

Supporting Information:

A simple model for calculating atomic charges in molecules

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Atomic charges in a.u.

Keywords:

File mol171.out

Molecule 171 LiF

SP Mol171 B3LYP/Def2TZVP VAC.

0 2

Dipole	0.0000	0.0000	-6.0320	6.0320								
Quadrupole	-1.9682	-1.9682	3.9364	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	0.3845	-0.7486	-0.6059	-0.5793	-0.9426	-0.7334	-0.8202	-0.9463	-0.9016	-0.6696
3	0.0000	0.0000	-1.1534	0.7486	0.6059	0.5794	0.9427	0.7334	0.8202	0.9463	0.9016	0.6696
Dipole moment (in D)	6.03 (DEN)		5.53	4.48	4.28	6.96	5.42	6.06	6.99	6.66	4.95	

File mol173.out

Molecule 173 LiS

SP Mol173 B3LYP/Def2TZVP VAC.

0 2

Dipole	0.0000	0.0000	-6.8056	6.8056								
Quadrupole	-6.0599	-2.7003	8.7602	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0000	0.0000	-1.7869	0.6526	0.3818	0.4678	0.8706	0.5647	0.6747	0.8692	0.8854	0.6657
16	0.0000	0.0000	0.3350	-0.6526	-0.3818	-0.4678	-0.8706	-0.5647	-0.6747	-0.8692	-0.8854	-0.6657
Dipole moment (in D)	6.81 (DEN)		6.65	3.89	4.77	8.87	5.76	6.88	8.86	9.02	6.78	

File mol174.out

Molecule 174 LiCl

SP Mol174 B3LYP/Def2TZVP VAC.

0 2

Dipole	0.0000	0.0000	-6.8593	6.8593								
Quadrupole	-4.4275	-4.4275	8.8549	0.0000	0.0000	0.0000						

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	0.2998	-0.6940	-0.4337	-0.5235	-0.9139	-0.6171	-0.7256	-0.9174	-0.9005	-0.6616
3	0.0000	0.0000	-1.6988	0.6940	0.4337	0.5236	0.9139	0.6171	0.7256	0.9174	0.9005	0.6616
Dipole moment (in D)			6.86 (DEN)	6.66	4.16	5.03	8.77	5.92	6.97	8.81	8.64	6.35

File mol175.out

Molecule 175 LiBr

SP Mol175 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -7.0857 7.0857

Quadrupole -6.0118 -6.0118 12.0235 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.0000	0.1714	-0.7036	-0.4222	-0.4985	-0.8953	-0.5640	-0.7197	-0.9063	-0.9002	-0.6552
3	0.0000	0.0000	-2.0001	0.7036	0.4222	0.4985	0.8953	0.5640	0.7197	0.9063	0.9002	0.6552
Dipole moment (in D)			7.09 (DEN)	7.34	4.40	5.20	9.34	5.88	7.51	9.45	9.39	6.83

File mol176.out

Molecule 176 LiI

SP Mol176 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -7.3360 7.3360

Quadrupole -7.6552 -7.6552 15.3105 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	0.0000	0.0000	0.1299	-0.6768	-0.3982	-0.4844	-0.8583	-0.5237	-0.6630	-0.8794	-0.8930	-0.6263
3	0.0000	0.0000	-2.2957	0.6768	0.3982	0.4844	0.8583	0.5237	0.6630	0.8794	0.8930	0.6263
Dipole moment (in D)			7.34 (DEN)	7.89	4.64	5.64	10.00	6.10	7.72	10.25	10.40	7.30

File mol177.out

Molecule 177 LiOH

SP Mol177 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 -4.1086 4.1086

Quadrupole -3.5328 -3.5328 7.0656 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0000	0.0000	-1.2507	0.6971	0.5367	0.5091	1.0046	0.7125	0.8813	0.9520	0.8907	0.6227
8	0.0000	0.0000	0.3119	-0.9726	-0.6469	-0.6028	-1.4481	-0.9801	-1.4385	-1.4035	-1.4380	-0.7979
1	0.0000	0.0000	1.2571	0.2755	0.1102	0.0937	0.4436	0.2676	0.5571	0.4515	0.5473	0.1752

Dipole moment (in D) 4.11 (DEN) 3.98 3.53 3.40 5.53 4.13 4.09 5.09 4.20 3.88

File mol178.out

Molecule 178 LiSH

SP Mol178 B3LYP/Def2TZVP VAC.

0 3

Dipole -0.4854 6.7189 0.0000 6.7364

Quadrupole -2.3789 8.8418 -6.4629 1.3129 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0665	1.8049	0.0000	0.6484	0.4144	0.4797	0.8970	0.5777	0.6770	0.8860	0.8884	0.6882
16	0.0665	-0.3105	0.0000	-0.7598	-0.4263	-0.4875	-1.0239	-0.6516	-0.7838	-1.0089	-0.7986	-0.7572
1	-1.2641	-0.4464	0.0000	0.1114	0.0120	0.0078	0.1269	0.0739	0.1068	0.1229	-0.0900	0.0690

Dipole moment (in D) 6.74 (DEN) 6.55 4.20 4.87 9.07 5.84 6.84 8.96 9.10 6.96

File mol179.out

Molecule 179 LiNH2

SP Mol179 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 -4.3874 0.0000 4.3874

