0452	0.1517	0.0992	0.1801	0.2305	0.0454	0.0909
1	-0.3054	2.1624	-0.8862	0.1277	0.1296	0.0452	0.1517	0.0992	0.1843	0.2305	0.0454	0.0909
1	-0.3054	2.1624	0.8862	0.1277	0.1296	0.0452	0.1517	0.0992	0.1843	0.2305	0.0454	0.0909

Dipole mement (in D)	1.80 (DEN)	1.89	2.00	1.02	0.49	1.45	1.86	1.50	3.29	1.63

File TZVPMol441.out
Molecule PMol441 pentachloroethane

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 SP Mol441 B3LYP/Def2TZVP VAC.
    0    8
Dipole          -0.8564   -0.2296    0.0000    0.8866
Quadrupole       2.0013   -1.9400   -0.0614    0.3743    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  17      1.8300   -0.3188    0.0000   -0.0431    0.3850   -0.0303   -0.0728   -0.0302    0.2023    0.0542   -0.1348   -0.1003
   6      0.0909   -0.6100    0.0000    0.1412   -1.1219    0.0974    0.2657    0.0932   -0.5617   -0.1450    0.3763    0.3023
   6     -0.7057    0.7168    0.0000   -0.0105   -0.8492    0.0358   -0.0298   -0.0128   -0.5389   -0.2906    0.2881    0.1191
  17     -0.3773   -1.5366    1.4421   -0.0519    0.3713   -0.0338   -0.0788   -0.0348    0.1479    0.0429   -0.1486   -0.0983
  17     -0.3773   -1.5366   -1.4421   -0.0519    0.3713   -0.0338   -0.0788   -0.0348    0.1479    0.0429   -0.1486   -0.0983
   1     -1.7634    0.4661    0.0000    0.1598    0.1325    0.0549    0.1027    0.1171    0.4084    0.2434    0.1204    0.0943
  17     -0.3773    1.6634   -1.4526   -0.0718    0.3555   -0.0452   -0.0543   -0.0490    0.0970    0.0261   -0.1768   -0.1094
  17     -0.3773    1.6634    1.4526   -0.0718    0.3555   -0.0452   -0.0543   -0.0490    0.0970    0.0261   -0.1768   -0.1094

 Dipole mement (in D)   0.89 (DEN)      1.25      2.03      0.57      0.85      0.91      1.02      0.97      1.86      1.27

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File TZVPMol442.out
Molecule PMol442    cyclopropylchloride
 SP Mol442 B3LYP/Def2TZVP VAC.
    0    9
Dipole           1.4181   -1.2807    0.0000    1.9108
Quadrupole       1.5783   -1.1641   -0.4143    0.6504    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.5931   -1.1837    0.7507   -0.2173   -0.2346   -0.0672   -0.2712   -0.1737   -0.2681   -0.4152   -0.0273   -0.1709
   6      0.5931    0.0990    0.0000    0.0001   -0.4934   -0.0016    0.0365   -0.0630   -0.1035   -0.2227    0.0856    0.0189
   6      0.5931   -1.1837   -0.7507   -0.2173   -0.2346   -0.0672   -0.2712   -0.1737   -0.2681   -0.4152   -0.0273   -0.1709
   1      1.4948   -1.4576    1.2798    0.1110    0.1292    0.0442    0.1223    0.0990    0.1427    0.2147    0.0348    0.0953
   1     -0.3222   -1.4673    1.2480    0.1193    0.1322    0.0449    0.1265    0.1009    0.1557    0.2227    0.0500    0.0911
   1      1.4834    0.7088    0.0000    0.1243    0.1301    0.0491    0.1002    0.1077    0.1736    0.2195    0.0663    0.0963
   1     -0.3222   -1.4673   -1.2480    0.1193    0.1322    0.0449    0.1265    0.1009    0.1557    0.2227    0.0500    0.0911
   1      1.4948   -1.4576   -1.2798    0.1110    0.1292    0.0442    0.1223    0.0990    0.1427    0.2147    0.0348    0.0953
  17     -0.8532    1.1031    0.0000   -0.1504    0.3097   -0.0913   -0.0918   -0.0971   -0.1307   -0.0411   -0.2661   -0.1462

 Dipole mement (in D)   1.91 (DEN)      1.88      1.84      1.16      1.15      1.50      2.00      1.51      2.84      1.83

-----------------------------------------
File TZVPMol443.out
Molecule PMol443    1-chloropropane(gauche)
 SP Mol443 B3LYP/Def2TZVP VAC.
    0   11
Dipole          -1.5997    1.2602    0.2816    2.0558
Quadrupole      -1.6488    1.2315    0.4173    0.1974    0.1328    0.4424
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.1796    0.8843    0.3039   -0.1111   -0.4815   -0.0016   -0.0754   -0.1069   -0.2457   -0.3433    0.1280   -0.0510
   1      0.0982    0.9110    1.3892    0.1171    0.1218    0.0410    0.0938    0.0970    0.1337    0.2012    0.0391    0.0909
   1      0.5822    1.8355   -0.0337    0.1290    0.1213    0.0426    0.0918    0.0982    0.1253    0.2089    0.0418    0.0936
   6     -1.1424    0.5643   -0.3501   -0.1346   -0.3249   -0.0459   -0.1655   -0.1576    0.2503   -0.4087    0.0667   -0.1339
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1	-1.0082	0.5334	-1.4330	0.0971	0.1358	0.0329	0.0944	0.0885	-0.0085	0.2042	0.0062	0.0793
1	-1.8060	1.4113	-0.1522	0.0892	0.1391	0.0354	0.0964	0.0902	-0.0249	0.2042	-0.0025	0.0852
6	-1.7755	-0.7210	0.1423	-0.3406	-0.3133	-0.0867	-0.3448	-0.2381	-0.2532	-0.5951	0.0125	-0.2511
1	-1.9382	-0.6957	1.2204	0.0981	0.1173	0.0287	0.1013	0.0806	0.0663	0.1958	-0.0073	0.0803
1	-1.1395	-1.5786	-0.0712	0.1231	0.1188	0.0265	0.1009	0.0795	0.0699	0.2130	0.0166	0.0722
1	-2.7394	-0.8967	-0.3313	0.1126	0.1184	0.0320	0.1070	0.0836	0.0538	0.2069	-0.0004	0.0857
17	1.4342	-0.3462	-0.0685	-0.1798	0.2472	-0.1050	-0.1000	-0.1151	-0.1670	-0.0869	-0.3002	-0.1510

Dipole mement (in D) 2.06 (DEN) 2.13 1.53 1.21 1.42 1.58 2.10 1.79 2.85 1.91

File TZVPMol444.out
Molecule PMol444 1-chloropropane(trans)
SP Mol444 B3LYP/Def2TZVP VAC.
0 11
Dipole 2.1284 0.2507 0.0000 2.1431
Quadrupole -1.9666 1.0183 0.9483 0.1380 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.5785	0.0000	-0.1095	-0.4877	-0.0034	-0.0748	-0.1084	-0.2300	-0.3448	0.1296	-0.0516
1	0.1586	1.1983	0.8807	0.1186	0.1211	0.0408	0.0940	0.0968	0.1263	0.2017	0.0386	0.0902
1	0.1586	1.1983	-0.8807	0.1186	0.1211	0.0408	0.0940	0.0968	0.1263	0.2017	0.0386	0.0902
6	0.8987	-0.6337	0.0000	-0.1395	-0.3256	-0.0480	-0.1731	-0.1599	0.3095	-0.4080	0.0693	-0.1369
1	0.6717	-1.2491	-0.8719	0.0972	0.1344	0.0325	0.0945	0.0881	-0.0301	0.2036	0.0064	0.0783
1	0.6717	-1.2491	0.8719	0.0972	0.1344	0.0325	0.0945	0.0881	-0.0301	0.2036	0.0064	0.0783
6	2.3621	-0.2296	0.0000	-0.3440	-0.3053	-0.0801	-0.3271	-0.2319	-0.2889	-0.5887	0.0092	-0.2455
1	2.6138	0.3655	0.8782	0.1066	0.1181	0.0305	0.1014	0.0823	0.0655	0.1979	-0.0037	0.0829
1	2.6138	0.3655	-0.8782	0.1066	0.1181	0.0305	0.1014	0.0823	0.0655	0.1979	-0.0037	0.0829
1	3.0135	-1.1012	0.0000	0.1194	0.1210	0.0355	0.1103	0.0870	0.0676	0.2115	0.0068	0.0894
17	-1.7333	0.1283	0.0000	-0.1713	0.2506	-0.1115	-0.1150	-0.1212	-0.1817	-0.0763	-0.2976	-0.1582

Dipole mement (in D) 2.14 (DEN) 2.16 1.23 1.37 1.43 1.75 2.22 1.88 3.00 1.99

File TZVPMol445.out
Molecule PMol445 1,3-dichloropropane
SP Mol445 B3LYP/Def2TZVP VAC.
0 11
Dipole 0.0000 0.0000 -1.8433 1.8433
Quadrupole 3.6423 -8.0416 4.3992 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	1.2413	-0.6800	-0.1284	-0.4880	-0.0021	-0.0773	-0.1068	-0.3024	-0.3522	0.1285	-0.0513
1	0.8809	1.2920	-1.3173	0.1241	0.1225	0.0432	0.0960	0.0993	0.1428	0.2051	0.0424	0.0930
1	-0.8809	1.2920	-1.3173	0.1241	0.1225	0.0432	0.0960	0.0993	0.1426	0.2051	0.0424	0.0930
6	0.0000	0.0000	0.1836	-0.1551	-0.3311	-0.0532	-0.2669	-0.1620	0.3743	-0.4264	0.0751	-0.1422
1	-0.8739	0.0000	0.8352	0.1119	0.1398	0.0378	0.1087	0.0945	-0.0219	0.2137	0.0277	0.0797
1	0.8739	0.0000	0.8352	0.1119	0.1398	0.0378	0.1087	0.0945	-0.0208	0.2137	0.0277	0.0797
6	0.0000	-1.2413	-0.6800	-0.1284	-0.4880	-0.0021	-0.0773	-0.1068	-0.3024	-0.3522	0.1287	-0.0513
1	0.8809	-1.2920	-1.3173	0.1241	0.1225	0.0432	0.0960	0.0993	0.1428	0.2051	0.0424	0.0930

1	-0.8809	-1.2920	-1.3173	0.1241	0.1225	0.0432	0.0960	0.0993	0.1426	0.2051	0.0424	0.0930
17	0.0000	-2.7246	0.3135	-0.1542	0.2687	-0.0956	-0.0901	-0.1053	-0.1488	-0.0584	-0.2787	-0.1433
17	0.0000	2.7246	0.3135	-0.1542	0.2687	-0.0956	-0.0901	-0.1053	-0.1488	-0.0584	-0.2787	-0.1433

Dipole mement (in D) 1.84 (DEN) 2.00 1.73 1.11 1.56 1.52 1.93 1.73 2.46 1.94

File TZVPMol446.out
Molecule PMol446 2-chloropropane
SP Mol446 B3LYP/Def2TZVP VAC.
0 11
Dipole -1.6814 -1.3845 0.0000 2.1781
Quadrupole 0.2477 -0.7139 0.4661 -0.7029 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.5697	-0.8965	1.2607	-0.3085	-0.3099	-0.0863	-0.4303	-0.2351	-0.3708	-0.6078	0.0275	-0.2498
1	-1.4650	-1.5192	1.2931	0.1031	0.1243	0.0361	0.1212	0.0882	0.1114	0.2073	0.0045	0.0882
1	0.2979	-1.5545	1.2940	0.1106	0.1228	0.0348	0.1217	0.0878	0.1200	0.2088	0.0148	0.0835
6	-0.5697	-0.0693	0.0000	0.0344	-0.5121	0.0351	0.1776	-0.0337	0.2231	-0.1520	0.1464	0.0641
1	-1.4095	0.6246	0.0000	0.1036	0.1366	0.0399	0.0773	0.0988	0.0701	0.2040	0.0361	0.0879
6	-0.5697	-0.8965	-1.2607	-0.3085	-0.3099	-0.0863	-0.4303	-0.2351	-0.3708	-0.6078	0.0273	-0.2498
1	-1.4650	-1.5192	-1.2931	0.1031	0.1243	0.0361	0.1212	0.0882	0.1114	0.2073	0.0045	0.0882
1	0.2979	-1.5545	-1.2940	0.1106	0.1228	0.0348	0.1217	0.0878	0.1200	0.2088	0.0148	0.0835
1	-0.5568	-0.2741	-2.1520	0.1222	0.1221	0.0359	0.1189	0.0885	0.1029	0.2173	0.0188	0.0854
17	0.8889	1.0144	0.0000	-0.1929	0.2570	-0.1159	-0.1179	-0.1240	-0.2204	-0.1031	-0.3138	-0.1666
1	-0.5568	-0.2741	2.1520	0.1222	0.1221	0.0359	0.1189	0.0885	0.1029	0.2173	0.0188	0.0854

Dipole mement (in D) 2.18 (DEN) 2.26 1.33 1.31 1.30 1.69 2.28 2.05 3.04 1.97

File TZVPMol447.out
Molecule PMol447 1-chloro-2-methylpropane
SP Mol447 B3LYP/Def2TZVP VAC.
0 14
Dipole 1.9549 -0.6021 0.2344 2.0589
Quadrupole -2.4579 1.3243 1.1336 -0.0393 -0.3493 -0.3213

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.1364	-0.7517	-0.0434	-0.3455	-0.2791	-0.0815	-0.3647	-0.2316	-0.4766	-0.5849	0.0037	-0.2494
6	0.8516	0.0134	-0.3336	-0.0023	-0.3471	-0.0134	0.0527	-0.0873	0.5208	-0.2363	0.0918	-0.0266
1	0.6764	0.0060	-1.4139	0.0706	0.1498	0.0310	0.0789	0.0901	-0.0293	0.1965	-0.0007	0.0738
1	2.0902	-1.7808	-0.3996	0.1115	0.1192	0.0305	0.1015	0.0825	0.1040	0.2032	-0.0042	0.0831
1	2.9907	-0.2745	-0.5213	0.1161	0.1226	0.0342	0.1123	0.0863	0.1153	0.2102	0.0043	0.0869
1	2.3411	-0.7823	1.0286	0.1036	0.1203	0.0295	0.1043	0.0819	0.1072	0.1971	-0.0054	0.0805
6	0.9500	1.4545	0.1351	-0.3431	-0.2878	-0.0885	-0.3834	-0.2380	-0.4251	-0.5922	0.0060	-0.2557
6	-0.3029	-0.7204	0.3210	-0.1076	-0.4619	-0.0040	-0.1067	-0.1071	-0.4008	-0.3390	0.1228	-0.0554
1	0.0367	2.0083	-0.0739	0.1278	0.1195	0.0257	0.1003	0.0791	0.1003	0.2187	0.0179	0.0713
1	1.1264	1.5008	1.2119	0.0950	0.1196	0.0277	0.1042	0.0802	0.1077	0.1944	-0.0095	0.0780
1	1.7754	1.9706	-0.3534	0.1085	0.1201	0.0308	0.1090	0.0829	0.0911	0.2048	-0.0036	0.0833
1	-0.2200	-0.6968	1.4077	0.1167	0.1240	0.0398	0.0962	0.0964	0.1719	0.2014	0.0373	0.0883

1	-0.3456	-1.7605	0.0048	0.1248	0.1236	0.0407	0.0936	0.0971	0.1664	0.2080	0.0393	0.0902
17	-1.8989	-0.0097	-0.0803	-0.1760	0.2572	-0.1023	-0.0981	-0.1126	-0.1528	-0.0818	-0.2992	-0.1481

Dipole mement (in D) 2.06 (DEN) 2.13 1.28 1.28 1.33 1.67 2.13 1.91 2.87 1.94

File TZVPMol448.out
Molecule PMol448 2-chlorobutane
SP Mol448 B3LYP/Def2TZVP VAC.
0 14
Dipole 0.7283 1.9814 0.3599 2.1415
Quadrupole -0.1229 -0.5594 0.6823 -1.1355 -0.3234 0.3851