Quadrupole -5.5834 6.8758 -1.2924 0.0001 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.0000	0.3208	0.0000	-1.0516	-0.7228	-0.5433	-1.5132	-1.1370	-1.8728	-1.5885	-1.4663	-1.0213
1	0.0000	0.9505	0.7931	0.1857	0.1054	0.0335	0.2907	0.2166	0.4887	0.3305	0.2882	0.1622

1	0.0000	0.9505	-0.7931	0.1857	0.1054	0.0335	0.2907	0.2166	0.4887	0.3305	0.2882	0.1622
3	-0.0000	-1.3823	0.0000	0.6802	0.5120	0.4763	0.9318	0.7039	0.8954	0.9274	0.8899	0.6970
Dipole moment (in D)		4.39 (DEN)	4.44	3.55	3.69	5.86	4.45	4.37	5.59	5.54	4.72	

File mol180.out

Molecule 180 LiCH3

SP Mol180 B3LYP/Def2TZVP VAC.

0 5

Dipole 0.0005 -5.5158 0.0000 5.5158

Quadrupole -3.3257 6.6514 -3.3258 -0.0006 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.0000	0.3690	0.0000	-1.0335	-0.8202	-0.4131	-1.2522	-0.6143	-1.6489	-1.4301	-0.7181	-0.6889
1	-1.0021	0.8182	0.0000	0.1019	0.0864	-0.0250	0.1176	0.0224	0.2826	0.1903	-0.0565	0.0086
1	0.5012	0.8178	0.8679	0.1019	0.0864	-0.0250	0.1176	0.0224	0.2894	0.1903	-0.0565	0.0086
1	0.5012	0.8178	-0.8679	0.1019	0.0864	-0.0250	0.1176	0.0224	0.2894	0.1903	-0.0565	0.0086
3	-0.0000	-1.5560	0.0000	0.7278	0.5612	0.4880	0.8995	0.5472	0.7875	0.8591	0.8876	0.6630

Dipole moment (in D)		5.52 (DEN)	6.07	4.63	4.67	7.56	4.91	5.42	6.71	8.57	6.07	
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File mol181.out

Molecule 181 LiCH3O

SP Mol181 B3LYP/Def2TZVP VAC.

0 6

Dipole -3.3690 1.2242 0.0000 3.5845

Quadrupole -2.5637 5.0621 -2.4984 -5.1102 -0.0002 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	-0.6331	1.3682	0.0000	0.7189	0.5075	0.4304	0.9700	0.6246	0.7851	0.8878	0.8879	0.6154
6	0.8197	0.1315	0.0000	-0.6030	-0.6474	-0.2752	-0.7939	-0.4200	-1.4886	-0.7378	-0.1964	-0.4321
8	-0.6176	-0.3706	-0.0000	-0.5846	-0.1709	-0.2784	-0.8386	-0.6152	-0.5111	-0.8902	-1.1730	-0.4829
1	-0.6884	-1.3236	-0.0000	0.3078	0.1565	0.1582	0.4678	0.3314	0.4288	0.4716	0.5689	0.2611
1	1.3050	-0.3027	-0.8805	0.0804	0.0771	-0.0175	0.0973	0.0396	0.3929	0.1343	-0.0438	0.0193
1	1.3050	-0.3027	0.8805	0.0804	0.0771	-0.0175	0.0973	0.0396	0.3929	0.1343	-0.0438	0.0193

Dipole moment (in D) 3.58 (DEN) 4.27 3.73 3.19 5.68 3.57 3.46 4.56 4.94 4.01

File mol182.out

Molecule 182 LiOCH3

SP Mol182 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0008 5.0398 0.0000 5.0398

Quadrupole -5.0614 10.1226 -5.0612 0.0019 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0002	2.0129	0.0000	0.7015	0.5517	0.5283	0.9725	0.7329	0.7973	0.9423	0.8851	0.6372
8	0.0000	0.4417	0.0000	-0.8166	-0.3235	-0.4905	-1.1985	-0.7482	-1.0256	-1.1104	-1.3862	-0.6491
6	-0.0001	-0.9188	0.0000	-0.0654	-0.4732	-0.0392	0.1712	-0.1573	0.4448	-0.2041	0.6369	-0.1164
1	-0.5078	-1.3530	0.8795	0.0602	0.0817	0.0005	0.0183	0.0575	-0.0728	0.1241	-0.0453	0.0428
1	-0.5078	-1.3530	-0.8795	0.0602	0.0817	0.0005	0.0183	0.0575	-0.0728	0.1241	-0.0453	0.0428
1	1.0155	-1.3531	0.0000	0.0602	0.0817	0.0005	0.0183	0.0575	-0.0710	0.1241	-0.0453	0.0428

Dipole moment (in D) 5.04 (DEN) 4.16 5.14 4.23 5.75 5.07 4.98 5.24 3.69 4.46

File mol183.out

Molecule 183 LiC2H

SP Mol183 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 -5.9091 5.9091

Quadrupole -7.4084 -7.4084 14.8167 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-0.2512	-0.4708	-0.4232	-0.4078	-1.0371	-0.4798	-0.9912	-0.7503	-0.5280	-0.5391
6	0.0000	0.0000	0.9723	-0.4848	-0.2509	-0.1792	-0.0683	-0.2331	0.0015	-0.3855	-0.5011	-0.2266
3	0.0000	0.0000	-2.1218	0.8123	0.5684	0.5286	0.9520	0.6015	0.8379	0.9329	0.9140	0.6644
1	0.0000	0.0000	2.0388	0.1433	0.1056	0.0583	0.1534	0.1114	0.1518	0.2029	0.1150	0.1013

Dipole moment (in D) 5.91 (DEN) 8.57 5.42 5.16 7.27 5.55 5.85 8.42 9.89 6.19

File mol185.out

Molecule 185 LiC3H5

SP Mol185 B3LYP/Def2TZVP VAC.