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.3485	1.4316	-0.0131	-0.3088	-0.3088	-0.0867	-0.4370	-0.2355	-0.4146	-0.6056	0.0274	-0.2498
6	-0.2733	0.4432	0.3600	0.0355	-0.4824	0.0339	0.1531	-0.0332	0.1161	-0.1445	0.1364	0.0591
6	1.0565	0.7204	-0.3097	-0.1435	-0.2996	-0.0481	-0.2046	-0.1579	0.1070	-0.4057	0.0617	-0.1385
17	-0.8426	-1.2309	-0.0702	-0.1989	0.2629	-0.1065	-0.1078	-0.1151	-0.2109	-0.1080	-0.3157	-0.1563
6	2.1787	-0.2048	0.1096	-0.3349	-0.3123	-0.0877	-0.3448	-0.2390	-0.2912	-0.5917	0.0132	-0.2516
1	-1.0473	2.4364	0.2874	0.1042	0.1241	0.0356	0.1184	0.0878	0.1157	0.2074	0.0040	0.0880
1	-1.5135	1.4381	-1.0898	0.1113	0.1232	0.0346	0.1192	0.0876	0.1185	0.2094	0.0147	0.0834
1	-2.2939	1.2016	0.4719	0.1237	0.1221	0.0356	0.1192	0.0883	0.1266	0.2177	0.0190	0.0850
1	-0.1459	0.4023	1.4427	0.0986	0.1384	0.0386	0.0765	0.0981	0.0831	0.2026	0.0335	0.0857
1	0.9155	0.6895	-1.3931	0.0936	0.1377	0.0317	0.0994	0.0879	0.0215	0.1997	0.0037	0.0772
1	1.3164	1.7567	-0.0706	0.0854	0.1408	0.0334	0.1006	0.0890	0.0112	0.2022	-0.0058	0.0818
1	3.1178	0.0689	-0.3677	0.1118	0.1182	0.0315	0.1075	0.0830	0.0787	0.2064	-0.0014	0.0851
1	2.3373	-0.1731	1.1883	0.0977	0.1175	0.0283	0.1006	0.0802	0.0634	0.1958	-0.0079	0.0798
1	1.9577	-1.2369	-0.1573	0.1243	0.1184	0.0255	0.0998	0.0787	0.0750	0.2141	0.0182	0.0713

Dipole mement (in D) 2.14 (DEN) 2.22 1.44 1.24 1.28 1.63 2.23 2.02 2.95 1.96

File TZVPMol449.out
Molecule PMol449 1-chlorobutane
SP Mol449 B3LYP/Def2TZVP VAC.
0 14
Dipole -1.8003 1.3144 0.0000 2.2291
Quadrupole -0.2344 -1.5595 1.7940 2.4784 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.1775	-0.9833	0.0000	-0.0995	-0.4852	-0.0035	-0.0761	-0.1085	-0.2436	-0.3412	0.1292	-0.0516
6	0.0000	0.5141	0.0000	-0.1640	-0.3011	-0.0504	-0.2096	-0.1606	0.1517	-0.4032	0.0600	-0.1423
1	-0.7174	-1.3263	0.8806	0.1194	0.1213	0.0406	0.0917	0.0966	0.1258	0.2022	0.0385	0.0901
1	-0.7174	-1.3263	-0.8806	0.1194	0.1213	0.0406	0.0917	0.0966	0.1258	0.2022	0.0385	0.0901
6	-1.3374	1.2400	0.0000	-0.1639	-0.2905	-0.0425	-0.1137	-0.1554	0.2269	-0.3810	0.0501	-0.1352
1	0.5875	0.8104	0.8721	0.0946	0.1362	0.0313	0.0951	0.0875	-0.0096	0.1990	0.0034	0.0757
6	-1.1802	2.7482	0.0000	-0.3271	-0.3067	-0.0817	-0.3280	-0.2336	-0.2845	-0.5824	0.0161	-0.2459
1	-1.9209	0.9279	-0.8708	0.0865	0.1322	0.0279	0.0820	0.0830	-0.0497	0.1910	-0.0151	0.0766
1	-1.9209	0.9279	0.8708	0.0865	0.1322	0.0279	0.0820	0.0830	-0.0497	0.1910	-0.0151	0.0766
1	-2.1428	3.2567	0.0000	0.1140	0.1177	0.0312	0.1018	0.0826	0.0722	0.2051	-0.0014	0.0849

1	-0.6300	3.0893	0.8773	0.1056	0.1180	0.0297	0.1010	0.0815	0.0569	0.1975	-0.0048	0.0821
1	-0.6300	3.0893	-0.8773	0.1056	0.1180	0.0297	0.1010	0.0815	0.0569	0.1975	-0.0048	0.0821
1	0.5875	0.8104	-0.8721	0.0946	0.1362	0.0313	0.0951	0.0875	-0.0096	0.1990	0.0034	0.0757
17	1.3927	-1.8455	0.0000	-0.1717	0.2502	-0.1122	-0.1140	-0.1219	-0.1695	-0.0767	-0.2979	-0.1589

Dipole mement (in D) 2.23 (DEN) 2.21 1.32 1.45 1.56 1.81 2.28 1.91 3.11 2.07

File TZVPMol450.out
Molecule PMol450 2-chloro-2-methylpropane
SP Mol450 B3LYP/Def2TZVP VAC.
0 14
Dipole -2.2461 0.0000 0.0000 2.2461
Quadrupole -1.4500 0.7250 0.7250 0.0004 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.8080	1.4474	0.0000	-0.3168	-0.2844	-0.0878	-0.4717	-0.2347	-0.4694	-0.6125	0.0271	-0.2539
6	-0.3644	-0.0000	0.0000	0.1506	-0.5405	0.0695	0.3903	0.0385	0.4438	0.0444	0.1447	0.1749
1	-0.4475	1.9733	0.8817	0.1181	0.1241	0.0347	0.1259	0.0880	0.1322	0.2152	0.0158	0.0837
1	-0.4475	1.9733	-0.8817	0.1181	0.1241	0.0347	0.1259	0.0880	0.1322	0.2152	0.0158	0.0837
1	-1.8987	1.4950	0.0000	0.1017	0.1257	0.0344	0.1273	0.0872	0.1334	0.2058	0.0015	0.0855
6	-0.8080	-0.7237	-1.2535	-0.3166	-0.2844	-0.0877	-0.4716	-0.2347	-0.4584	-0.6125	0.0273	-0.2539
6	-0.8080	-0.7237	1.2535	-0.3166	-0.2844	-0.0877	-0.4716	-0.2347	-0.4584	-0.6125	0.0275	-0.2539
1	-0.4479	-1.7505	-1.2679	0.1181	0.1241	0.0347	0.1259	0.0880	0.1281	0.2152	0.0158	0.0837
1	-1.8987	-0.7472	-1.2949	0.1017	0.1257	0.0344	0.1273	0.0872	0.1320	0.2058	0.0015	0.0855
1	-0.4472	-0.2234	-2.1499	0.1181	0.1241	0.0347	0.1259	0.0880	0.1293	0.2152	0.0158	0.0837
1	-1.8987	-0.7472	1.2949	0.1017	0.1257	0.0344	0.1273	0.0872	0.1320	0.2058	0.0015	0.0855
1	-0.4472	-0.2234	2.1499	0.1181	0.1241	0.0347	0.1259	0.0880	0.1293	0.2152	0.0158	0.0837
1	-0.4479	-1.7505	1.2679	0.1181	0.1241	0.0347	0.1259	0.0880	0.1281	0.2152	0.0158	0.0837
17	1.4771	0.0001	0.0000	-0.2141	0.2721	-0.1176	-0.1126	-0.1239	-0.2342	-0.1158	-0.3260	-0.1719

Dipole mement (in D) 2.25 (DEN) 2.40 1.15 1.32 1.10 1.73 2.36 2.17 3.13 1.99

File TZVPMol451.out
Molecule PMol451 1-chloropentane
SP Mol451 B3LYP/Def2TZVP VAC.
0 17
Dipole 1.5072 -1.6623 0.0000 2.2439
Quadrupole -2.0965 -0.7257 2.8223 4.0181 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.3765	0.0000	-0.1500	-0.2988	-0.0505	-0.2129	-0.1607	0.1878	-0.4009	0.0596	-0.1422
6	0.8074	-0.9122	0.0000	-0.2012	-0.2654	-0.0445	-0.1452	-0.1557	-0.0030	-0.3759	0.0397	-0.1403
1	0.2580	0.9815	0.8723	0.0952	0.1365	0.0312	0.0931	0.0874	-0.0204	0.1994	0.0034	0.0757
1	0.2580	0.9815	-0.8723	0.0952	0.1365	0.0312	0.0931	0.0874	-0.0204	0.1994	0.0034	0.0757
6	2.3086	-0.6758	0.0000	-0.1396	-0.2913	-0.0433	-0.1204	-0.1564	0.2361	-0.3768	0.0560	-0.1352
1	0.5350	-1.5174	0.8711	0.0844	0.1340	0.0268	0.0823	0.0826	-0.0150	0.1866	-0.0177	0.0741
1	0.5350	-1.5174	-0.8711	0.0844	0.1340	0.0268	0.0823	0.0826	-0.0150	0.1866	-0.0177	0.0741
6	3.1101	-1.9626	0.0000	-0.3264	-0.3089	-0.0838	-0.3291	-0.2356	-0.2540	-0.5838	0.0140	-0.2474

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   1      2.5770   -0.0702   -0.8701    0.0860    0.1326    0.0276    0.0831    0.0828   -0.0533    0.1910   -0.0150    0.0764
   1      2.5770   -0.0702    0.8701    0.0860    0.1326    0.0276    0.0831    0.0828   -0.0533    0.1910   -0.0150    0.0764
   1      4.1826   -1.7751    0.0000    0.1136    0.1173    0.0304    0.1009    0.0817    0.0599    0.2048   -0.0027    0.0839
   1      2.8855   -2.5704    0.8773    0.1023    0.1168    0.0277    0.0974    0.0795    0.0513    0.1955   -0.0083    0.0799
   1      2.8855   -2.5704   -0.8773    0.1023    0.1168    0.0277    0.0974    0.0795    0.0513    0.1955   -0.0083    0.0799
   6     -1.4830    0.1040    0.0000   -0.0999   -0.4847   -0.0035   -0.0740   -0.1085   -0.2246   -0.3399    0.1295   -0.0516
   1     -1.7909   -0.4567   -0.8806    0.1199    0.1213    0.0405    0.0918    0.0966    0.1235    0.2024    0.0385    0.0900
   1     -1.7909   -0.4567    0.8806    0.1199    0.1213    0.0405    0.0918    0.0966    0.1235    0.2024    0.0385    0.0900
  17     -2.4453    1.6154    0.0000   -0.1722    0.2495   -0.1128   -0.1148   -0.1225   -0.1745   -0.0773   -0.2986   -0.1594

 Dipole mement (in D)   2.24 (DEN)      2.16      1.14      1.49      1.54      1.86      2.31      1.96      3.14      2.10

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File TZVPMol452.out
Molecule PMol452    chlorocyclohexane(axial)
 SP Mol452 B3LYP/Def2TZVP VAC.
    0   18
Dipole         -2.1258    0.0009    0.0000    2.1258
Quadrupole     -2.3753    1.2951    1.0802    1.9953    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -0.6086    1.0222    1.2563   -0.1854   -0.2636   -0.0512   -0.1614   -0.1610    0.0153   -0.3936    0.0392   -0.1490
   6     -1.2699    1.5725    0.0000   -0.1688   -0.2603   -0.0487   -0.1501   -0.1588   -0.0061   -0.3862    0.0395   -0.1459
   6     -0.6086    1.0222   -1.2563   -0.1854   -0.2636   -0.0512   -0.1614   -0.1610    0.0153   -0.3936    0.0400   -0.1490
   6     -0.6086   -0.4992   -1.2583   -0.1726   -0.2652   -0.0515   -0.2431   -0.1587   -0.0673   -0.4111    0.0494   -0.1479
   6      0.0088   -1.0802    0.0000    0.0444   -0.4456    0.0315    0.1288   -0.0330   -0.0948   -0.1408    0.1230    0.0503
   6     -0.6086   -0.4992    1.2583   -0.1726   -0.2652   -0.0515   -0.2431   -0.1587   -0.0673   -0.4111    0.0490   -0.1479
   1     -1.1097    1.3931   -2.1514    0.0943    0.1329    0.0296    0.0866    0.0844    0.0005    0.2045   -0.0110    0.0798
   1     -2.3313    1.2993    0.0000    0.0761    0.1325    0.0231    0.0770    0.0788    0.0099    0.1840   -0.0248    0.0699
   1     -1.2391    2.6632    0.0000    0.0941    0.1328    0.0296    0.0834    0.0844    0.0010    0.2048   -0.0103    0.0799
   1      0.4234    1.3790    1.3121    0.1010    0.1364    0.0243    0.0826    0.0813    0.0272    0.2041    0.0022    0.0668
   1     -1.1097    1.3931    2.1514    0.0943    0.1329    0.0296    0.0866    0.0844    0.0005    0.2045   -0.0110    0.0798
   1     -1.6411   -0.8649   -1.2995    0.0848    0.1425    0.0320    0.0955    0.0881    0.0545    0.2003   -0.0095    0.0791
   1     -0.1045   -0.8955   -2.1396    0.1040    0.1369    0.0323    0.0945    0.0883    0.0458    0.2160    0.0080    0.0787
   1     -0.0630   -2.1661    0.0000    0.1109    0.1376    0.0394    0.0708    0.0986    0.1179    0.2136    0.0355    0.0877
   1     -1.6411   -0.8649    1.2995    0.0848    0.1425    0.0320    0.0955    0.0881    0.0545    0.2003   -0.0095    0.0791
   1     -0.1045   -0.8955    2.1396    0.1040    0.1369    0.0323    0.0945    0.0883    0.0458    0.2160    0.0080    0.0787
   1      0.4234    1.3790   -1.3121    0.1010    0.1364    0.0243    0.0826    0.0813    0.0272    0.2041    0.0022    0.0668
  17      1.8042   -0.7676    0.0000   -0.2090    0.2631   -0.1060   -0.1190   -0.1146   -0.1799   -0.1158   -0.3206   -0.1567

 Dipole mement (in D)   2.13 (DEN)      2.18      1.43      1.23      1.35      1.63      2.17      2.03      2.95      1.96

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File TZVPMol453.out
Molecule PMol453    chlorocyclohexane(equato
 SP Mol453 B3LYP/Def2TZVP VAC.
    0   18
Dipole          0.2223   -2.4365    0.0000    2.4466
Quadrupole      1.7958   -3.7548    1.9589    1.0583    0.0000    0.0000
```

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.1646	-1.5453	1.2540	-0.1834	-0.2561	-0.0459	-0.1470	-0.1561	0.0593	-0.3857	0.0368	-0.1441
6	0.8259	-2.0985	0.0000	-0.1595	-0.2611	-0.0483	-0.1602	-0.1587	-0.0924	-0.3877	0.0407	-0.1460
6	0.1646	-1.5453	-1.2540	-0.1834	-0.2561	-0.0459	-0.1470	-0.1561	0.0593	-0.3857	0.0365	-0.1441
6	0.1646	-0.0200	-1.2557	-0.1735	-0.2670	-0.0535	-0.2515	-0.1609	-0.1285	-0.4082	0.0506	-0.1503
6	-0.5008	0.5042	0.0000	0.0240	-0.4637	0.0272	0.1278	-0.0367	-0.0726	-0.1485	0.1281	0.0488
6	0.1646	-0.0200	1.2557	-0.1735	-0.2670	-0.0535	-0.2515	-0.1609	-0.1285	-0.4082	0.0509	-0.1503
1	0.6622	-1.9151	-2.1516	0.0994	0.1348	0.0322	0.0895	0.0870	0.0034	0.2085	-0.0050	0.0826
1	1.8861	-1.8246	0.0000	0.0821	0.1354	0.0271	0.0843	0.0829	0.0421	0.1899	-0.0169	0.0744
1	0.7935	-3.1891	0.0000	0.0962	0.1331	0.0299	0.0840	0.0846	0.0171	0.2051	-0.0097	0.0801
1	-0.8672	-1.9078	1.3095	0.0857	0.1352	0.0267	0.0811	0.0825	0.0098	0.1890	-0.0178	0.0739
1	0.6622	-1.9151	2.1516	0.0994	0.1348	0.0322	0.0895	0.0870	0.0034	0.2085	-0.0050	0.0826
1	1.1923	0.3537	-1.2885	0.0901	0.1389	0.0297	0.0957	0.0867	0.0778	0.1972	0.0004	0.0730
1	-0.3381	0.3734	-2.1392	0.1051	0.1362	0.0320	0.0949	0.0879	0.0578	0.2145	0.0066	0.0779
1	-1.5597	0.2364	0.0000	0.0984	0.1399	0.0368	0.0721	0.0969	0.1421	0.2017	0.0289	0.0818
1	1.1923	0.3537	1.2885	0.0901	0.1389	0.0297	0.0957	0.0867	0.0778	0.1972	0.0004	0.0730
1	-0.3381	0.3734	2.1392	0.1051	0.1362	0.0320	0.0949	0.0879	0.0578	0.2145	0.0066	0.0779
1	-0.8672	-1.9078	-1.3095	0.0857	0.1352	0.0267	0.0811	0.0825	0.0098	0.1890	-0.0178	0.0739
17	-0.4894	2.3128	0.0000	-0.1879	0.2725	-0.1149	-0.1333	-0.1230	-0.1956	-0.0911	-0.3142	-0.1650
Dipole mement (in D)	2.45 (DEN)			2.47	1.34	1.56	1.74	1.93	2.52	2.10	3.40	2.21

File TZVPMol454.out
Molecule PMol454 chloroethene
SP Mol454 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.5419 1.2538 0.0000 1.3659
Quadrupole 0.9905 1.4725 -2.4630 -0.1554 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.7506	0.0000	-0.0333	-0.4991	-0.0087	0.0056	-0.0658	-0.0938	-0.2174	0.0566	0.0110
6	1.2892	1.0360	0.0000	-0.2637	-0.2370	-0.0832	-0.3290	-0.1847	-0.3609	-0.4049	-0.0177	-0.1865
1	1.6051	2.0696	0.0000	0.1240	0.1291	0.0482	0.1332	0.1014	0.1685	0.2086	0.0523	0.0976
1	-0.7806	1.4981	0.0000	0.1379	0.1245	0.0541	0.1081	0.1106	0.1704	0.2075	0.0808	0.0994
17	-0.6243	-0.8564	0.0000	-0.0955	0.3585	-0.0580	-0.0519	-0.0628	-0.0753	-0.0001	-0.2321	-0.1130
1	2.0534	0.2724	0.0000	0.1306	0.1240	0.0476	0.1340	0.1014	0.1911	0.2062	0.0601	0.0915
Dipole mement (in D)	1.37 (DEN)			1.41	2.25	0.78	0.88	1.12	1.43	1.10	2.59	1.46

File TZVPMol455.out
Molecule PMol455 1,1-dichloroethene
SP Mol455 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 1.2295 1.2295
Quadrupole -2.1882 0.0597 2.1284 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.4191	0.1035	-0.8275	0.0427	0.2117	0.0342	0.0400	-0.1191	0.1664	0.1871

6	0.0000	0.0000	1.7428	-0.2695	-0.2409	-0.0900	-0.4355	-0.1883	-0.3125	-0.4149	0.0278	-0.1972
1	0.0000	0.9304	2.2887	0.1405	0.1307	0.0524	0.1534	0.1068	0.1673	0.2200	0.0731	0.0966
17	0.0000	1.4442	-0.5161	-0.0575	0.4035	-0.0288	-0.0416	-0.0298	-0.0311	0.0470	-0.1702	-0.0916
17	0.0000	-1.4442	-0.5161	-0.0575	0.4035	-0.0288	-0.0416	-0.0298	-0.0311	0.0470	-0.1702	-0.0916
1	0.0000	-0.9304	2.2887	0.1405	0.1307	0.0524	0.1534	0.1068	0.1673	0.2200	0.0731	0.0966

Dipole mement (in D)	1.23	(DEN)	1.33	2.81	0.63	0.36	0.99	1.30	0.89	3.02	1.30	

File TZVPMol456.out
Molecule PMol456 Z-1,2-dichloroethene
SP Mol456 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.0000 0.0000 1.7779 1.7779
Quadrupole -2.2541 -1.1899 3.4440 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6632	0.9524	-0.0822	-0.5282	-0.0235	-0.1165	-0.0767	-0.1367	-0.2577	0.1048	-0.0062
6	0.0000	-0.6632	0.9524	-0.0822	-0.5282	-0.0235	-0.1165	-0.0767	-0.1367	-0.2577	0.1043	-0.0062
1	0.0000	-1.2086	1.8845	0.1463	0.1323	0.0590	0.1257	0.1158	0.1672	0.2223	0.0922	0.1040
1	0.0000	1.2086	1.8845	0.1463	0.1323	0.0590	0.1257	0.1158	0.1672	0.2223	0.0922	0.1040
17	0.0000	1.6398	-0.4470	-0.0641	0.3958	-0.0355	-0.0092	-0.0392	-0.0305	0.0355	-0.1967	-0.0978
17	0.0000	-1.6398	-0.4470	-0.0641	0.3958	-0.0355	-0.0092	-0.0392	-0.0305	0.0355	-0.1967	-0.0978

Dipole mement (in D)	1.78	(DEN)	2.17	4.14	1.01	1.25	1.56	1.91	1.51	3.47	2.25	

File TZVPMol457.out
Molecule PMol457 1-chloropropene(cis)
SP Mol457 B3LYP/Def2TZVP VAC.
0 9
Dipole -1.5516 0.3806 0.0000 1.5976
Quadrupole 0.4138 1.6769 -2.0908 0.0889 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2327	0.4256	0.0000	-0.1385	-0.2361	-0.0358	-0.0486	-0.0986	0.0209	-0.1933	0.0070	-0.0667
6	0.0000	0.9129	0.0000	-0.0665	-0.4762	-0.0255	-0.0912	-0.0808	-0.3036	-0.2282	0.0423	-0.0138
17	1.4291	-0.0613	0.0000	-0.1097	0.3497	-0.0605	-0.0398	-0.0659	-0.0548	-0.0172	-0.2483	-0.1132
6	-1.6372	-0.9995	0.0000	-0.2948	-0.2926	-0.0822	-0.3755	-0.2288	-0.0370	-0.6378	0.0212	-0.2456
1	-2.0227	1.1699	0.0000	0.1146	0.1478	0.0437	0.1007	0.0998	0.0687	0.2073	0.0353	0.0895
1	0.2197	1.9697	0.0000	0.1360	0.1252	0.0494	0.1050	0.1061	0.1959	0.2107	0.0757	0.0941
1	-0.7764	-1.6636	0.0000	0.1235	0.1233	0.0314	0.1090	0.0856	0.0457	0.2223	0.0318	0.0751
1	-2.2480	-1.2340	0.8729	0.1176	0.1294	0.0397	0.1203	0.0913	0.0321	0.2181	0.0174	0.0904
1	-2.2480	-1.2340	-0.8729	0.1176	0.1294	0.0397	0.1203	0.0913	0.0321	0.2181	0.0174	0.0904

Dipole mement (in D)	1.60	(DEN)	1.64	2.35	0.93	1.07	1.27	1.58	1.37	2.74	1.63	

File TZVPMol458.out
Molecule PMol458 1-chloropropene(trans)

```
 SP Mol458 B3LYP/Def2TZVP VAC.
    0    9
Dipole          1.8838    0.0097    0.0000    1.8838
Quadrupole      0.2214    1.5492   -1.7706   -0.0607    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.9154   -0.5123    0.0000   -0.1093   -0.2283   -0.0353   -0.0547   -0.0981    0.0627   -0.1944    0.0127   -0.0672
   6      0.0000    0.4451    0.0000   -0.0578   -0.4788   -0.0245   -0.0803   -0.0793   -0.3008   -0.2253    0.0451   -0.0122
   1      0.2403    1.4999    0.0000    0.1264    0.1238    0.0482    0.1074    0.1051    0.2181    0.2027    0.0703    0.0919
   6      2.3769   -0.2438    0.0000   -0.3117   -0.2860   -0.0771   -0.3568   -0.2241   -0.2414   -0.6173    0.0264   -0.2406
   1      0.5913   -1.5474    0.0000    0.1152    0.1402    0.0434    0.1017    0.1001    0.0955    0.2016    0.0443    0.0835
  17     -1.7000    0.1446    0.0000   -0.1103    0.3502   -0.0705   -0.0642   -0.0752   -0.0793   -0.0051   -0.2436   -0.1245
   1      2.5942    0.8228    0.0000    0.1083    0.1247    0.0379    0.1142    0.0904    0.0797    0.2080    0.0109    0.0891
   1      2.8602   -0.6840    0.8736    0.1196    0.1271    0.0390    0.1164    0.0905    0.0827    0.2149    0.0167    0.0900
   1      2.8602   -0.6840   -0.8736    0.1196    0.1271    0.0390    0.1164    0.0905    0.0827    0.2149    0.0167    0.0900

 Dipole mement (in D)   1.88 (DEN)      1.97      1.59      1.26      1.24      1.64      1.96      1.45      3.15      1.91

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File TZVPMol459.out
Molecule PMol459    2-chloropropene
 SP Mol459 B3LYP/Def2TZVP VAC.
    0    9
Dipole          0.6797    1.4419    0.0000    1.5941
Quadrupole      1.4815    0.4546   -1.9360    0.0733    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.4584    0.0000    0.1276   -0.5045    0.0350    0.2620    0.0160    0.2259   -0.0105    0.0542    0.1297
   6     -1.0164    1.3075    0.0000   -0.3015   -0.2199   -0.0976   -0.4067   -0.1970   -0.5088   -0.4119   -0.0223   -0.2067
   1     -0.8216    2.3712    0.0000    0.1175    0.1281    0.0423    0.1376    0.0961    0.1989    0.2031    0.0415    0.0906
   6      1.4422    0.8051    0.0000   -0.3099   -0.2870   -0.0821   -0.4595   -0.2267   -0.2830   -0.6364    0.0420   -0.2455
  17     -0.3031   -1.2615    0.0000   -0.1263    0.3682   -0.0672   -0.0679   -0.0703   -0.1335   -0.0188   -0.2541   -0.1259
   1     -2.0448    0.9808    0.0000    0.1304    0.1243    0.0431    0.1361    0.0973    0.1934    0.2114    0.0567    0.0865
   1      1.5763    1.8847    0.0000    0.1109    0.1300    0.0429    0.1361    0.0957    0.1076    0.2170    0.0203    0.0944
   1      1.9438    0.3915    0.8748    0.1256    0.1304    0.0418    0.1311    0.0944    0.0997    0.2230    0.0306    0.0885
   1      1.9438    0.3915   -0.8748    0.1256    0.1304    0.0418    0.1311    0.0944    0.0997    0.2230    0.0306    0.0885

 Dipole mement (in D)   1.59 (DEN)      1.68      2.13      0.94      0.77      1.29      1.70      1.28      2.83      1.57