0 9

Dipole 0.1633 3.5699 0.0000 3.5736

Quadrupole 0.3797 5.0405 -5.4202 2.0662 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.1428	-0.0773	1.2441	-0.6357	-0.4175	-0.2212	-0.7937	-0.3668	-1.3744	-0.8304	-0.3748	-0.3931
6	-0.4034	-0.3894	0.0000	-0.0241	-0.3001	-0.0607	0.0413	-0.1704	0.8135	-0.2332	-0.1064	-0.1210
6	0.1428	-0.0773	-1.2441	-0.6357	-0.4175	-0.2212	-0.7937	-0.3668	-1.3744	-0.8304	-0.3749	-0.3931
1	-0.3649	-0.3610	-2.1534	0.1053	0.1142	0.0144	0.1386	0.0672	0.3163	0.2099	0.0095	0.0553
1	1.2267	0.0136	-1.3307	0.1411	0.1249	0.0142	0.1098	0.0671	0.3359	0.1839	-0.0265	0.0404
1	-1.4454	-0.7087	0.0000	0.0911	0.1505	0.0404	0.1102	0.0961	-0.0424	0.1994	0.0138	0.0773
1	-0.3649	-0.3610	2.1534	0.1053	0.1142	0.0144	0.1386	0.0672	0.3163	0.2099	0.0095	0.0553
1	1.2267	0.0136	1.3307	0.1411	0.1249	0.0142	0.1098	0.0671	0.3359	0.1839	-0.0265	0.0404
3	0.1428	1.5557	0.0000	0.7116	0.5064	0.4056	0.9392	0.5393	0.6734	0.9070	0.8765	0.6383

Dipole moment (in D) 3.57 (DEN) 5.19 3.78 3.12 6.71 4.07 3.62 6.45 6.94 4.84

File mol186.out

Molecule 186 LiC2H2F

SP Mol186 B3LYP/Def2TZVP VAC.

0 6

Dipole -3.5323 2.3485 0.0013 4.2418

Quadrupole 7.1852 -2.1887 -4.9965 -7.6466 -0.0014 0.0014

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.2159	0.5484	-0.0002	-0.2419	-0.3150	-0.1753	-0.4997	-0.2417	-0.6910	-0.1801	-0.2212	-0.2402
6	1.3818	-0.0609	0.0001	-0.3463	-0.2949	-0.1275	-0.2738	-0.2261	0.0111	-0.5893	-0.1015	-0.2300
3	-1.6091	1.0143	0.0002	0.7851	0.5407	0.4837	0.9368	0.6462	0.7581	0.9266	0.9077	0.6468
9	-0.9498	-0.6005	-0.0000	-0.4228	-0.1831	-0.2635	-0.4423	-0.3678	-0.2778	-0.5832	-0.6848	-0.3430
1	1.5274	-1.1333	0.0002	0.1152	0.1215	0.0431	0.1441	0.0967	0.1062	0.2111	0.0582	0.0835
1	2.2624	0.5696	0.0001	0.1106	0.1309	0.0394	0.1349	0.0927	0.0935	0.2150	0.0418	0.0829

Dipole moment (in D) 4.24 (DEN) 6.25 3.93 3.81 6.55 4.75 4.16 7.12 6.87 4.99

File mol188.out

Molecule 188 LiC2H6N

SP Mol188 B3LYP/Def2TZVP VAC.

0 10

Dipole -0.0001 5.4372 0.0000 5.4372

Quadrupole -4.7788 11.0431 -6.2643 -0.0002 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	-0.0000	2.1218	-0.0000	0.6824	0.5390	0.4943	0.9166	0.7296	0.7874	0.9188	0.8834	0.7090
7	-0.0000	0.4062	-0.0000	-0.7492	-0.2701	-0.3756	-1.1500	-0.7865	-0.9590	-1.0026	-1.3297	-0.7479
6	-1.1665	-0.4284	0.0000	-0.1681	-0.4096	-0.0698	0.0287	-0.1583	-0.0239	-0.3981	0.3658	-0.1392
6	1.1665	-0.4284	0.0000	-0.1681	-0.4096	-0.0698	0.0287	-0.1583	-0.0348	-0.3981	0.3660	-0.1392
1	1.2284	-1.0988	-0.8790	0.0720	0.0893	-0.0000	0.0286	0.0583	0.0497	0.1402	-0.0447	0.0503
1	1.2284	-1.0987	0.8790	0.0720	0.0893	-0.0000	0.0286	0.0583	0.0497	0.1402	-0.0447	0.0503
1	2.0892	0.1636	-0.0000	0.0574	0.0965	0.0106	0.0309	0.0703	0.0204	0.1595	-0.0533	0.0581
1	-1.2284	-1.0988	-0.8790	0.0720	0.0893	-0.0000	0.0286	0.0583	0.0454	0.1402	-0.0447	0.0503
1	-2.0892	0.1636	-0.0000	0.0574	0.0965	0.0106	0.0309	0.0703	0.0198	0.1595	-0.0533	0.0581
1	-1.2284	-1.0988	0.8790	0.0720	0.0893	-0.0000	0.0286	0.0583	0.0454	0.1402	-0.0447	0.0503

Dipole moment (in D) 5.44 (DEN) 4.75 4.92 4.61 6.42 5.43 5.30 6.34 5.76 5.37

File Lix_9.out

Molecule _9 (CH3)HNLi

SP Lix_9 B3LYP/Def2TZVP VAC.