-----------------------------------------
File TZVPMol460.out
Molecule PMol460    3-chloropropene
 SP Mol460 B3LYP/Def2TZVP VAC.
    0    9
Dipole          1.3675    1.2403    0.0000    1.8462
Quadrupole     -0.7696    2.6590   -1.8894    0.2488    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      1.3432    0.3293    0.0000   -0.1431   -0.2412   -0.0386   -0.0549   -0.1018    0.0543   -0.2091   -0.0377   -0.0681
   6      1.6193   -0.9641    0.0000   -0.2425   -0.2093   -0.0853   -0.2844   -0.1875   -0.4659   -0.3756   -0.0528   -0.1908
   1      0.8346   -1.7092    0.0000    0.1256    0.1197    0.0312    0.1061    0.0863    0.2042    0.2037    0.0564    0.0713
```

6	0.0000	0.9630	0.0000	-0.0730	-0.4763	-0.0030	-0.1203	-0.1030	-0.1857	-0.3938	0.1325	-0.0498
1	2.1530	1.0548	0.0000	0.1114	0.1449	0.0431	0.0994	0.0988	0.0849	0.2025	0.0301	0.0888
1	2.6404	-1.3179	0.0000	0.1166	0.1226	0.0402	0.1167	0.0932	0.1735	0.1987	0.0361	0.0894
17	-1.3614	-0.1879	0.0000	-0.1565	0.2780	-0.0842	-0.0714	-0.0939	-0.1424	-0.0634	-0.2770	-0.1329
1	-0.1301	1.5989	0.8756	0.1307	0.1309	0.0484	0.1044	0.1040	0.1386	0.2185	0.0561	0.0961
1	-0.1301	1.5989	-0.8756	0.1307	0.1309	0.0484	0.1044	0.1040	0.1386	0.2185	0.0561	0.0961

Dipole mement (in D)	1.85	(DEN)	1.91	1.85	1.07	1.42	1.45	1.89	1.70	2.49	1.85	

File TZVPMol461.out
Molecule PMol461 chlorobenzene
SP Mol461 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -1.6672 1.6672
Quadrupole -4.4758 3.9777 0.4982 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	0.5068	0.1683	-0.4263	0.0242	0.1621	0.0166	0.0037	-0.0434	0.0704	0.1033
6	0.0000	1.2090	-0.1740	-0.1630	-0.1427	-0.0432	-0.1891	-0.0960	-0.0201	-0.2249	0.0051	-0.0900
6	0.0000	-1.2090	-0.1740	-0.1630	-0.1427	-0.0432	-0.1891	-0.0960	-0.0201	-0.2249	0.0051	-0.0900
6	0.0000	1.2005	-1.5615	-0.1007	-0.1327	-0.0326	-0.0637	-0.0884	-0.1822	-0.1914	-0.0185	-0.0772
6	0.0000	-1.2005	-1.5615	-0.1007	-0.1327	-0.0326	-0.0637	-0.0884	-0.1822	-0.1914	-0.0185	-0.0772
6	0.0000	0.0000	-2.2583	-0.1094	-0.1407	-0.0397	-0.1046	-0.0958	-0.0687	-0.2137	-0.0217	-0.0848
1	0.0000	2.1377	0.3793	0.1204	0.1465	0.0460	0.1122	0.1034	0.0980	0.2226	0.0541	0.0844
1	0.0000	-2.1377	0.3793	0.1204	0.1465	0.0460	0.1122	0.1034	0.0980	0.2226	0.0541	0.0844
1	0.0000	2.1409	-2.0974	0.1151	0.1452	0.0453	0.1005	0.1015	0.1339	0.2123	0.0375	0.0899
1	0.0000	-2.1409	-2.0974	0.1151	0.1452	0.0453	0.1005	0.1015	0.1339	0.2123	0.0375	0.0899
1	0.0000	0.0000	-3.3402	0.1144	0.1437	0.0433	0.0979	0.0995	0.1121	0.2117	0.0350	0.0878
17	0.0000	0.0000	2.2418	-0.1170	0.3908	-0.0589	-0.0753	-0.0611	-0.1063	0.0082	-0.2401	-0.1204

Dipole mement (in D)	1.67	(DEN)	1.60	2.23	1.02	1.20	1.36	1.76	1.31	3.03	1.73	

File TZVPMol462.out
Molecule PMol462 1,2-dichlorobenzene
SP Mol462 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 2.3630 2.3630
Quadrupole -4.3989 1.6045 2.7944 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6974	-0.0298	0.1053	-0.4437	0.0171	0.0829	0.0128	0.0452	-0.0741	0.1057	0.0943
6	0.0000	-0.6974	-0.0298	0.1053	-0.4437	0.0171	0.0829	0.0128	0.0452	-0.0741	0.1057	0.0943
6	0.0000	1.3868	1.1769	-0.1591	-0.1381	-0.0388	-0.1676	-0.0914	-0.0539	-0.2073	0.0117	-0.0857
6	0.0000	-1.3868	1.1769	-0.1591	-0.1381	-0.0388	-0.1676	-0.0914	-0.0539	-0.2073	0.0115	-0.0857
6	0.0000	0.6940	2.3761	-0.1045	-0.1346	-0.0341	-0.0820	-0.0900	-0.1501	-0.2001	-0.0133	-0.0794
6	0.0000	-0.6940	2.3761	-0.1045	-0.1346	-0.0341	-0.0820	-0.0900	-0.1501	-0.2001	-0.0134	-0.0794
17	0.0000	-1.5854	-1.5062	-0.0833	0.4208	-0.0404	-0.0529	-0.0414	-0.0780	0.0401	-0.2060	-0.1088
1	0.0000	2.4676	1.1580	0.1235	0.1490	0.0486	0.1140	0.1062	0.1008	0.2257	0.0596	0.0871

1	0.0000	-2.4676	1.1580	0.1235	0.1490	0.0486	0.1140	0.1062	0.1008	0.2257	0.0596	0.0871
1	0.0000	1.2421	3.3087	0.1181	0.1466	0.0476	0.1055	0.1038	0.1361	0.2157	0.0424	0.0924
1	0.0000	-1.2421	3.3087	0.1181	0.1466	0.0476	0.1055	0.1038	0.1361	0.2157	0.0424	0.0924
17	0.0000	1.5854	-1.5062	-0.0833	0.4208	-0.0404	-0.0529	-0.0414	-0.0780	0.0401	-0.2060	-0.1088

Dipole mement (in D) 2.36 (DEN) 2.12 4.28 1.42 1.60 1.99 2.53 1.90 4.79 2.67

File TZVPMol463.out
Molecule PMol463 1,3-dichlorobenzene
SP Mol463 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 1.5628 1.5628
Quadrupole -2.9086 -2.5037 5.4123 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	1.1911	-0.0049	0.1690	-0.4250	0.0289	0.1858	0.0214	-0.0313	-0.0313	0.0812	0.1081
6	0.0000	0.0000	-0.7161	-0.2160	-0.1453	-0.0482	-0.2970	-0.0976	0.0497	-0.2445	0.0371	-0.0974
6	0.0000	1.2074	1.3824	-0.1625	-0.1428	-0.0439	-0.2013	-0.0968	-0.0378	-0.2317	0.0100	-0.0916
6	0.0000	-1.1911	-0.0049	0.1690	-0.4250	0.0289	0.1858	0.0214	-0.0313	-0.0313	0.0809	0.1081
6	0.0000	0.0000	2.0648	-0.0934	-0.1252	-0.0261	-0.0343	-0.0817	-0.1962	-0.1764	-0.0099	-0.0712
6	0.0000	-1.2074	1.3824	-0.1625	-0.1428	-0.0439	-0.2013	-0.0968	-0.0378	-0.2317	0.0100	-0.0916
1	0.0000	0.0000	-1.7958	0.1323	0.1509	0.0506	0.1324	0.1092	0.0846	0.2343	0.0775	0.0835
1	0.0000	2.1498	1.9109	0.1248	0.1481	0.0485	0.1170	0.1059	0.1117	0.2264	0.0595	0.0873
17	0.0000	-2.6873	-0.8763	-0.1032	0.4052	-0.0467	-0.0561	-0.0488	-0.0855	0.0214	-0.2260	-0.1088
1	0.0000	0.0000	3.1468	0.1208	0.1486	0.0501	0.1082	0.1064	0.1476	0.2174	0.0462	0.0951
1	0.0000	-2.1498	1.9109	0.1248	0.1481	0.0485	0.1170	0.1059	0.1117	0.2264	0.0595	0.0873
17	0.0000	2.6873	-0.8763	-0.1032	0.4052	-0.0467	-0.0561	-0.0488	-0.0855	0.0214	-0.2260	-0.1088

Dipole mement (in D) 1.56 (DEN) 1.50 2.36 0.93 1.11 1.26 1.65 1.26 2.93 1.64

File TZVPMol464.out
Molecule PMol464 ortho-chlorotoluene
SP Mol464 B3LYP/Def2TZVP VAC.
0 15
Dipole -1.2654 0.6325 0.0000 1.4147
Quadrupole 0.5814 3.6440 -4.2254 1.4102 0.0002 0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.0867	0.9374	-0.0000	0.0897	-0.1742	0.0034	0.1039	-0.0112	0.3965	-0.0399	0.0214	0.0343
6	0.3577	-0.3865	0.0000	0.0986	-0.3921	0.0202	0.1065	0.0146	-0.0846	-0.0377	0.0602	0.0929
6	-1.4662	1.1371	-0.0001	-0.1588	-0.1120	-0.0396	-0.1291	-0.0934	-0.3185	-0.1905	-0.0244	-0.0901
6	-0.5185	-1.4611	-0.0000	-0.1659	-0.1445	-0.0451	-0.1827	-0.0978	-0.0355	-0.2164	0.0050	-0.0914
6	-2.3601	0.0769	-0.0001	-0.1061	-0.1406	-0.0416	-0.0985	-0.0975	-0.0590	-0.2060	-0.0230	-0.0861
6	-1.8848	-1.2259	-0.0001	-0.1084	-0.1397	-0.0393	-0.0821	-0.0951	-0.2063	-0.2028	-0.0199	-0.0837
17	2.0668	-0.7071	0.0001	-0.1162	0.3993	-0.0499	-0.0501	-0.0527	-0.1027	-0.0002	-0.2475	-0.1097
6	0.8659	2.0847	0.0000	-0.3407	-0.2609	-0.0861	-0.4326	-0.2305	-0.5181	-0.6134	0.0216	-0.2534
1	-1.8374	2.1553	-0.0001	0.1057	0.1460	0.0402	0.1008	0.0972	0.1471	0.2067	0.0281	0.0836
1	-0.1255	-2.4683	-0.0000	0.1170	0.1463	0.0446	0.1096	0.1021	0.1071	0.2218	0.0521	0.0827

1	-3.4250	0.2691	-0.0001	0.1104	0.1435	0.0424	0.0982	0.0985	0.1174	0.2107	0.0330	0.0866
1	-2.5714	-2.0623	-0.0001	0.1118	0.1441	0.0437	0.1003	0.0998	0.1379	0.2119	0.0354	0.0880
1	1.5210	2.0589	0.8716	0.1267	0.1299	0.0354	0.1182	0.0884	0.1393	0.2228	0.0255	0.0794
1	0.3367	3.0346	-0.0000	0.1096	0.1251	0.0362	0.1192	0.0891	0.1402	0.2101	0.0074	0.0878
1	1.5211	2.0589	-0.8714	0.1267	0.1299	0.0354	0.1182	0.0884	0.1393	0.2228	0.0255	0.0794

Dipole mement (in D) 1.41 (DEN) 1.30 2.87 0.73 0.83 1.04 1.50 1.11 2.72 1.46

File TZVPMol465.out
Molecule PMol465 para-chlorotoluene
SP Mol465 B3LYP/Def2TZVP VAC.
0 15
Dipole 2.1344 0.0000 0.0277 2.1346
Quadrupole -0.0652 3.9020 -3.8368 -0.0001 0.0846 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.7973	0.0000	-0.0104	0.1601	-0.1690	0.0070	0.1538	-0.0107	0.3798	-0.0268	0.0000	0.0386
6	1.0780	1.1936	-0.0100	-0.1681	-0.1095	-0.0385	-0.1217	-0.0921	-0.3321	-0.1908	-0.0254	-0.0890
6	1.0780	-1.1936	-0.0100	-0.1681	-0.1095	-0.0385	-0.1217	-0.0921	-0.3321	-0.1908	-0.0253	-0.0890
6	-0.3084	1.2049	-0.0033	-0.1553	-0.1421	-0.0444	-0.1783	-0.0971	-0.0045	-0.2164	0.0045	-0.0909
6	-0.3084	-1.2049	-0.0033	-0.1553	-0.1421	-0.0444	-0.1783	-0.0971	-0.0045	-0.2164	0.0045	-0.0909
6	-0.9946	0.0000	0.0013	0.1626	-0.4312	0.0189	0.1503	0.0113	-0.0223	-0.0528	0.0696	0.0978
1	1.6118	2.1370	-0.0176	0.1068	0.1466	0.0414	0.1039	0.0983	0.1567	0.2072	0.0291	0.0849
1	1.6118	-2.1370	-0.0176	0.1068	0.1466	0.0414	0.1039	0.0983	0.1567	0.2072	0.0291	0.0849
1	-0.8562	2.1370	-0.0055	0.1167	0.1464	0.0452	0.1115	0.1026	0.1041	0.2217	0.0522	0.0834
1	-0.8562	-2.1370	-0.0055	0.1167	0.1464	0.0452	0.1115	0.1026	0.1041	0.2217	0.0522	0.0834
17	-2.7297	-0.0000	0.0060	-0.1227	0.3867	-0.0633	-0.0795	-0.0654	-0.1123	0.0052	-0.2442	-0.1246
6	3.2930	-0.0000	0.0128	-0.3607	-0.2521	-0.0807	-0.4054	-0.2259	-0.4656	-0.6097	0.0174	-0.2492
1	3.6732	-0.0002	1.0363	0.1247	0.1297	0.0374	0.1181	0.0893	0.1278	0.2162	0.0156	0.0857
1	3.7047	-0.8806	-0.4773	0.1179	0.1265	0.0366	0.1159	0.0891	0.1222	0.2121	0.0102	0.0874
1	3.7047	0.8807	-0.4771	0.1179	0.1265	0.0366	0.1159	0.0891	0.1222	0.2121	0.0102	0.0874

Dipole mement (in D) 2.13 (DEN) 2.32 1.31 1.49 1.41 1.90 2.24 1.72 3.53 2.16

File TZVPMol466.out
Molecule PMol466 chloroacetylene
SP Mol466 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 -0.2656 0.2656
Quadrupole -2.2692 -2.2692 4.5385 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.8642	0.1913	0.1261	0.0912	0.2147	0.1452	0.2806	0.2374	0.1752	0.1380
6	0.0000	0.0000	-1.8033	-0.1422	-0.1362	-0.1056	-0.3141	-0.1569	-0.3552	-0.2424	-0.0268	-0.1615
6	0.0000	0.0000	-0.6030	-0.0692	-0.5247	-0.0465	0.0118	-0.0494	-0.0105	-0.1470	-0.0802	0.0264
17	0.0000	0.0000	1.0178	0.0201	0.5348	0.0608	0.0876	0.0610	0.0851	0.1520	-0.0681	-0.0029

Dipole mement (in D) 0.27 (DEN) 1.10 3.58 0.09 0.16 0.20 0.34 0.00 2.28 0.59

File TZVPMol467.out
Molecule PMol467 3-chloropropyne
 SP Mol467 B3LYP/Def2TZVP VAC.
  0 7
Dipole 1.2391 1.1527 0.0000 1.6924
Quadrupole 0.8693 0.8368 -1.7061 -2.4356 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.2904	-0.4806	0.0000	-0.0686	-0.0756	-0.0920	-0.2869	-0.1437	-0.5199	-0.1924	-0.1240	-0.1497
6	1.2440	0.1058	0.0000	-0.1076	-0.1509	-0.0473	0.0381	-0.0579	0.2340	-0.0389	-0.1679	-0.0283
1	3.2158	-1.0012	0.0000	0.1941	0.1280	0.0911	0.2092	0.1450	0.3284	0.2339	0.1702	0.1383
6	0.0000	0.8247	0.0000	-0.1865	-0.4604	0.0137	-0.1299	-0.0826	-0.3204	-0.4330	0.2033	-0.0319
17	-1.4255	-0.2712	0.0000	-0.1340	0.2740	-0.0873	-0.0807	-0.0949	-0.1032	-0.0431	-0.2476	-0.1423
1	-0.0940	1.4558	0.8812	0.1513	0.1425	0.0609	0.1251	0.1170	0.1906	0.2367	0.0830	0.1069
1	-0.0940	1.4558	-0.8812	0.1513	0.1425	0.0609	0.1251	0.1170	0.1906	0.2367	0.0830	0.1069

Dipole mement (in D)	1.69 (DEN)	2.49	1.90	1.01	1.26	1.35	1.81	1.65	2.52	1.71

File TZVPMol468.out
Molecule PMol468 chlorofluoromethane
 SP Mol468 B3LYP/Def2TZVP VAC.
  0 5
Dipole 0.3676 1.7525 0.0000 1.7906
Quadrupole -1.7285 1.0192 0.7093 1.9398 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.5638	0.5677	0.0000	0.0828	-0.6045	0.0951	0.1671	0.0170	-0.0040	0.0407	0.7262	0.1091
1	0.6740	1.1680	-0.9007	0.1222	0.1029	0.0534	0.0727	0.1101	0.1332	0.1703	0.0786	0.1011
1	0.6739	1.1680	0.9008	0.1222	0.1029	0.0534	0.0727	0.1101	0.1332	0.1703	0.0786	0.1011
17	-1.0687	-0.1166	-0.0000	-0.1230	0.2839	-0.0809	-0.1218	-0.0870	-0.1182	-0.0587	-0.2376	-0.1351
9	1.4930	-0.4178	0.0000	-0.2041	0.1148	-0.1210	-0.1906	-0.1502	-0.1442	-0.3226	-0.6460	-0.1762

Dipole mement (in D)	1.79 (DEN)	2.08	1.83	1.16	1.73	1.64	1.89	2.82	4.39	1.90

File TZVPMol469.out
Molecule PMol469 chlorodifluoromethane
 SP Mol469 B3LYP/Def2TZVP VAC.
  0 5
Dipole -1.0779 0.9253 0.0000 1.4206
Quadrupole 2.2368 -0.6399 -1.5968 -0.9595 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.5646	-0.0916	0.0000	0.3230	-0.7811	0.2056	0.5847	0.1957	0.0980	0.5179	1.3663	0.3610
1	-1.4481	0.5479	0.0000	0.1004	0.1066	0.0608	0.0300	0.1219	0.1702	0.1452	0.1119	0.1008
17	0.8823	0.9268	0.0000	-0.0898	0.3296	-0.0629	-0.1535	-0.0630	-0.0687	-0.0501	-0.1941	-0.1281
9	-0.5646	-0.8752	1.0808	-0.1668	0.1725	-0.1018	-0.2306	-0.1273	-0.0998	-0.3065	-0.6419	-0.1668
9	-0.5646	-0.8752	-1.0808	-0.1668	0.1725	-0.1018	-0.2306	-0.1273	-0.0998	-0.3065	-0.6419	-0.1668

Dipole mement (in D) 1.42 (DEN) 1.54 1.95 0.95 1.61 1.40 1.52 2.69 4.60 1.62

File TZVPMol470.out
Molecule PMol470 fluorotrichloromethane
SP Mol470 B3LYP/Def2TZVP VAC.
0 5
Dipole -0.0011 0.0000 -0.3672 0.3672
Quadrupole 0.6849 0.6831 -1.3681 0.0007 -0.0003 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0001	-0.0001	0.2509	0.2366	-1.2769	0.1876	0.5663	0.2062	-0.3324	0.1956	1.0030	0.4582
17	1.5303	-0.6839	-0.3092	-0.0376	0.3618	-0.0347	-0.1181	-0.0326	0.0888	0.0326	-0.1253	-0.1026
17	-1.3579	-0.9832	-0.3082	-0.0375	0.3617	-0.0346	-0.1181	-0.0325	0.0895	0.0327	-0.1253	-0.1025
17	-0.1731	1.6670	-0.3087	-0.0375	0.3619	-0.0346	-0.1181	-0.0325	0.0889	0.0327	-0.1253	-0.1025
9	0.0014	0.0001	1.5820	-0.1240	0.1915	-0.0838	-0.2120	-0.1085	0.0652	-0.2937	-0.6264	-0.1507

Dipole mement (in D) 0.37 (DEN) 0.49 1.69 0.26 0.40 0.43 0.30 2.14 2.99 0.14

File TZVPMol471.out
Molecule PMol471 chloropentaflouroethane
SP Mol471 B3LYP/Def2TZVP VAC.
0 8
Dipole -0.4087 -0.2842 0.0000 0.4978
Quadrupole 0.8689 -0.1118 -0.7571 0.8386 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.4497	0.4641	0.0000	0.3421	-0.8231	0.2053	0.4907	0.2479	-0.0054	0.5509	1.4010	0.4349
6	0.9386	-0.2272	0.0000	0.4594	-0.7338	0.2627	0.7894	0.3240	0.4612	0.8921	1.9042	0.5110
17	-1.7432	-0.7281	0.0000	-0.0545	0.4171	-0.0274	-0.1029	-0.0225	0.0252	0.0057	-0.1399	-0.1117
9	1.8855	0.7051	-0.0001	-0.1527	0.2306	-0.0899	-0.2509	-0.1108	-0.1133	-0.2923	-0.6307	-0.1704
9	-0.5375	1.2373	-1.0808	-0.1445	0.2219	-0.0860	-0.2074	-0.1085	-0.0443	-0.2866	-0.6287	-0.1631
9	-0.5375	1.2373	1.0808	-0.1445	0.2219	-0.0860	-0.2074	-0.1085	-0.0443	-0.2866	-0.6287	-0.1631
9	1.0782	-0.9812	-1.0811	-0.1527	0.2326	-0.0894	-0.2557	-0.1108	-0.1396	-0.2916	-0.6381	-0.1687
9	1.0783	-0.9810	1.0813	-0.1526	0.2327	-0.0894	-0.2557	-0.1108	-0.1396	-0.2916	-0.6381	-0.1687

Dipole mement (in D) 0.50 (DEN) 0.55 2.10 0.39 0.58 0.59 0.41 1.99 3.12 0.19

File TZVPMol472.out
Molecule PMol472 1-chloro-1-fluoroethane
SP Mol472 B3LYP/Def2TZVP VAC.
0 8
Dipole -1.3755 -1.4498 0.9174 2.1990
Quadrupole -0.0690 -1.1638 1.2328 1.6884 -0.6797 0.5627

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.2492	-1.0325	-0.1099	-0.2977	-0.3096	-0.0883	-0.5247	-0.2343	-0.3049	-0.6423	0.0338	-0.2533
1	-0.9222	-1.9691	0.3328	0.1185	0.1297	0.0453	0.1408	0.0982	0.0961	0.2233	0.0327	0.0955

1	-2.2888	-0.8592	0.1627	0.1179	0.1290	0.0450	0.1406	0.0978	0.1207	0.2197	0.0276	0.0946
1	-1.1785	-1.1140	-1.1916	0.1233	0.1285	0.0446	0.1430	0.0983	0.1285	0.2239	0.0398	0.0897
6	-0.4095	0.1030	0.3840	0.1838	-0.6204	0.1218	0.3860	0.0806	0.1923	0.2102	0.7022	0.2137
1	-0.4220	0.2177	1.4682	0.1019	0.1215	0.0482	0.0527	0.1081	0.1096	0.1730	0.0712	0.0924
9	-0.8384	1.2759	-0.1646	-0.2059	0.1287	-0.1243	-0.2060	-0.1523	-0.1896	-0.3330	-0.6486	-0.1830
17	1.3123	-0.1283	-0.0550	-0.1418	0.2926	-0.0922	-0.1324	-0.0965	-0.1528	-0.0749	-0.2583	-0.1494

Dipole mement (in D) 2.20 (DEN) 2.44 1.68 1.43 1.63 1.95 2.27 3.19 4.95 2.14

File TZVPMol473.out
Molecule PMol473 1,1-dichloro-2-fluoropro
SP Mol473 B3LYP/Def2TZVP VAC.
0 9
Dipole 1.5058 1.2144 0.0000 1.9345
Quadrupole 2.2603 -1.5798 -0.6805 2.6858 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.2465	0.0411	0.0000	0.0093	-0.8063	0.0032	-0.0756	0.0032	-0.2595	-0.2069	0.2146	0.1349
6	1.0613	-0.2319	0.0000	0.2270	-0.3768	0.0862	0.3377	0.0937	0.4925	0.3631	0.5928	0.1879
6	2.1999	0.7026	0.0000	-0.3215	-0.2623	-0.0823	-0.5110	-0.2247	-0.4491	-0.6599	0.0385	-0.2509
1	2.8255	0.5351	0.8774	0.1307	0.1374	0.0493	0.1467	0.1021	0.1458	0.2288	0.0398	0.0962
1	2.8255	0.5351	-0.8773	0.1307	0.1374	0.0493	0.1467	0.1021	0.1458	0.2288	0.0398	0.0962
1	1.8676	1.7346	-0.0000	0.1307	0.1322	0.0415	0.1337	0.0964	0.1274	0.2366	0.0503	0.0867
9	1.4304	-1.5196	0.0000	-0.1925	0.2013	-0.0967	-0.1644	-0.1218	-0.2196	-0.3034	-0.6530	-0.1642
17	-0.8345	1.6533	-0.0000	-0.0644	0.4131	-0.0224	0.0010	-0.0239	0.0015	0.0483	-0.1723	-0.0848
17	-1.4291	-1.1944	0.0000	-0.0499	0.4240	-0.0282	-0.0149	-0.0273	0.0153	0.0647	-0.1507	-0.1019

Dipole mement (in D) 1.93 (DEN) 2.37 2.08 1.28 1.19 1.77 1.98 2.80 4.81 1.94

File TZVPMol474.out
Molecule PMol474 chlorotrifluoromethane
SP Mol474 B3LYP/Def2TZVP VAC.
0 5
Dipole 0.3952 -0.0002 0.0000 0.3952
Quadrupole 1.1042 -0.5520 -0.5521 -0.0001 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.3508	0.0001	0.0000	0.4813	-1.0297	0.3034	1.0364	0.3620	0.2050	0.9057	2.0304	0.6036
9	-0.8093	1.2407	0.0000	-0.1420	0.2160	-0.0887	-0.2852	-0.1101	-0.0659	-0.2934	-0.6319	-0.1632
9	-0.8093	-0.6201	1.0744	-0.1420	0.2160	-0.0887	-0.2852	-0.1101	-0.0640	-0.2934	-0.6319	-0.1632
9	-0.8093	-0.6201	-1.0744	-0.1420	0.2160	-0.0887	-0.2852	-0.1101	-0.0640	-0.2934	-0.6319	-0.1632
17	1.4091	-0.0003	0.0000	-0.0553	0.3818	-0.0372	-0.1809	-0.0316	-0.0111	-0.0255	-0.1337	-0.1141

Dipole mement (in D) 0.40 (DEN) 0.47 1.80 0.27 0.36 0.46 0.33 1.72 3.04 0.11

File TZVPMol475.out
Molecule PMol475 dichlorofluoromethane

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 SP Mol475 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -1.1336    0.5407    0.0000    1.2559
Quadrupole     -0.0380    0.2887   -0.2507   -1.9106    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6     -0.1763    0.5190    0.0000    0.1748   -0.9296    0.1439    0.3629    0.1141   -0.1643    0.1320    0.8727    0.2857
   1     -1.0787    1.1242    0.0000    0.1299    0.1072    0.0603    0.0602    0.1212    0.2357    0.1872    0.1215    0.1032
  17     -0.1763   -0.4718    1.4617   -0.0729    0.3309   -0.0530   -0.1141   -0.0549   -0.0155   -0.0086   -0.1786   -0.1144
   9      0.9035    1.3115    0.0000   -0.1588    0.1608   -0.0984   -0.1950   -0.1256   -0.0404   -0.3021   -0.6365   -0.1601
  17     -0.1763   -0.4718   -1.4617   -0.0729    0.3309   -0.0530   -0.1141   -0.0549   -0.0155   -0.0086   -0.1786   -0.1144

 Dipole mement (in D)   1.26 (DEN)      1.46      2.26      0.83      1.37      1.24      1.41      2.44      3.85      1.50

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File TZVPMol476.out
Molecule PMol476    1-chloro-1,1-difluoroeth
 SP Mol476 B3LYP/Def2TZVP VAC.
    0    8
Dipole          0.6648    2.0858    0.0000    2.1892
Quadrupole      0.1733    1.3064   -1.4796    1.7837    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   6      0.8115    1.4274    0.0000   -0.3280   -0.2813   -0.0910   -0.6560   -0.2326   -0.4406   -0.6624    0.0472   -0.2604
   1      0.4435    1.9367    0.8847    0.1303    0.1352    0.0510    0.1623    0.1052    0.1587    0.2321    0.0501    0.0974
   1      0.4435    1.9367   -0.8847    0.1303    0.1352    0.0510    0.1623    0.1052    0.1587    0.2321    0.0501    0.0974
   1      1.8991    1.4437    0.0000    0.1269    0.1353    0.0512    0.1628    0.1054    0.1840    0.2289    0.0461    0.0964
   6      0.3527    0.0038    0.0000    0.3974   -0.8254    0.2285    0.8179    0.2543    0.3005    0.6636    1.3082    0.4659
   9      0.8115   -0.6543   -1.0787   -0.1711    0.1835   -0.1068   -0.2447   -0.1310   -0.1339   -0.3162   -0.6438   -0.1756
   9      0.8115   -0.6543    1.0787   -0.1711    0.1835   -0.1068   -0.2447   -0.1310   -0.1339   -0.3162   -0.6438   -0.1756
  17     -1.4340   -0.1250    0.0000   -0.1149    0.3338   -0.0772   -0.1597   -0.0754   -0.0936   -0.0618   -0.2136   -0.1456

 Dipole mement (in D)   2.19 (DEN)      2.28      1.56      1.46      1.31      2.01      2.24      3.43      5.80      2.02

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File TZVPMol477.out
Molecule PMol477    acetylchloride
 SP Mol477 B3LYP/Def2TZVP VAC.
    0    7
Dipole          2.8215    0.1151    0.0000    2.8238
Quadrupole      0.9939   -2.0732    1.0793    2.6507    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP      NPA       AIM       ACP
   1      1.7273    1.7663    0.0000    0.1341    0.1352    0.0550    0.1642    0.1100    0.1147    0.2339    0.0536    0.1008
   6      1.4763    0.7099    0.0000   -0.2989   -0.2838   -0.0725   -0.5841   -0.2149   -0.2689   -0.7070    0.0206   -0.2408
   6      0.0000    0.5372    0.0000    0.2138   -0.6111    0.1996    0.6993    0.2275    0.5435    0.5618    1.1921    0.4162
   8     -0.8355    1.3709    0.0000   -0.1916    0.1857   -0.2021   -0.4403   -0.2511   -0.3933   -0.4646   -1.1256   -0.3304
   1      1.9040    0.2216    0.8732    0.1423    0.1429    0.0579    0.1638    0.1115    0.0985    0.2468    0.0622    0.1062
   1      1.9040    0.2216   -0.8732    0.1423    0.1429    0.0579    0.1638    0.1115    0.0985    0.2468    0.0622    0.1062
  17     -0.4535   -1.2153    0.0000   -0.1420    0.2883   -0.0958   -0.1666   -0.0946   -0.1930   -0.1176   -0.2646   -0.1581
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 Dipole mement (in D)   2.82 (DEN)      2.73      1.59      2.02      2.38      2.64      2.85      3.66      7.15      2.74

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File TZVPMol478.out
Molecule PMol478    phosgene
 SP Mol478 B3LYP/Def2TZVP VAC.
    0    4
Dipole          0.0000    0.0000   -1.3184    1.3184
Quadrupole      1.0635    1.6532   -2.7167    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.0000    0.4981    0.2009   -0.9776    0.1987    0.6157    0.2381    0.3733    0.4137    1.3562    0.4651
   8      0.0000    0.0000    1.6730   -0.1569    0.1833   -0.1867   -0.4334   -0.2333   -0.2897   -0.4485   -1.0989   -0.3173
  17      0.0000    1.4402   -0.4815   -0.0220    0.3972   -0.0061   -0.0912   -0.0025   -0.0418    0.0174   -0.1286   -0.0739
  17      0.0000   -1.4402   -0.4815   -0.0220    0.3972   -0.0061   -0.0912   -0.0025   -0.0418    0.0174   -0.1286   -0.0739

 Dipole mement (in D)   1.32 (DEN)      0.68      2.70      1.00      1.59      1.29      1.24      2.69      4.99      1.09

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File TZVPMol479.out
Molecule PMol479    para-chlorophenol
 SP Mol479 B3LYP/Def2TZVP VAC.
    0   13
Dipole         -1.3155   -1.8273    0.0000    2.2516
Quadrupole      5.5189   -1.2535   -4.2654    5.5082    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.9595    0.0000    0.1564   -0.4409    0.0099    0.1240    0.0023   -0.0803   -0.0759    0.0737    0.0878
   6     -1.2013    0.2685    0.0000   -0.1738   -0.1417   -0.0412   -0.1360   -0.0938    0.0377   -0.2010    0.0142   -0.0869
   6     -1.1936   -1.1183    0.0000   -0.1861   -0.1390   -0.0609   -0.2597   -0.1129   -0.4091   -0.2756   -0.0255   -0.1127
   6      0.0118   -1.8116    0.0000    0.2704   -0.2756    0.0734    0.4154    0.0849    0.4436    0.2836    0.5152    0.1796
   6      1.2132   -1.1102    0.0000   -0.1773   -0.1122   -0.0489   -0.2238   -0.0995   -0.3187   -0.2448   -0.0065   -0.1013
   6      1.2075    0.2734    0.0000   -0.1459   -0.1379   -0.0386   -0.1392   -0.0911   -0.0147   -0.1998    0.0139   -0.0846
   1      2.1441   -1.6607    0.0000    0.1186    0.1508    0.0496    0.1332    0.1090    0.1914    0.2239    0.0566    0.0859
   1      2.1378    0.8240    0.0000    0.1201    0.1483    0.0478    0.1142    0.1052    0.1207    0.2233    0.0562    0.0861
   1     -2.1364    0.8109    0.0000    0.1211    0.1478    0.0472    0.1144    0.1047    0.1127    0.2233    0.0559    0.0856
   1     -2.1317   -1.6617    0.0000    0.1045    0.1429    0.0413    0.1124    0.0996    0.1725    0.2061    0.0250    0.0852
  17     -0.0044    2.6945    0.0000   -0.1250    0.3834   -0.0662   -0.0827   -0.0682   -0.0988    0.0038   -0.2454   -0.1274
   8      0.0803   -3.1693    0.0000   -0.3921    0.0893   -0.1850   -0.6080   -0.3873   -0.5679   -0.6391   -1.1109   -0.3669
   1     -0.8080   -3.5332    0.0000    0.3094    0.1848    0.1716    0.4359    0.3471    0.4109    0.4722    0.5774    0.2697

 Dipole mement (in D)   2.25 (DEN)      2.09      0.78      1.52      1.87      2.02      2.31      1.77      2.21      1.91

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File TZVPMol480.out
Molecule PMol480    cyanogen_chloride
 SP Mol480 B3LYP/Def2TZVP VAC.
    0    3
Dipole          0.0000    0.0000    3.0442    3.0442
Quadrupole      1.3538    1.3538   -2.7076    0.0000    0.0000    0.0000
```