0 7

Dipole 4.5444 -1.8936 -0.0007 4.9231

Quadrupole 8.0511 -1.3505 -6.7006 -4.7098 -0.0007 -0.0008

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.4530	0.3134	0.0001	-0.9007	-0.4734	-0.4563	-1.3220	-0.9417	-1.6570	-1.2885	-1.3857	-0.8852
6	-0.9204	-0.1598	-0.0000	-0.1515	-0.4355	-0.0741	0.0500	-0.1670	0.7977	-0.3841	0.3641	-0.1370
3	1.9597	-0.5387	-0.0001	0.6696	0.5229	0.4825	0.9137	0.7007	0.8415	0.9172	0.8846	0.6967
1	0.4271	1.3290	-0.0002	0.1736	0.1219	0.0413	0.2724	0.2279	0.4538	0.3197	0.2764	0.1629

1	-1.5048	0.1548	0.8819	0.0760	0.0855	-0.0009	0.0273	0.0562	-0.1552	0.1424	-0.0448	0.0524
1	-0.9450	-1.2569	0.0003	0.0571	0.0932	0.0083	0.0314	0.0677	-0.1255	0.1510	-0.0496	0.0579
1	-1.5045	0.1542	-0.8823	0.0760	0.0855	-0.0009	0.0273	0.0562	-0.1553	0.1424	-0.0448	0.0524

Dipole moment (in D) 4.92 (DEN) 4.53 4.62 4.27 6.20 5.03 4.90 6.06 5.79 5.08

File Lix_10.out

Molecule_10 (CH3)2NLi

SP Lix_10 B3LYP/Def2TZVP VAC.

0 10

Dipole 0.0070 5.4907 0.0000 5.4907

Quadrupole -6.3651 11.2374 -4.8723 0.0181 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.0002	0.3998	0.0000	-0.7539	-0.2779	-0.3756	-1.1471	-0.7709	-1.0212	-1.0025	-1.3221	-0.7468
3	0.0018	2.1394	0.0000	0.6803	0.5414	0.4938	0.9128	0.7154	0.7941	0.9171	0.8838	0.7065
6	-0.0002	-0.4312	1.1788	-0.1653	-0.4065	-0.0703	0.0262	-0.1593	0.0507	-0.3991	0.3568	-0.1394
6	-0.0002	-0.4312	-1.1788	-0.1653	-0.4065	-0.0703	0.0262	-0.1593	0.0507	-0.3991	0.3567	-0.1394
1	0.8821	-1.0981	1.2392	0.0723	0.0892	0.0002	0.0295	0.0583	0.0298	0.1409	-0.0431	0.0506
1	-0.8830	-1.0974	1.2398	0.0723	0.0892	0.0002	0.0295	0.0583	0.0305	0.1409	-0.0431	0.0506
1	0.0003	0.1746	2.0936	0.0575	0.0965	0.0109	0.0320	0.0705	0.0025	0.1599	-0.0513	0.0584
1	0.8821	-1.0981	-1.2392	0.0723	0.0892	0.0002	0.0295	0.0583	0.0298	0.1409	-0.0431	0.0506
1	-0.8830	-1.0974	-1.2398	0.0723	0.0892	0.0002	0.0295	0.0583	0.0305	0.1409	-0.0431	0.0506
1	0.0003	0.1746	-2.0936	0.0575	0.0965	0.0109	0.0320	0.0705	0.0025	0.1599	-0.0513	0.0584

Dipole moment (in D) 5.49 (DEN) 4.80 4.99 4.66 6.50 5.42 5.36 6.45 5.89 5.43

File Lix_11.out

Molecule_11 CH3-OLi

SP Lix_11 B3LYP/Def2TZVP VAC.

0 6

Dipole -0.0180 4.9815 0.0000 4.9815

Quadrupole -5.1054 10.2106 -5.1052 -0.0445 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
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8	0.0000	0.4459	0.0000	-0.8215	-0.3398	-0.4948	-1.2021	-0.7488	-1.0129	-1.1168	-1.3713	-0.6497
6	0.0016	-0.9301	0.0000	-0.0670	-0.4587	-0.0386	0.1611	-0.1578	0.3993	-0.2077	0.6085	-0.1201
1	0.5120	-1.3504	0.8833	0.0631	0.0827	0.0025	0.0232	0.0596	-0.0591	0.1274	-0.0408	0.0452
1	0.5120	-1.3504	-0.8833	0.0631	0.0827	0.0025	0.0232	0.0596	-0.0591	0.1274	-0.0408	0.0452
1	-1.0178	-1.3521	0.0000	0.0630	0.0826	0.0025	0.0231	0.0596	-0.0612	0.1274	-0.0408	0.0451
3	-0.0053	2.0221	0.0000	0.6994	0.5505	0.5259	0.9716	0.7278	0.7929	0.9423	0.8849	0.6344

Dipole moment (in D) 4.98 (DEN) 4.11 5.06 4.17 5.69 5.01 4.91 5.21 3.73 4.43

File Lix_16.out

Molecule_16 LiS
SP Lix_16 B3LYP/Def2TZVP VAC.
0 2

Dipole	0.0000	0.0000	-6.8900	6.8900								
Quadrupole	-2.8074	-6.1682	8.9756	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0000	0.0000	-1.8091	0.6512	0.3891	0.4698	0.8679	0.5606	0.6751	0.8675	0.8859	0.6647
16	0.0000	0.0000	0.3392	-0.6512	-0.3891	-0.4698	-0.8679	-0.5606	-0.6751	-0.8675	-0.8859	-0.6647

Dipole moment (in D) 6.89 (DEN) 6.72 4.02 4.85 8.96 5.78 6.97 8.95 9.14 6.86

File Lix_17.out

Molecule_17 Li+_CH3
SP Lix_17 B3LYP/Def2TZVP VAC.
1 5

Dipole	0.0000	-6.5762	0.0000	6.5762								
Quadrupole	-4.6088	9.2165	-4.6077	-0.0002	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0000	-1.7424	0.0000	0.9321	0.8370	0.7767	0.9860	0.8006	0.8726	0.9770	0.9552	0.8662
6	0.0000	0.5379	0.0000	-0.5748	-0.2161	-0.0204	-0.5040	-0.1907	-0.4849	-0.5898	-0.2901	-0.2564
1	-1.0772	0.6666	0.0000	0.2142	0.1264	0.0812	0.1726	0.1300	0.2029	0.2042	0.1117	0.1301
1	0.5385	0.6667	0.9330	0.2142	0.1264	0.0812	0.1727	0.1301	0.2047	0.2043	0.1117	0.1301
1	0.5385	0.6667	-0.9330	0.2142	0.1264	0.0812	0.1727	0.1301	0.2047	0.2043	0.1117	0.1301

Dipole moment (in D) 6.58 (DEN) 7.23 6.35 5.77 7.89 5.94 6.60 7.74 7.67 6.66

File Lix_18.out

Molecule_18 Li+_C2H5

SP Lix_18 B3LYP/Def2TZVP VAC.

1 8

Dipole -7.4487 -2.8470 0.0000 7.9742

Quadrupole 12.2743 -4.8109 -7.4634 7.1539 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.9260	-0.2696	0.0000	-0.2951	-0.3198	-0.0556	-0.3891	-0.2064	-0.0975	-0.6954	-0.0101	-0.2282
6	-0.3129	0.5416	-0.0000	-0.5615	-0.2303	-0.0300	-0.3566	-0.1657	-0.3402	-0.4345	-0.2810	-0.1984
1	-0.6291	1.0271	0.9224	0.2158	0.1389	0.0664	0.1324	0.1178	0.1369	0.2010	0.0719	0.1083
1	1.0399	-0.8837	-0.8950	0.1520	0.1405	0.0616	0.1500	0.1127	0.0578	0.2354	0.0503	0.1119
1	1.0399	-0.8836	0.8950	0.1520	0.1405	0.0616	0.1500	0.1127	0.0578	0.2354	0.0503	0.1119
1	1.7910	0.4168	-0.0000	0.1922	0.1719	0.0851	0.2016	0.1351	0.1803	0.2819	0.0980	0.1364
1	-0.6291	1.0271	-0.9224	0.2158	0.1389	0.0664	0.1324	0.1178	0.1369	0.2010	0.0719	0.1083
3	-2.0970	-0.7786	0.0000	0.9288	0.8194	0.7444	0.9792	0.7759	0.8681	0.9753	0.9488	0.8499

Dipole moment (in D) 7.97 (DEN) 8.62 7.78 7.20 9.36 7.38 7.87 9.32 9.09 8.21

File Lix_19.out

Molecule_19 Li+_C2H3

SP Lix_19 B3LYP/Def2TZVP VAC.

1 6

Dipole -6.0426 -2.7364 1.0252 6.7121

Quadrupole 9.6137 -2.2690 -7.3447 4.7153 -0.7541 0.6715

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.7591	-0.3025	0.0133	-0.2156	-0.1649	0.0079	-0.2312	-0.1000	-0.1900	-0.4430	-0.0470	-0.1178
6	-0.1617	0.6131	-0.1501	-0.3419	-0.1203	-0.0230	-0.3469	-0.1125	-0.2921	-0.2679	-0.3399	-0.1432
1	0.8678	-1.1711	-0.6349	0.2072	0.1612	0.0936	0.1778	0.1455	0.2055	0.2429	0.1172	0.1383
1	1.4927	-0.2251	0.8218	0.2055	0.1711	0.1023	0.2091	0.1537	0.2011	0.2628	0.1445	0.1513
1	-0.3515	1.6219	0.1980	0.2352	0.1569	0.1064	0.2160	0.1581	0.2473	0.2306	0.1772	0.1519

3	-1.8645	-0.6963	0.1452	0.9097	0.7959	0.7127	0.9751	0.7553	0.8282	0.9746	0.9478	0.8196
Dipole moment (in D)	6.71 (DEN)	7.60	6.63	5.90	8.33	6.19	6.73	8.41	8.10	6.90		

File Lix_21.out

Molecule _21 Li+_propene

SP Lix_21 B3LYP/Def2TZVP VAC.