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	0.9711	0.0842	0.5805	0.1235	0.1028	0.1282	0.1086	0.1737	0.0045	0.0622
6	0.0000	0.0000	-0.6456	-0.0660	-0.6224	0.0748	0.2667	0.1915	0.2648	0.1224	1.0884	0.2903
7	0.0000	0.0000	-1.8049	-0.0183	0.0418	-0.1983	-0.3694	-0.3198	-0.3734	-0.2961	-1.0928	-0.3525
Dipole mement (in D)	3.04 (DEN)			0.76	4.28	2.06	2.86	2.78	2.92	3.00	6.12	2.45

File TZVPMol481.out
Molecule PMol481 1-chloro-2-nitrobenzene
SP Mol481 B3LYP/Def2TZVP VAC.
0 14
Dipole 4.8619 0.2072 0.0722 4.8668
Quadrupole 0.2609 2.0636 -2.3245 -3.6289 0.7771 -2.0882

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.3628	0.7787	-0.0159	0.0206	-0.4056	0.0323	0.1344	0.0328	-0.1547	-0.0432	0.1195	0.1123
6	-0.0797	-0.5442	0.0226	0.1425	-0.1551	0.0237	-0.0681	0.0785	0.2384	0.0069	0.2437	0.1162
6	0.8253	-1.5962	0.0544	-0.1675	-0.0876	-0.0228	-0.0991	-0.0695	-0.2926	-0.1706	0.0162	-0.0673
6	2.1830	-1.3432	0.0851	-0.0776	-0.1255	-0.0279	-0.0951	-0.0835	-0.0149	-0.2063	-0.0034	-0.0746
6	2.6335	-0.0298	0.0531	-0.1059	-0.1133	-0.0167	-0.0440	-0.0724	-0.2136	-0.1677	-0.0075	-0.0622
6	1.7331	1.0196	-0.0091	-0.1304	-0.1303	-0.0339	-0.1838	-0.0865	0.0754	-0.2110	0.0175	-0.0820
1	0.4319	-2.6028	0.0606	0.1544	0.1606	0.0544	0.1296	0.1194	0.1849	0.2437	0.0925	0.0884
1	2.8844	-2.1648	0.1289	0.1281	0.1497	0.0528	0.1118	0.1091	0.1206	0.2213	0.0522	0.0984
1	3.6941	0.1840	0.0685	0.1275	0.1503	0.0539	0.1105	0.1101	0.1503	0.2195	0.0520	0.0995
1	2.0764	2.0432	-0.0588	0.1294	0.1516	0.0520	0.1189	0.1098	0.0792	0.2301	0.0675	0.0912
7	-1.5061	-0.9064	0.0389	0.4051	-0.0339	0.2429	0.7345	0.0784	0.6180	0.5011	0.4488	0.2242
8	-1.8141	-1.9384	-0.5402	-0.3024	-0.0163	-0.2013	-0.4204	-0.1620	-0.4056	-0.3605	-0.4765	-0.2285
8	-2.2714	-0.1789	0.6469	-0.2800	-0.0051	-0.1949	-0.4263	-0.1520	-0.3730	-0.3374	-0.4577	-0.2270
17	-0.6946	2.1243	-0.1451	-0.0437	0.4604	-0.0144	-0.0030	-0.0121	-0.0125	0.0739	-0.1655	-0.0887
Dipole mement (in D)	4.87 (DEN)			4.63	2.89	3.68	4.81	4.60	4.94	5.97	9.16	5.00

File TZVPMol482.out
Molecule PMol482 1-chloro-3-nitrobenzene
SP Mol482 B3LYP/Def2TZVP VAC.
0 14
Dipole -2.7967 2.8293 0.0001 3.9782
Quadrupole -8.3509 6.5061 1.8448 1.7627 0.0003 -0.0001

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.4256	0.0015	0.0000	0.2111	-0.4234	0.0323	0.1633	0.0252	0.0132	-0.0471	0.0923	0.1108
6	-0.2025	-0.6486	0.0000	-0.2350	-0.0936	-0.0313	-0.2186	-0.0750	-0.1290	-0.2032	0.0389	-0.0779
6	0.9412	0.1309	0.0000	0.0941	-0.1509	0.0305	0.0336	0.0811	0.1107	0.0365	0.2089	0.1261
6	0.9076	1.5145	0.0000	-0.1692	-0.0903	-0.0260	-0.1275	-0.0733	-0.2191	-0.1907	0.0128	-0.0715
6	-0.3300	2.1376	0.0000	-0.0620	-0.1166	-0.0206	-0.0577	-0.0759	-0.1213	-0.1867	-0.0007	-0.0673
6	-1.4988	1.3899	0.0000	-0.1661	-0.1177	-0.0244	-0.1562	-0.0771	-0.0493	-0.1924	0.0145	-0.0722
1	1.8339	2.0689	0.0000	0.1627	0.1598	0.0542	0.1325	0.1188	0.1792	0.2491	0.1009	0.0872
1	-0.3891	3.2176	-0.0000	0.1302	0.1515	0.0547	0.1141	0.1111	0.1489	0.2222	0.0553	0.1005