1 10

Dipole 5.2260 5.8154 0.2246 7.8218

Quadrupole 4.8699 2.3261 -7.1960 10.2802 -0.1922 -0.0423

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.0438	-0.5356	-0.2175	-0.6084	-0.2520	-0.0808	-0.5479	-0.2125	-0.4039	-0.5894	-0.2456	-0.2473
6	-0.0770	-0.2134	0.4491	-0.1212	-0.1887	0.0335	0.0647	-0.0467	0.1573	-0.1258	-0.0802	-0.0273
6	-1.3867	0.1437	-0.1679	-0.2979	-0.2624	-0.0572	-0.4207	-0.2054	-0.4195	-0.6636	-0.0039	-0.2336
1	-1.3333	0.2176	-1.2540	0.1379	0.1367	0.0563	0.1471	0.1084	0.1300	0.2245	0.0403	0.1065
1	-1.7916	1.0716	0.2447	0.1479	0.1412	0.0599	0.1435	0.1110	0.1166	0.2360	0.0457	0.1099
1	-2.1159	-0.6323	0.0853	0.1803	0.1585	0.0757	0.1816	0.1271	0.2251	0.2651	0.0834	0.1283
1	-0.0620	-0.2700	1.5367	0.1918	0.1645	0.0716	0.1264	0.1268	0.0667	0.2197	0.0716	0.1155
1	1.9165	-0.9165	0.3068	0.2310	0.1513	0.0698	0.1584	0.1224	0.1434	0.2335	0.0715	0.1107
1	1.0554	-0.5978	-1.3033	0.2238	0.1507	0.0684	0.1658	0.1214	0.1644	0.2261	0.0704	0.1097
3	1.6166	1.5865	0.0005	0.9149	0.8000	0.7027	0.9810	0.7475	0.8199	0.9737	0.9465	0.8275

Dipole moment (in D)	7.82 (DEN)	8.71	7.80	6.91	9.57	7.28	7.64	9.54	9.27	8.16		
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File Lix_22.out

Molecule _22 Li+_propyne

SP Lix_22 B3LYP/Def2TZVP VAC.

1 8

Dipole -4.5135 5.8558 0.0000 7.3934

Quadrupole 7.0878 3.2372 -10.3251 -8.6483 0.0001 -0.0001

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-1.1780	-0.5479	-0.0000	-0.2825	-0.1098	-0.0769	-0.5385	-0.1613	-0.6812	-0.4027	-0.2392	-0.1973
6	-0.0117	-0.2315	0.0000	-0.0557	-0.1049	0.0340	0.1626	-0.0008	0.3053	0.0387	-0.2771	0.0175

1	-2.1413	-1.0127	0.0000	0.2641	0.1657	0.1280	0.2745	0.1813	0.3981	0.2836	0.2243	0.1736
6	1.4100	0.0821	-0.0000	-0.3776	-0.2371	-0.0283	-0.4337	-0.1731	-0.4480	-0.7020	0.0634	-0.2041
1	1.7021	0.6393	-0.8916	0.1756	0.1558	0.0772	0.1733	0.1288	0.1571	0.2588	0.0835	0.1273
1	1.7018	0.6410	0.8906	0.1755	0.1558	0.0772	0.1733	0.1288	0.1570	0.2587	0.0835	0.1273
1	1.9660	-0.8589	0.0010	0.1996	0.1728	0.0922	0.2077	0.1441	0.2592	0.2862	0.1173	0.1439
3	-1.5168	1.5916	-0.0000	0.9010	0.8018	0.6967	0.9808	0.7522	0.8525	0.9788	0.9445	0.8118

Dipole moment (in D) 7.39 (DEN) 8.51 7.31 6.38 9.00 6.82 7.30 9.16 8.65 7.49

File Lix_26.out

Molecule_26 Li(NH3)+
SP Lix_26 B3LYP/Def2TZVP VAC.

1 5

Dipole 0.0000 4.5558 0.0000 4.5558

Quadrupole -3.9101 7.8196 -3.9094 -0.0003 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	-0.0000	1.6043	0.0000	0.9176	0.7931	0.7368	0.9987	0.8555	0.9308	0.9808	0.9494	0.8715
7	-0.0000	-0.3589	0.0000	-0.8036	-0.3183	-0.1968	-1.2038	-0.8546	-1.2277	-1.1867	-1.1614	-0.7040
1	0.9346	-0.7669	0.0000	0.2953	0.1751	0.1533	0.4017	0.3330	0.4310	0.4020	0.4040	0.2775
1	-0.4673	-0.7669	0.8095	0.2953	0.1751	0.1533	0.4017	0.3330	0.4330	0.4020	0.4040	0.2775
1	-0.4673	-0.7669	-0.8095	0.2953	0.1751	0.1533	0.4017	0.3330	0.4330	0.4020	0.4040	0.2775

Dipole moment (in D) 4.56 (DEN) 5.19 4.73 4.32 5.33 4.39 4.51 5.16 4.85 4.86

File Lix_27.out

Molecule_27 Li+_N(CH3)H2
SP Lix_27 B3LYP/Def2TZVP VAC.

1 8

Dipole 5.9658 2.7148 0.0000 6.5545

Quadrupole 9.6470 -3.6022 -6.0448 4.9510 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	1.9520	0.7102	0.0000	0.9079	0.7828	0.7145	0.9952	0.8409	0.9019	0.9798	0.9465	0.8611
7	0.0000	0.5890	0.0000	-0.6954	-0.1963	-0.1732	-1.0282	-0.7395	-1.0270	-0.9683	-1.1242	-0.6315

6	-0.5212	-0.8146	0.0000	-0.2643	-0.3215	-0.0055	-0.1190	-0.1125	0.2542	-0.4159	0.2633	-0.1123
1	-0.3992	1.0741	0.8024	0.2812	0.1798	0.1411	0.3739	0.3256	0.3901	0.3878	0.3820	0.2619
1	-0.3992	1.0741	-0.8024	0.2812	0.1798	0.1411	0.3739	0.3256	0.3901	0.3878	0.3820	0.2619
1	-1.6102	-0.8437	0.0000	0.1741	0.1248	0.0626	0.1442	0.1212	0.0506	0.2161	0.0628	0.1246
1	-0.1600	-1.3351	0.8857	0.1576	0.1253	0.0597	0.1300	0.1194	0.0200	0.2064	0.0441	0.1171
1	-0.1600	-1.3351	-0.8857	0.1576	0.1253	0.0597	0.1300	0.1194	0.0200	0.2064	0.0441	0.1171

Dipole moment (in D) 6.55 (DEN) 6.92 7.03 6.09 7.34 6.33 6.51 7.28 6.56 6.61

File Lix_28.out

Molecule _28 Li+_N(CH3)2H

SP Lix_28 B3LYP/Def2TZVP VAC.

1 11

Dipole -4.0628 5.4432 0.0000 6.7923

Quadrupole 1.3988 4.0095 -5.4083 -8.9803 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	-1.3726	1.6678	0.0000	0.9010	0.7722	0.6917	0.9867	0.8268	0.8848	0.9809	0.9446	0.8513
7	0.1259	0.4191	0.0000	-0.5700	-0.0978	-0.1435	-0.7789	-0.6203	-0.7325	-0.7589	-1.0987	-0.5464
1	1.0038	0.9351	0.0000	0.2621	0.1900	0.1324	0.3402	0.3222	0.3643	0.3803	0.3674	0.2497
6	0.1259	-0.4213	1.2279	-0.2678	-0.3108	-0.0129	-0.1617	-0.1167	-0.0192	-0.4256	0.2651	-0.1205
6	0.1259	-0.4213	-1.2279	-0.2678	-0.3108	-0.0129	-0.1617	-0.1167	-0.0192	-0.4256	0.2651	-0.1205
1	0.9514	-1.1366	1.2250	0.1638	0.1259	0.0583	0.1394	0.1178	0.1190	0.2113	0.0539	0.1179
1	-0.8076	-0.9820	1.2878	0.1510	0.1266	0.0559	0.1234	0.1164	0.0830	0.2024	0.0349	0.1107
1	0.2169	0.2103	2.1116	0.1564	0.1261	0.0584	0.1249	0.1182	0.0588	0.2108	0.0394	0.1147
1	0.9514	-1.1366	-1.2250	0.1638	0.1259	0.0583	0.1394	0.1178	0.1190	0.2113	0.0539	0.1179
1	-0.8076	-0.9820	-1.2878	0.1510	0.1266	0.0559	0.1234	0.1164	0.0830	0.2024	0.0349	0.1107
1	0.2169	0.2103	-2.1116	0.1564	0.1261	0.0584	0.1249	0.1182	0.0588	0.2108	0.0394	0.1147

Dipole moment (in D) 6.79 (DEN) 7.18 7.14 6.17 7.85 6.52 6.68 7.67 6.79 6.85

File Lix_29.out

Molecule _29 Li+_N(CH3)3

SP Lix_29 B3LYP/Def2TZVP VAC.

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1 14
Dipole      -1.8820    6.5535    0.0000    6.8184
Quadrupole  -4.5073   10.3484   -5.8410   -4.6496    0.0000    0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
3  -0.6008    2.0937    0.0000    0.8977    0.7620    0.6698    0.9752    0.8147    0.8836    0.9855    0.9435    0.8427
7  -0.0637    0.2239    0.0000   -0.4770   -0.0265   -0.1103   -0.4390   -0.4979   -0.3263   -0.5633   -1.0818   -0.4521
6  1.4165    0.1345    0.0000   -0.2646   -0.2955   -0.0182   -0.2214   -0.1191   -0.4203   -0.4309    0.2672   -0.1273
6  -0.6008   -0.4420    1.2114   -0.2648   -0.2955   -0.0181   -0.2215   -0.1192   -0.3113   -0.4310    0.2667   -0.1273
6  -0.6008   -0.4420   -1.2114   -0.2648   -0.2955   -0.0181   -0.2215   -0.1192   -0.3113   -0.4310    0.2668   -0.1273
1  1.7489   -0.9086    0.0000    0.1575    0.1284    0.0551    0.1371    0.1155    0.2138    0.2082    0.0483    0.1124
1  1.8217    0.6203    0.8884    0.1501    0.1276    0.0549    0.1195    0.1157    0.1683    0.2077    0.0321    0.1090
1  1.8217    0.6203   -0.8884    0.1501    0.1276    0.0549    0.1195    0.1157    0.1683    0.2077    0.0321    0.1090
1  -0.3164   -1.4989    1.2398    0.1575    0.1284    0.0552    0.1372    0.1155    0.1900    0.2083    0.0484    0.1124
1  -1.6899   -0.3828    1.2204    0.1501    0.1276    0.0549    0.1194    0.1157    0.1372    0.2076    0.0320    0.1090
1  -0.2098    0.0394    2.1086    0.1502    0.1277    0.0549    0.1195    0.1157    0.1405    0.2077    0.0321    0.1090
1  -0.3164   -1.4989   -1.2398    0.1575    0.1284    0.0552    0.1372    0.1155    0.1900    0.2083    0.0484    0.1124
1  -0.2098    0.0394   -2.1086    0.1502    0.1277    0.0549    0.1195    0.1157    0.1405    0.2077    0.0321    0.1090
1  -1.6899   -0.3828   -1.2204    0.1501    0.1276    0.0549    0.1194    0.1157    0.1372    0.2076    0.0320    0.1090