1	-2.4661	1.8725	-0.0000	0.1328	0.1516	0.0544	0.1198	0.1118	0.1215	0.2291	0.0685	0.0940
17	-2.8811	-0.9280	0.0000	-0.0860	0.4207	-0.0335	-0.0455	-0.0355	-0.0615	0.0352	-0.2104	-0.0966
1	-0.1255	-1.7253	0.0000	0.1673	0.1626	0.0559	0.1452	0.1216	0.1508	0.2596	0.1175	0.0829
7	2.2524	-0.5514	0.0000	0.4291	-0.0242	0.2462	0.7265	0.0817	0.6636	0.5035	0.4500	0.2291
8	3.2497	0.1534	-0.0000	-0.3051	-0.0150	-0.1966	-0.4172	-0.1576	-0.4055	-0.3577	-0.4743	-0.2229
8	2.2511	-1.7725	-0.0000	-0.3039	-0.0144	-0.1957	-0.4125	-0.1568	-0.4022	-0.3574	-0.4739	-0.2222

Dipole mement (in D) 3.98 (DEN) 4.10 4.30 3.05 4.05 3.70 3.98 5.14 6.90 3.69

File TZVPMol483.out
Molecule PMol483 1-chloro-4-nitrobenzene
SP Mol483 B3LYP/Def2TZVP VAC.
0 14
Dipole 0.0000 0.0000 3.3082 3.3082
Quadrupole 3.2682 8.6924 -11.9606 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	1.6416	0.1677	-0.4163	0.0395	0.1782	0.0320	-0.0877	-0.0244	0.0841	0.1191
6	0.0000	1.2125	0.9602	-0.1293	-0.1269	-0.0319	-0.1818	-0.0842	0.0692	-0.2192	0.0220	-0.0806
6	0.0000	1.2119	-0.4225	-0.1571	-0.0825	-0.0186	-0.0833	-0.0655	-0.3046	-0.1671	0.0163	-0.0634
6	0.0000	0.0000	-1.0943	0.0863	-0.1578	0.0246	-0.0052	0.0762	0.2208	0.0152	0.2162	0.1206
6	0.0000	-1.2119	-0.4225	-0.1571	-0.0825	-0.0186	-0.0833	-0.0655	-0.3046	-0.1671	0.0164	-0.0634
6	0.0000	-1.2125	0.9602	-0.1293	-0.1269	-0.0319	-0.1818	-0.0842	0.0692	-0.2192	0.0219	-0.0806
1	0.0000	-2.1317	-0.9889	0.1633	0.1616	0.0561	0.1340	0.1207	0.1845	0.2500	0.1036	0.0890
1	0.0000	-2.1405	1.5135	0.1342	0.1523	0.0546	0.1244	0.1122	0.0996	0.2317	0.0704	0.0943
17	0.0000	0.0000	3.3654	-0.0817	0.4289	-0.0275	-0.0411	-0.0296	-0.0507	0.0416	-0.2072	-0.0904
1	0.0000	2.1405	1.5135	0.1342	0.1523	0.0546	0.1244	0.1122	0.0996	0.2317	0.0703	0.0943
7	0.0000	0.0000	-2.5644	0.4225	-0.0246	0.2442	0.7289	0.0789	0.6144	0.5021	0.4390	0.2255
8	0.0000	-1.0851	-3.1278	-0.3085	-0.0196	-0.2007	-0.4236	-0.1619	-0.3971	-0.3625	-0.4780	-0.2266
8	0.0000	1.0851	-3.1278	-0.3085	-0.0196	-0.2007	-0.4236	-0.1619	-0.3971	-0.3625	-0.4780	-0.2266
1	0.0000	2.1317	-0.9889	0.1633	0.1616	0.0561	0.1340	0.1207	0.1845	0.2500	0.1036	0.0890

Dipole mement (in D) 3.31 (DEN) 3.46 5.22 2.80 3.72 3.24 3.26 4.76 5.31 2.91

File TZVPMol587.out
Molecule PMol587 HBr
SP Mol587 B3LYP/Def2TZVP VAC.
0 2
Dipole 0.0000 0.0000 -0.9193 0.9193
Quadrupole -1.4230 -1.4230 2.8459 0.0000 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.0000	0.0394	-0.1927	-0.0482	-0.0898	-0.1745	-0.1338	-0.1629	-0.1966	-0.1201	-0.1214
1	0.0000	0.0000	-1.3794	0.1927	0.0482	0.0898	0.1745	0.1338	0.1629	0.1966	0.1201	0.1214

Dipole mement (in D) 0.92 (DEN) 1.31 0.33 0.61 1.19 0.91 1.11 1.34 0.82 0.83

File TZVPMol588.out
Molecule PMol588 bromomethane
 SP Mol588 B3LYP/Def2TZVP VAC.
  0 5
Dipole -1.8947 0.0000 0.0003 1.8947
Quadrupole 2.4248 -1.2121 -1.2126 0.0000 0.0002 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.4184	0.0000	-0.0000	-0.1189	0.1875	-0.0850	-0.0257	-0.0812	-0.0860	-0.0096	-0.1424	-0.1249
6	-1.5120	0.0000	-0.0000	-0.3057	-0.5075	-0.0552	-0.3619	-0.2139	-0.6290	-0.6296	-0.0298	-0.1928
1	-1.8574	0.9213	-0.4534	0.1415	0.1067	0.0467	0.1292	0.0984	0.2385	0.2131	0.0575	0.1059
1	-1.8573	-0.8534	-0.5711	0.1415	0.1067	0.0467	0.1292	0.0984	0.2386	0.2131	0.0575	0.1059
1	-1.8572	-0.0680	1.0246	0.1415	0.1066	0.0467	0.1292	0.0984	0.2379	0.2130	0.0575	0.1059

Dipole mement (in D)	1.89 (DEN)	1.81	1.21	1.02	0.88	1.24	1.98	1.15	1.61	1.69	

File TZVPMol589.out
Molecule PMol589 dibromomethane
 SP Mol589 B3LYP/Def2TZVP VAC.
  0 5
Dipole 0.0000 1.4994 0.0000 1.4994
Quadrupole -0.2851 2.0808 -1.7957 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	-0.1227	1.6205	-0.0627	0.2429	-0.0477	-0.0088	-0.0410	0.0433	0.0437	-0.0785	-0.0870
6	0.0000	0.9208	0.0000	-0.1928	-0.7094	-0.0117	-0.2340	-0.1352	-0.7917	-0.5327	-0.0433	-0.0541
35	0.0000	-0.1227	-1.6205	-0.0627	0.2429	-0.0477	-0.0088	-0.0410	0.0433	0.0437	-0.0785	-0.0870
1	-0.8922	1.5334	0.0000	0.1591	0.1118	0.0535	0.1258	0.1086	0.3535	0.2226	0.1002	0.1141
1	0.8922	1.5333	0.0000	0.1591	0.1118	0.0535	0.1258	0.1086	0.3517	0.2226	0.1002	0.1141

Dipole mement (in D)	1.50 (DEN)	1.56	1.78	0.79	0.83	1.05	1.64	0.87	1.38	1.54	

File TZVPMol590.out
Molecule PMol590 bromoform
 SP Mol590 B3LYP/Def2TZVP VAC.
  0 5
Dipole -0.7699 0.4626 0.0000 0.8982
Quadrupole 0.4714 -0.0807 -0.3907 -0.5236 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.3657	0.8238	0.0000	0.1679	0.1143	0.0545	0.1026	0.1131	0.4344	0.2242	0.1363	0.1162
6	-0.4398	0.2649	0.0000	-0.1037	-0.9481	0.0206	-0.0215	-0.0668	-0.8591	-0.4884	-0.0584	0.0718
35	0.9941	1.5616	0.0000	-0.0216	0.2776	-0.0252	-0.0272	-0.0155	0.1417	0.0878	-0.0261	-0.0629
35	-0.4398	-0.8153	1.6029	-0.0212	0.2781	-0.0250	-0.0270	-0.0154	0.1415	0.0882	-0.0257	-0.0626
35	-0.4398	-0.8153	-1.6029	-0.0212	0.2781	-0.0250	-0.0270	-0.0154	0.1415	0.0882	-0.0257	-0.0626

Dipole mement (in D)	0.90 (DEN)	1.04	1.64	0.48	0.75	0.71	1.12	0.46	0.92	1.11	

File TZVPMol591.out
Molecule PMol591 bromoethane
 SP Mol591 B3LYP/Def2TZVP VAC.
  0 8
Dipole 0.4659 -2.0995 0.0000 2.1506
Quadrupole -0.4978 1.2659 -0.7681 -0.9895 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.7929	0.0000	-0.1440	0.1973	-0.0938	-0.0710	-0.0883	-0.1860	-0.0374	-0.1750	-0.1433
6	0.5922	-1.0684	0.0000	-0.1521	-0.4736	-0.0157	-0.0998	-0.1349	-0.0565	-0.3992	0.0032	-0.0818
6	-0.5672	-2.0252	0.0000	-0.3078	-0.3362	-0.0842	-0.3819	-0.2358	-0.0683	-0.6160	0.0324	-0.2392
1	1.2191	-1.1747	0.8807	0.1278	0.1228	0.0420	0.1005	0.0968	0.0904	0.2088	0.0464	0.0980
1	1.2191	-1.1747	-0.8807	0.1278	0.1228	0.0420	0.1005	0.0968	0.0904	0.2088	0.0464	0.0980
1	-0.1991	-3.0521	0.0000	0.1099	0.1240	0.0387	0.1196	0.0901	0.0424	0.2117	0.0098	0.0920
1	-1.1945	-1.8950	-0.8795	0.1193	0.1215	0.0355	0.1161	0.0877	0.0439	0.2117	0.0185	0.0882
1	-1.1945	-1.8950	0.8795	0.1193	0.1215	0.0355	0.1161	0.0877	0.0439	0.2117	0.0185	0.0882

 Dipole mement (in D) 2.15 (DEN) 2.04 1.15 1.17 1.15 1.39 2.26 1.46 2.02 1.92

File TZVPMol592.out
Molecule PMol592 1-bromopropane
 SP Mol592 B3LYP/Def2TZVP VAC.
  0 11
Dipole 1.3181 1.8092 0.0000 2.2384
Quadrupole -0.2957 0.3678 -0.0722 -0.0367 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	2.1871	2.0308	0.0000	-0.3400	-0.3044	-0.0798	-0.3260	-0.2317	-0.3255	-0.5874	0.0093	-0.2453
6	1.5014	0.6755	0.0000	-0.1483	-0.3264	-0.0487	-0.1648	-0.1618	0.3850	-0.4153	0.0704	-0.1319
6	0.0000	0.8271	0.0000	-0.1576	-0.4514	-0.0192	-0.1369	-0.1365	-0.3526	-0.3973	-0.0063	-0.0880
1	1.8084	0.0948	0.8714	0.1016	0.1352	0.0316	0.0937	0.0870	-0.0411	0.2042	0.0068	0.0808
1	1.8084	0.0948	-0.8714	0.1016	0.1352	0.0316	0.0937	0.0870	-0.0411	0.2042	0.0068	0.0808
35	-0.9182	-0.8932	0.0000	-0.1419	0.2054	-0.0932	-0.0760	-0.0877	-0.1595	-0.0308	-0.1740	-0.1424
1	3.2703	1.9262	0.0000	0.1202	0.1213	0.0359	0.1107	0.0874	0.0710	0.2120	0.0076	0.0899
1	1.9157	2.6170	0.8782	0.1072	0.1182	0.0307	0.1023	0.0825	0.0768	0.1981	-0.0033	0.0831
1	1.9157	2.6170	-0.8782	0.1072	0.1182	0.0307	0.1023	0.0825	0.0768	0.1981	-0.0033	0.0831
1	-0.3569	1.3559	-0.8809	0.1250	0.1244	0.0403	0.1004	0.0956	0.1551	0.2071	0.0429	0.0949
1	-0.3569	1.3559	0.8809	0.1250	0.1244	0.0403	0.1004	0.0956	0.1551	0.2071	0.0429	0.0949

 Dipole mement (in D) 2.24 (DEN) 2.08 0.98 1.29 1.23 1.52 2.35 1.52 2.12 2.01

File TZVPMol593.out
Molecule PMol593 2-bromopropane
 SP Mol593 B3LYP/Def2TZVP VAC.
  0 11
Dipole 1.7614 -1.4818 0.0000 2.3018
Quadrupole 0.7533 -0.4336 -0.3197 -0.5558 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP

6	0.9068	-0.4357	0.0000	-0.0041	-0.4713	0.0217	0.1407	-0.0584	0.2252	-0.1888	0.0248	0.0293
35	-0.6727	0.7550	0.0000	-0.1699	0.2097	-0.0982	-0.0833	-0.0908	-0.2202	-0.0586	-0.1993	-0.1580
1	1.7416	0.2632	0.0000	0.1081	0.1392	0.0393	0.0807	0.0975	0.0643	0.2085	0.0398	0.0922
6	0.9068	-1.2633	1.2608	-0.3148	-0.3100	-0.0871	-0.4303	-0.2370	-0.3460	-0.6165	0.0273	-0.2443
6	0.9068	-1.2633	-1.2608	-0.3148	-0.3100	-0.0871	-0.4303	-0.2370	-0.3460	-0.6165	0.0269	-0.2443
1	0.9033	-0.6459	2.1556	0.1263	0.1227	0.0351	0.1178	0.0875	0.0946	0.2181	0.0194	0.0882
1	0.9033	-0.6459	-2.1556	0.1263	0.1227	0.0351	0.1178	0.0875	0.0946	0.2181	0.0194	0.0882
1	0.0383	-1.9197	1.3004	0.1150	0.1235	0.0342	0.1210	0.0870	0.1115	0.2094	0.0156	0.0859
1	0.0383	-1.9197	-1.3004	0.1150	0.1235	0.0342	0.1210	0.0870	0.1115	0.2094	0.0156	0.0859
1	1.7996	-1.8909	1.2863	0.1064	0.1249	0.0364	0.1224	0.0884	0.1053	0.2085	0.0053	0.0885
1	1.7996	-1.8909	-1.2863	0.1064	0.1249	0.0364	0.1224	0.0884	0.1053	0.2085	0.0053	0.0885

Dipole mement (in D)	2.30 (DEN)	2.24	1.06	1.23	1.09	1.47	2.45	1.70	2.22	2.06

File TZVPMol594.out
Molecule PMol594 1-bromobutane
SP Mol594 B3LYP/Def2TZVP VAC.
0 14
Dipole 2.2320 0.6843 0.0000 2.3345
Quadrupole -1.3477 0.6863 0.6614 0.5661 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	3.6051	-0.6295	0.0000	-0.3278	-0.3063	-0.0814	-0.3285	-0.2333	-0.2949	-0.5825	0.0159	-0.2457
6	2.4800	0.3870	0.0000	-0.1584	-0.2898	-0.0423	-0.1123	-0.1553	0.1801	-0.3799	0.0494	-0.1350
1	4.5835	-0.1519	0.0000	0.1148	0.1180	0.0316	0.1023	0.0829	0.0782	0.2057	-0.0006	0.0852
1	3.5562	-1.2751	0.8773	0.1059	0.1182	0.0299	0.1013	0.0817	0.0586	0.1977	-0.0043	0.0823
1	3.5562	-1.2751	-0.8773	0.1059	0.1182	0.0299	0.1013	0.0817	0.0586	0.1977	-0.0043	0.0823
6	1.1039	-0.2654	0.0000	-0.1772	-0.3021	-0.0512	-0.2012	-0.1625	0.2422	-0.4106	0.0612	-0.1373
1	2.5711	1.0424	0.8709	0.0872	0.1323	0.0280	0.0829	0.0831	-0.0309	0.1911	-0.0146	0.0767
1	2.5711	1.0424	-0.8709	0.0872	0.1323	0.0280	0.0829	0.0831	-0.0309	0.1911	-0.0146	0.0767
6	0.0000	0.7619	0.0000	-0.1444	-0.4485	-0.0192	-0.1383	-0.1365	-0.5325	-0.3927	-0.0066	-0.0877
1	1.0008	-0.9160	-0.8718	0.0993	0.1370	0.0304	0.0942	0.0864	-0.0069	0.1993	0.0038	0.0782
1	1.0008	-0.9160	0.8718	0.0993	0.1370	0.0304	0.0942	0.0864	-0.0069	0.1993	0.0038	0.0782
1	0.0345	1.3988	-0.8810	0.1256	0.1246	0.0401	0.0983	0.0954	0.2026	0.2076	0.0428	0.0948
1	0.0345	1.3988	0.8810	0.1256	0.1246	0.0401	0.0983	0.0954	0.2026	0.2076	0.0428	0.0948
35	-1.7727	-0.0535	0.0000	-0.1430	0.2045	-0.0943	-0.0752	-0.0887	-0.1200	-0.0314	-0.1748	-0.1435

Dipole mement (in D)	2.33 (DEN)	2.14	1.07	1.38	1.37	1.60	2.41	1.56	2.25	2.11

File TZVPMol595.out
Molecule PMol595 2-bromobutane
SP Mol595 B3LYP/Def2TZVP VAC.
0 14
Dipole -1.8793 1.2583 0.2956 2.2809
Quadrupole -0.3974 0.5251 -0.1276 -0.3557 -0.2237 0.6334

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.1605	2.1292	-0.0146	-0.3104	-0.3092	-0.0876	-0.4374	-0.2376	-0.4206	-0.6147	0.0273	-0.2443

6	-0.4772	0.7053	0.3669	-0.0067	-0.4421	0.0206	0.1157	-0.0577	0.1239	-0.1800	0.0160	0.0246
1	0.7264	2.5008	0.4927	0.1274	0.1226	0.0347	0.1180	0.0872	0.1251	0.2185	0.0197	0.0878
1	0.0024	2.2213	-1.0878	0.1153	0.1238	0.0339	0.1184	0.0867	0.1176	0.2100	0.0153	0.0857
1	-0.9987	2.7760	0.2522	0.1073	0.1245	0.0358	0.1192	0.0878	0.1211	0.2083	0.0047	0.0881
6	-1.7059	0.1578	-0.3290	-0.1485	-0.2994	-0.0484	-0.1994	-0.1593	0.0783	-0.4154	0.0609	-0.1337
1	-0.5816	0.6080	1.4478	0.1022	0.1409	0.0379	0.0798	0.0967	0.0815	0.2068	0.0368	0.0896
6	-2.1290	-1.2263	0.1149	-0.3357	-0.3113	-0.0883	-0.3486	-0.2400	-0.2509	-0.5922	0.0118	-0.2499
1	-2.5138	0.8716	-0.1345	0.0882	0.1420	0.0341	0.1021	0.0897	0.0154	0.2041	-0.0040	0.0824
1	-1.5427	0.1829	-1.4095	0.0986	0.1385	0.0312	0.0982	0.0872	0.0263	0.2002	0.0048	0.0796
1	-3.0502	-1.5351	-0.3757	0.1126	0.1186	0.0320	0.1087	0.0835	0.0720	0.2073	-0.0006	0.0856
1	-1.3652	-1.9671	-0.1162	0.1289	0.1187	0.0235	0.0961	0.0765	0.0622	0.2142	0.0170	0.0762
1	-2.3029	-1.2616	1.1911	0.0990	0.1179	0.0284	0.1013	0.0803	0.0554	0.1961	-0.0073	0.0803
35	1.0989	-0.4284	-0.0311	-0.1781	0.2145	-0.0879	-0.0722	-0.0808	-0.2073	-0.0633	-0.2014	-0.1519
Dipole mement (in D)	2.28 (DEN)		2.23	1.15	1.16	1.09	1.41	2.39	1.69	2.15	2.06	

File TZVPMol596.out
Molecule PMol596 1-bromopentane
SP Mol596 B3LYP/Def2TZVP VAC.
0 17
Dipole 1.5552 1.7706 0.0000 2.3566
Quadrupole 0.2247 -1.8241 1.5994 -2.0403 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.6258	0.0000	-0.1650	-0.2999	-0.0512	-0.2045	-0.1625	0.1276	-0.4082	0.0610	-0.1372
6	1.1982	1.5637	0.0000	-0.1954	-0.2647	-0.0443	-0.1437	-0.1556	0.0546	-0.3748	0.0403	-0.1401
1	-0.6281	0.8238	0.8718	0.1000	0.1373	0.0303	0.0922	0.0863	0.0004	0.1996	0.0038	0.0782
1	-0.6281	0.8238	-0.8718	0.1000	0.1373	0.0303	0.0922	0.0863	0.0004	0.1996	0.0038	0.0782
6	0.8055	3.0319	0.0000	-0.1396	-0.2911	-0.0430	-0.1206	-0.1561	0.1328	-0.3769	0.0566	-0.1349
1	1.8282	1.3555	0.8711	0.0852	0.1341	0.0269	0.0832	0.0827	-0.0108	0.1868	-0.0173	0.0742
1	1.8282	1.3555	-0.8711	0.0852	0.1341	0.0269	0.0832	0.0827	-0.0108	0.1868	-0.0173	0.0742
6	2.0009	3.9639	0.0000	-0.3267	-0.3087	-0.0835	-0.3290	-0.2354	-0.2203	-0.5836	0.0139	-0.2472
1	0.1749	3.2351	-0.8701	0.0863	0.1328	0.0278	0.0833	0.0830	-0.0269	0.1912	-0.0147	0.0766
1	0.1749	3.2351	0.8701	0.0863	0.1328	0.0278	0.0833	0.0830	-0.0269	0.1912	-0.0147	0.0766
1	1.7018	5.0108	0.0000	0.1140	0.1174	0.0306	0.1012	0.0819	0.0599	0.2050	-0.0024	0.0842
1	2.6290	3.8046	0.8772	0.1025	0.1168	0.0278	0.0976	0.0796	0.0447	0.1956	-0.0081	0.0800
1	2.6290	3.8046	-0.8772	0.1025	0.1168	0.0278	0.0976	0.0796	0.0447	0.1956	-0.0081	0.0800
6	0.4262	-0.8205	0.0000	-0.1437	-0.4482	-0.0192	-0.1362	-0.1364	-0.3257	-0.3916	-0.0056	-0.0877
1	1.0109	-1.0748	-0.8810	0.1263	0.1246	0.0400	0.0983	0.0954	0.1516	0.2078	0.0427	0.0947
1	1.0109	-1.0748	0.8810	0.1263	0.1246	0.0400	0.0983	0.0954	0.1516	0.2078	0.0427	0.0947
35	-1.0948	-2.0425	0.0000	-0.1441	0.2040	-0.0949	-0.0761	-0.0894	-0.1470	-0.0320	-0.1757	-0.1441
Dipole mement (in D)	2.36 (DEN)		2.11	0.88	1.43	1.35	1.66	2.46	1.61	2.30	2.14	

File TZVPMol597.out
Molecule PMol597 1-bromoheptane
SP Mol597 B3LYP/Def2TZVP VAC.

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    0   23
Dipole          2.2968    0.7253    0.0002    2.4086
Quadrupole     -6.4351    2.8729    3.5622   -1.5444   -0.0006   -0.0001
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6     -1.7126    0.7646    0.0000   -0.1417   -0.4480   -0.0192   -0.1362   -0.1365   -0.4972   -0.3911   -0.0055   -0.0877
   6     -0.5480   -0.1934   -0.0000   -0.1668   -0.2994   -0.0513   -0.2032   -0.1626    0.3129   -0.4074    0.0611   -0.1372
   1     -1.7170    1.4023    0.8810    0.1262    0.1246    0.0400    0.0982    0.0953    0.1922    0.2077    0.0427    0.0946
   1     -1.7169    1.4024   -0.8809    0.1262    0.1246    0.0400    0.0982    0.0953    0.1922    0.2077    0.0426    0.0946
   6      0.7841    0.5428    0.0001   -0.1875   -0.2622   -0.0444   -0.1445   -0.1556    0.0650   -0.3715    0.0401   -0.1401
   1     -0.6117   -0.8489    0.8718    0.1006    0.1373    0.0301    0.0923    0.0862   -0.0292    0.1999    0.0037    0.0780
   1     -0.6116   -0.8487   -0.8720    0.1006    0.1373    0.0301    0.0923    0.0862   -0.0292    0.1999    0.0037    0.0780
   6      1.9818   -0.3915    0.0001   -0.1622   -0.2636   -0.0450   -0.1550   -0.1565   -0.0548   -0.3694    0.0461   -0.1400
   1      0.8377    1.2041   -0.8711    0.0868    0.1344    0.0267    0.0811    0.0825   -0.0243    0.1873   -0.0173    0.0741
   1      0.8377    1.2040    0.8714    0.0868    0.1344    0.0267    0.0811    0.0825   -0.0243    0.1873   -0.0173    0.0741
   1      1.9259   -1.0535    0.8706    0.0849    0.1348    0.0268    0.0815    0.0825   -0.0120    0.1872   -0.0173    0.0742
   1      1.9259   -1.0533   -0.8706    0.0849    0.1348    0.0268    0.0815    0.0825   -0.0120    0.1872   -0.0173    0.0742
   6      3.3157    0.3337    0.0002   -0.1721   -0.2676   -0.0468   -0.1529   -0.1581    0.0756   -0.3726    0.0448   -0.1413
   6      4.5158   -0.5982    0.0001   -0.1355   -0.2930   -0.0451   -0.1207   -0.1582    0.2251   -0.3775    0.0542   -0.1364
   1      3.3705    0.9964    0.8708    0.0804    0.1332    0.0249    0.0800    0.0806   -0.0235    0.1848   -0.0208    0.0720
   1      3.3705    0.9965   -0.8703    0.0804    0.1332    0.0249    0.0800    0.0806   -0.0235    0.1848   -0.0208    0.0720
   6      5.8413    0.1378    0.0002   -0.3264   -0.3101   -0.0845   -0.3274   -0.2363   -0.3429   -0.5833    0.0136   -0.2477
   1      4.4583   -1.2591    0.8701    0.0824    0.1314    0.0257    0.0794    0.0808   -0.0418    0.1891   -0.0183    0.0742
   1      4.4583   -1.2589   -0.8700    0.0824    0.1314    0.0257    0.0794    0.0808   -0.0418    0.1891   -0.0183    0.0742
   1      6.6896   -0.5451    0.0002    0.1120    0.1164    0.0291    0.0987    0.0804    0.0821    0.2033   -0.0049    0.0825
   1      5.9392    0.7790   -0.8768    0.1011    0.1163    0.0269    0.0962    0.0787    0.0717    0.1948   -0.0094    0.0790
   1      5.9391    0.7789    0.8774    0.1011    0.1163    0.0269    0.0962    0.0787    0.0717    0.1948   -0.0094    0.0790
  35     -3.4333   -0.1563   -0.0002   -0.1445    0.2034   -0.0953   -0.0767   -0.0898   -0.1319   -0.0323   -0.1760   -0.1444

 Dipole mement (in D)   2.41 (DEN)      2.12      0.83      1.48      1.40      1.71      2.51      1.65      2.36      2.19

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File TZVPMol598.out
Molecule PMol598    bromoethene
 SP Mol598 B3LYP/Def2TZVP VAC.
    0    6
Dipole          0.2398   -1.4030    0.0000    1.4233
Quadrupole      0.6722    2.4662   -3.1384   -0.5021    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.4509   -1.1030    0.0000   -0.0907   -0.4553   -0.0288   -0.0606   -0.1002   -0.2198   -0.2764   -0.1039   -0.0332
   6     -0.4369   -2.0802    0.0000   -0.2592   -0.2317   -0.0794   -0.3067   -0.1821   -0.2668   -0.4006   -0.0153   -0.1761
   1     -0.1005   -3.1085    0.0000    0.1267    0.1296    0.0491    0.1339    0.1021    0.1550    0.2096    0.0533    0.0986
   1      1.5194   -1.2654    0.0000    0.1429    0.1276    0.0533    0.1155    0.1089    0.2107    0.2112    0.0844    0.1040
  35      0.0000    0.7250    0.0000   -0.0538    0.3055   -0.0412   -0.0136   -0.0291   -0.0502    0.0498   -0.0786   -0.0886
   1     -1.5031   -1.9033    0.0000    0.1341    0.1244    0.0471    0.1317    0.1006    0.1710    0.2063    0.0603    0.0953

 Dipole mement (in D)   1.42 (DEN)      1.16      2.02      0.70      0.66      0.88      1.54      0.69      1.43      1.39

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File TZVPMol599.out
Molecule PMol599 bromobenzene
 SP Mol599 B3LYP/Def2TZVP VAC.
  0 12
Dipole 0.0000 0.0000 -1.7754 1.7754
Quadrupole -5.4059 3.1610 2.2448 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-0.0973	0.1010	-0.3778	0.0050	0.1080	-0.0166	-0.0807	-0.0856	-0.0835	0.0582
6	0.0000	1.2086	-0.7794	-0.1526	-0.1429	-0.0428	-0.1732	-0.0969	0.0223	-0.2305	0.0065	-0.0829
6	0.0000	-1.2086	-0.7794	-0.1526	-0.1429	-0.0428	-0.1732	-0.0969	0.0223	-0.2305	0.0065	-0.0829
6	0.0000	1.2004	-2.1675	-0.1007	-0.1320	-0.0322	-0.0669	-0.0881	-0.1888	-0.1901	-0.0187	-0.0769
6	0.0000	-1.2004	-2.1675	-0.1007	-0.1320	-0.0322	-0.0669	-0.0881	-0.1888	-0.1901	-0.0188	-0.0769
6	0.0000	0.0000	-2.8640	-0.1086	-0.1388	-0.0380	-0.1010	-0.0941	-0.0566	-0.2109	-0.0211	-0.0830
1	0.0000	2.1409	-0.2319	0.1268	0.1469	0.0446	0.1079	0.1017	0.0910	0.2203	0.0535	0.0880
1	0.0000	-2.1409	-0.2319	0.1268	0.1469	0.0446	0.1079	0.1017	0.0910	0.2203	0.0535	0.0880
1	0.0000	2.1409	-2.7035	0.1159	0.1455	0.0457	0.1008	0.1018	0.1330	0.2130	0.0383	0.0903
1	0.0000	-2.1409	-2.7035	0.1159	0.1455	0.0457	0.1008	0.1018	0.1330	0.2130	0.0383	0.0903
1	0.0000	0.0000	-3.9460	0.1150	0.1440	0.0439	0.0983	0.1000	0.1103	0.2120	0.0357	0.0884
35	0.0000	0.0000	1.7985	-0.0860	0.3377	-0.0415	-0.0424	-0.0265	-0.0881	0.0589	-0.0903	-0.1007

Dipole mement (in D)	1.78 (DEN)	1.53	1.99	0.96	1.06	1.13	1.93	0.91	1.90	1.75	

File TZVPMol600.out
Molecule PMol600 bromoacetylene
 SP Mol600 B3LYP/Def2TZVP VAC.
  0 4
Dipole 0.0000 0.0000 -0.1660 0.1660
Quadrupole -2.6679 -2.6679 5.3357 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-3.3633	0.1913	0.1259	0.0917	0.2112	0.1457	0.2527	0.2383	0.1745	0.1387
6	0.0000	0.0000	-2.3018	-0.1031	-0.1323	-0.1002	-0.2728	-0.1525	-0.2376	-0.2307	-0.0818	-0.1520
6	0.0000	0.0000	-1.1001	-0.1997	-0.4702	-0.0768	-0.0770	-0.0982	-0.1466	-0.2251	-0.2622	-0.0343
35	0.0000	0.0000	0.6793	0.1114	0.4765	0.0853	0.1385	0.1050	0.1316	0.2175	0.1694	0.0476

Dipole mement (in D)	0.17 (DEN)	0.53	3.47	0.31	0.46	0.19	0.25	0.60	0.02	0.22	

File TZVPMol601.out
Molecule PMol601 3-bromopropyne
 SP Mol601 B3LYP/Def2TZVP VAC.
  0 7
Dipole 0.8209 -1.4489 0.0000 1.6653
Quadrupole 1.2977 1.1181 -2.4158 1.5130 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.9264	-2.6930	0.0000	-0.0817	-0.0745	-0.0919	-0.2878	-0.1438	-0.5443	-0.1895	-0.1217	-0.1489
6	-0.1279	-1.7969	0.0000	-0.1034	-0.1530	-0.0489	0.0490	-0.0608	0.3233	-0.0448	-0.1690	-0.0199
1	-1.6329	-3.4854	0.0000	0.1947	0.1280	0.0911	0.2095	0.1450	0.3327	0.2344	0.1707	0.1384

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   6      0.8364   -0.7373    0.0000   -0.2187   -0.4224   -0.0041   -0.1992   -0.1124   -0.5390   -0.4869    0.0690   -0.0685
  35      0.0000    1.0395    0.0000   -0.1029    0.2311   -0.0662   -0.0364   -0.0590   -0.0675    0.0032   -0.1229   -0.1234
   1      1.4701   -0.7663    0.8827    0.1560    0.1454    0.0601    0.1324    0.1155    0.2473    0.2418    0.0868    0.1112
   1      1.4701   -0.7663   -0.8827    0.1560    0.1454    0.0601    0.1324    0.1155    0.2473    0.2418    0.0868    0.1112

 Dipole mement (in D)   1.67 (DEN)      2.21      1.73      0.87      0.95      1.07      1.83      1.23      1.55      1.67

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File TZVPMol602.out
Molecule PMol602    bromotrifluoromethane
 SP Mol602 B3LYP/Def2TZVP VAC.
    0    5
Dipole         -0.4358   -0.0004    0.0000    0.4358
Quadrupole      1.3763   -0.6881   -0.6883    0.0001    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  35     -1.1238    0.0000    0.0000   -0.0379    0.3154   -0.0212   -0.1385    0.0009    0.0003    0.0005   -0.0033   -0.0961
   6      0.8161   -0.0001    0.0000    0.4540   -0.9718    0.2860    0.9701    0.3320    0.1420    0.8887    1.9028    0.5614
   9      1.2754    1.2411    0.0000   -0.1387    0.2188   -0.0883   -0.2772   -0.1110   -0.0472   -0.2964   -0.6330   -0.1551
   9      1.2754   -0.6206    1.0750   -0.1387    0.2188   -0.0883   -0.2772   -0.1110   -0.0476   -0.2964   -0.6330   -0.1551
   9      1.2754   -0.6206   -1.0750   -0.1387    0.2188   -0.0883   -0.2772   -0.1110   -0.0476   -0.2964   -0.6330   -0.1551

 Dipole mement (in D)   0.44 (DEN)      0.57      1.49      0.39      0.54      0.74      0.32      1.97      4.16      0.13

-----------------------------------------
File TZVPMol603.out
Molecule PMol603    dibromodifluoromethane
 SP Mol603 B3LYP/Def2TZVP VAC.
    0    5
Dipole          0.0000    0.0000   -0.4645    0.4645
Quadrupole      2.0445   -1.5528   -0.4917    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
   6      0.0000    0.0000    0.6593    0.3100   -1.0361    0.2114    0.6559    0.2252   -0.3704    0.5170    1.2687    0.4472
   9      0.0000    1.0729    1.4409   -0.1259    0.2113   -0.0845   -0.2266   -0.1103    0.0867   -0.3024   -0.6328   -0.1398
   9      0.0000   -1.0729    1.4409   -0.1259    0.2113   -0.0845   -0.2266   -0.1103    0.0867   -0.3024   -0.6328   -0.1398
  35      1.6144    0.0000   -0.4270   -0.0291    0.3068   -0.0213   -0.1013   -0.0024    0.0987    0.0439   -0.0017   -0.0838
  35     -1.6144    0.0000   -0.4270   -0.0291    0.3068   -0.0213   -0.1013   -0.0024    0.0984    0.0439   -0.0017   -0.0838

 Dipole mement (in D)   0.46 (DEN)      0.64      1.61      0.41      0.64      0.80      0.38      2.73      4.73      0.17

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File TZVPMol604.out
Molecule PMol604    hydrogen_iodide
 SP Mol604 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000   -0.4619    0.4619
Quadrupole     -1.5942   -1.5942    3.1884    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  53      0.0000    0.0000    0.0299   -0.1200   -0.0164   -0.0640   -0.1147   -0.0965   -0.0962   -0.0960    0.0780   -0.0519
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   1      0.0000    0.0000   -1.5841    0.1200    0.0164    0.0640    0.1146    0.0965    0.0962    0.0960   -0.0780    0.0519

 Dipole mement (in D)   0.46 (DEN)      0.93      0.13      0.50      0.89      0.75      0.75      0.74      0.60      0.40

-----------------------------------------
File TZVPMol605.out
Molecule PMol605    iodine_monofluoride
 SP Mol605 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000    2.0661    2.0661
Quadrupole     -0.2003   -0.2003    0.4006    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  53      0.0000    0.0000    0.2805    0.3584    0.3252    0.1853    0.2694    0.2290    0.1989    0.5146    0.5767    0.1673
   9      0.0000    0.0000   -1.6519   -0.3584   -0.3252   -0.1854   -0.2695   -0.2292   -0.1989   -0.5146   -0.5766   -0.1673

 Dipole mement (in D)   2.07 (DEN)      3.33      3.02      1.72      2.50      2.13      1.85      4.78      5.35      1.55

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File TZVPMol606.out
Molecule PMol606    iodine_monochloride
 SP Mol606 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000    1.1669    1.1669
Quadrupole     -1.2860   -1.2860    2.5719    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  53      0.0000    0.0000    0.5644    0.1886    0.0644    0.0813    0.1133    0.1058    0.0902    0.2285    0.3125    0.0737
  17      0.0000    0.0000   -1.7596   -0.1886   -0.0644   -0.0814   -0.1135   -0.1059   -0.0902   -0.2285   -0.3125   -0.0737

 Dipole mement (in D)   1.17 (DEN)      2.10      0.72      0.91      1.27      1.18      1.01      2.55      3.49      0.82

-----------------------------------------
File TZVPMol607.out
Molecule PMol607    iodine_monobromide
 SP Mol607 B3LYP/Def2TZVP VAC.
    0    2
Dipole          0.0000    0.0000    0.7498    0.7498
Quadrupole     -1.9460   -1.9460    3.8921    0.0000    0.0000    0.0000
        Atomic coordinates (in A)        Mul.      Lowdin    Hirsch.   I-Hirsch  CM5       ESP       NPA       AIM       ACP
  53      0.0000    0.0000    0.9890    0.1218    0.0642    0.0411    0.0562    0.0515    0.0618    0.1321    0.1789    0.0478
  35      0.0000    0.0000   -1.4977   -0.1218   -0.0642   -0.0411   -0.0562   -0.0515   -0.0618   -0.1321   -0.1789   -0.0477

 Dipole mement (in D)   0.75 (DEN)      1.46      0.77      0.49      0.67      0.61      0.74      1.58      2.14      0.57

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File TZVPMol608.out
Molecule PMol608    cyanic_iodide
 SP Mol608 B3LYP/Def2TZVP VAC.
    0    3
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Dipole 0.0000 0.0000 3.8163 3.8163
Quadrupole 2.3832 2.3832 -4.7664 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	0.0000	0.0000	0.5141	0.2611	0.5195	0.1717	0.1805	0.2084	0.1998	0.3228	0.4339	0.1608
6	0.0000	0.0000	-1.4706	-0.2231	-0.5551	0.0224	0.1475	0.1082	0.1040	-0.0199	0.6768	0.1851
7	0.0000	0.0000	-2.6316	-0.0381	0.0356	-0.1941	-0.3280	-0.3166	-0.3038	-0.3029	-1.1107	-0.3459

Dipole mement (in D) 3.82 (DEN) 2.70 4.75 2.72 3.55 3.75 3.60 4.77 10.33 3.46

File TZVPMol609.out
Molecule PMol609 iodomethane
SP Mol609 B3LYP/Def2TZVP VAC.
0 5
Dipole -0.0002 -0.0087 1.6844 1.6844
Quadrupole -1.7503 -1.7501 3.5004 0.0001 0.0005 -0.0291

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	-0.0000	0.0018	-0.3262	-0.0469	0.2043	-0.0706	0.0003	-0.0563	-0.0484	0.0681	0.0192	-0.0955
6	0.0001	-0.0099	1.8066	-0.3925	-0.5250	-0.0665	-0.3977	-0.2336	-0.7657	-0.7180	-0.1912	-0.2135
1	0.8369	-0.6080	2.1459	0.1465	0.1069	0.0457	0.1325	0.0966	0.2717	0.2167	0.0573	0.1030
1	-0.9347	-0.4384	2.1467	0.1465	0.1069	0.0457	0.1325	0.0966	0.2711	0.2167	0.0573	0.1030
1	0.0979	1.0111	2.1547	0.1465	0.1069	0.0457	0.1325	0.0966	0.2713	0.2167	0.0573	0.1030

Dipole mement (in D) 1.68 (DEN) 1.20 1.57 0.95 0.65 1.05 1.84 0.37 0.09 1.49

File TZVPMol610.out
Molecule PMol610 iodoacetylene
SP Mol610 B3LYP/Def2TZVP VAC.
0 4
Dipole 0.0000 0.0000 0.1509 0.1509
Quadrupole -3.0943 -3.0943 6.1886 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	0.0000	0.0000	0.5334	0.1980	0.4786	0.0953	0.1600	0.1282	0.1658	0.3123	0.3663	0.0795
6	0.0000	0.0000	-1.4443	-0.2284	-0.4650	-0.0909	-0.1182	-0.1249	-0.2304	-0.3246	-0.3874	-0.0697
6	0.0000	0.0000	-2.6490	-0.1597	-0.1387	-0.0955	-0.2492	-0.1482	-0.1650	-0.2253	-0.1510	-0.1476
1	0.0000	0.0000	-3.7113	0.1901	0.1251	0.0911	0.2074	0.1449	0.2296	0.2376	0.1722	0.1378

Dipole mement (in D) 0.15 (DEN) 0.74 3.99 0.47 0.70 0.50 0.03 1.68 2.48 0.11

File TZVPMol611.out
Molecule PMol611 iodoethene
SP Mol611 B3LYP/Def2TZVP VAC.
0 6
Dipole 0.1490 -1.2456 0.0000 1.2545
Quadrupole 0.0503 3.6894 -3.7397 -0.6952 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP

53	0.0000	0.5780	0.0000	0.0161	0.3102	-0.0323	0.0049	-0.0089	-0.0243	0.1345	0.0995	-0.0630
6	0.4577	-1.4559	0.0000	-0.1637	-0.4526	-0.0381	-0.0921	-0.1188	-0.2801	-0.3574	-0.2675	-0.0551
6	-0.4407	-2.4248	0.0000	-0.2531	-0.2367	-0.0750	-0.2867	-0.1784	-0.2044	-0.3991	-0.0201	-0.1721
1	-0.1180	-3.4592	0.0000	0.1267	0.1286	0.0484	0.1307	0.1011	0.1387	0.2084	0.0514	0.0975
1	-1.5069	-2.2436	0.0000	0.1352	0.1236	0.0456	0.1269	0.0988	0.1512	0.2035	0.0560	0.0927
1	1.5225	-1.6454	0.0000	0.1388	0.1270	0.0515	0.1164	0.1063	0.2190	0.2101	0.0806	0.1000

Dipole mement (in D)	1.25 (DEN)	0.54	2.37	0.66	0.53	0.71	1.41	0.20	0.48	1.22	

File TZVPMol612.out
Molecule PMol612 iodoethane
SP Mol612 B3LYP/Def2TZVP VAC.
0 8
Dipole 0.3803 -1.9829 0.0000 2.0190
Quadrupole -1.2017 2.7007 -1.4990 -1.3165 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	0.0000	0.6389	0.0000	-0.0801	0.2068	-0.0822	-0.0489	-0.0662	-0.1469	0.0331	-0.0235	-0.1174
6	0.6010	-1.4349	0.0000	-0.2310	-0.4762	-0.0239	-0.1279	-0.1508	-0.1803	-0.4661	-0.1409	-0.0983
6	-0.5731	-2.3771	0.0000	-0.3144	-0.3421	-0.0834	-0.3749	-0.2357	0.0156	-0.6223	0.0314	-0.2391
1	-0.2188	-3.4096	0.0000	0.1128	0.1236	0.0382	0.1188	0.0894	0.0283	0.2120	0.0096	0.0912
1	-1.2005	-2.2421	0.8788	0.1230	0.1214	0.0345	0.1142	0.0865	0.0258	0.2108	0.0165	0.0863
1	-1.2005	-2.2421	-0.8788	0.1230	0.1214	0.0345	0.1142	0.0865	0.0258	0.2108	0.0165	0.0863
1	1.2262	-1.5474	-0.8807	0.1334	0.1225	0.0412	0.1023	0.0952	0.1158	0.2109	0.0455	0.0956
1	1.2262	-1.5474	0.8807	0.1334	0.1225	0.0412	0.1023	0.0952	0.1158	0.2109	0.0454	0.0956

Dipole mement (in D)	2.02 (DEN)	1.56	1.46	1.14	1.01	1.24	2.18	0.75	0.67	1.77	

File TZVPMol613.out
Molecule PMol613 iodopropane
SP Mol613 B3LYP/Def2TZVP VAC.
0 11
Dipole -0.2978 -2.1002 0.0000 2.1212
Quadrupole -0.7839 1.7562 -0.9723 0.7111 0.0000 0.0000

Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0821	-3.4182	0.0000	-0.3324	-0.3041	-0.0800	-0.3266	-0.2318	-0.2742	-0.5863	0.0091	-0.2453
6	0.5609	-1.9755	0.0000	-0.1575	-0.3330	-0.0477	-0.1550	-0.1615	0.4405	-0.4172	0.0700	-0.1317
1	0.9200	-4.1130	0.0000	0.1192	0.1212	0.0358	0.1103	0.0872	0.0535	0.2117	0.0072	0.0897
1	-0.5252	-3.6371	0.8783	0.1071	0.1181	0.0306	0.1026	0.0824	0.0618	0.1981	-0.0031	0.0830
1	-0.5252	-3.6371	-0.8783	0.1071	0.1181	0.0306	0.1026	0.0824	0.0618	0.1981	-0.0031	0.0830
6	-0.6071	-1.0171	0.0000	-0.2382	-0.4540	-0.0272	-0.1672	-0.1524	-0.4465	-0.4676	-0.1519	-0.1046
1	1.1910	-1.7882	0.8711	0.1054	0.1353	0.0307	0.0916	0.0859	-0.0575	0.1998	0.0047	0.0789
1	1.1910	-1.7882	-0.8711	0.1054	0.1353	0.0307	0.0916	0.0859	-0.0575	0.1998	0.0047	0.0789
1	-1.2336	-1.1348	-0.8809	0.1304	0.1241	0.0395	0.1025	0.0941	0.1722	0.2099	0.0420	0.0925
1	-1.2336	-1.1348	0.8809	0.1304	0.1241	0.0395	0.1025	0.0941	0.1722	0.2099	0.0420	0.0925
53	0.0000	1.0509	0.0000	-0.0769	0.2149	-0.0822	-0.0546	-0.0661	-0.1262	0.0438	-0.0216	-0.1167

Dipole mement (in D) 2.12 (DEN) 1.62 1.30 1.26 1.11 1.37 2.27 0.78 0.79 1.87

File TZVPMol614.out
Molecule PMol614 iodobenzene
SP Mol614 B3LYP/Def2TZVP VAC.
0 12
Dipole 0.0000 0.0000 -1.6475 1.6475
Quadrupole -6.3643 2.2018 4.1624 0.0000 0.0000 0.0000

	Atomic coordinates (in A)			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-3.3278	-0.1152	-0.1372	-0.0367	-0.0972	-0.0928	0.0080	-0.2085	-0.0210	-0.0815
6	0.0000	1.1999	-2.6308	-0.0858	-0.1327	-0.0326	-0.0716	-0.0885	-0.2591	-0.1914	-0.0200	-0.0773
6	0.0000	1.2074	-1.2425	-0.2065	-0.1516	-0.0412	-0.1590	-0.0962	0.1592	-0.2383	0.0025	-0.0821
6	0.0000	0.0000	-0.5542	0.1177	-0.3622	-0.0039	0.0793	-0.0344	-0.2661	-0.1477	-0.2385	0.0379
6	0.0000	-1.2074	-1.2425	-0.2065	-0.1516	-0.0412	-0.1590	-0.0962	0.1592	-0.2383	0.0025	-0.0821
6	0.0000	-1.1999	-2.6308	-0.0858	-0.1327	-0.0326	-0.0716	-0.0885	-0.2591	-0.1914	-0.0200	-0.0773
1	0.0000	0.0000	-4.4099	0.1152	0.1440	0.0441	0.0983	0.1002	0.0996	0.2120	0.0358	0.0887
1	0.0000	2.1410	-3.1660	0.1158	0.1455	0.0455	0.1005	0.1016	0.1399	0.2131	0.0379	0.0900
1	0.0000	2.1446	-0.7026	0.1293	0.1462	0.0427	0.1027	0.0996	0.0585	0.2180	0.0487	0.0848
1	0.0000	-2.1446	-0.7026	0.1293	0.1462	0.0427	0.1027	0.0996	0.0585	0.2180	0.0487	0.0848
1	0.0000	-2.1410	-3.1660	0.1158	0.1455	0.0455	0.1005	0.1016	0.1399	0.2131	0.0379	0.0900
53	0.0000	0.0000	1.5456	-0.0233	0.3404	-0.0323	-0.0256	-0.0060	-0.0386	0.1414	0.0856	-0.0761

Dipole mement (in D) 1.65 (DEN) 0.85 2.38 0.93 0.97 0.97 1.82 0.01 0.16 1.62