Dipole moment (in D)  6.82 (DEN)    7.19    6.90    6.03    8.20    6.48    6.73    7.80    6.81    6.89

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File Lix_30.out

Molecule_30 C5H5N-Li+

SP Lix_30 B3LYP/Def2TZVP VAC.

```

1 12
Dipole      -8.5566    0.0000   -0.0021    8.5566
Quadrupole  27.1501   -7.8992  -19.2509    0.0000    0.0061    0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
7  -1.1897   -0.0005    0.0001   -0.5485    0.0572   -0.1656   -0.7562   -0.4905   -0.8709   -0.6370   -1.2987   -0.5008
6  -0.4939   -1.1529    0.0001    0.0831   -0.1729    0.0521    0.2108    0.0672    0.4650    0.0386    0.4651    0.0891
6  0.8890   -1.1961    0.0000   -0.1172   -0.1032   -0.0048   -0.1406   -0.0557   -0.3571   -0.2190    0.0060   -0.0489
6  1.5945    0.0005   -0.0001   -0.0821   -0.0620    0.0279    0.0235   -0.0259    0.2538   -0.1140    0.0120   -0.0171
6  -0.4947    1.1525    0.0002    0.0832   -0.1729    0.0521    0.2107    0.0671    0.4647    0.0384    0.4645    0.0890
6  0.8880    1.1966   -0.0001   -0.1174   -0.1032   -0.0048   -0.1405   -0.0557   -0.3570   -0.2190    0.0059   -0.0489

```

1	-1.0677	-2.0726	0.0000	0.1484	0.1492	0.0657	0.0913	0.1315	0.0172	0.2017	0.0591	0.1141
1	1.3975	-2.1500	0.0002	0.1682	0.1629	0.0743	0.1440	0.1309	0.1803	0.2435	0.0931	0.1230
1	2.6766	0.0010	-0.0004	0.1702	0.1636	0.0782	0.1386	0.1343	0.0937	0.2398	0.0966	0.1270
1	-1.0696	2.0716	0.0002	0.1483	0.1492	0.0656	0.0912	0.1315	0.0173	0.2017	0.0590	0.1141
1	1.3961	2.1507	-0.0001	0.1682	0.1629	0.0743	0.1440	0.1309	0.1803	0.2435	0.0931	0.1230
3	-3.1008	-0.0002	-0.0005	0.8958	0.7692	0.6850	0.9830	0.8343	0.9128	0.9819	0.9442	0.8365

Dipole moment (in D) 8.56 (DEN) 9.31 9.56 8.00 9.56 8.48 8.48 9.63 6.82 8.46

File Lix_31.out

Molecule_31 HCN-Li+

SP Lix_31 B3LYP/Def2TZVP VAC.

1 4

Dipole 0.0000 0.0000 4.9085 4.9085

Quadrupole -8.9727 -8.9727 17.9454 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.0200	0.2742	0.1676	0.1811	0.2586	0.2402	0.2550	0.2734	0.3076	0.2431
6	0.0000	0.0000	-0.9466	0.0379	0.0151	0.2157	0.3500	0.2845	0.3554	0.3008	1.0912	0.2839
7	0.0000	0.0000	0.1948	-0.2478	0.0245	-0.1405	-0.6048	-0.4070	-0.5462	-0.5623	-1.3579	-0.3944
3	0.0000	0.0000	2.1118	0.9358	0.7928	0.7437	0.9963	0.8823	0.9358	0.9881	0.9591	0.8674

Dipole moment (in D) 4.91 (DEN) 6.43 6.37 4.67 5.44 4.94 4.89 5.48 0.51 4.78

File Lix_32.out

Molecule_32 CH3CN-Li+

SP Lix_32 B3LYP/Def2TZVP VAC.

1 7

Dipole 6.8870 -0.0006 -0.0005 6.8870

Quadrupole 26.0742 -13.0370 -13.0372 -0.0016 -0.0010 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.1205	-0.0001	-0.0000	0.0811	-0.0903	0.1982	0.6564	0.3023	0.6615	0.4952	1.0217	0.3432
6	-1.5661	-0.0000	-0.0000	-0.2389	-0.2141	-0.0110	-0.5093	-0.1506	-0.5169	-0.7298	0.0784	-0.1812
1	-1.9324	-0.8453	0.5847	0.1910	0.1710	0.0952	0.2094	0.1479	0.2200	0.2852	0.1227	0.1493

1	-1.9324	0.9291	0.4397	0.1910	0.1710	0.0952	0.2094	0.1479	0.2201	0.2852	0.1227	0.1493
1	-1.9325	-0.0837	-1.0244	0.1910	0.1710	0.0952	0.2094	0.1479	0.2201	0.2852	0.1227	0.1493
7	1.0276	0.0001	0.0001	-0.3348	0.0147	-0.1962	-0.7757	-0.4704	-0.7486	-0.6060	-1.4227	-0.4658
3	2.9080	-0.0001	-0.0001	0.9196	0.7766	0.7234	1.0006	0.8752	0.9438	0.9850	0.9545	0.8560

Dipole moment (in D) 6.89 (DEN) 7.62 7.82 6.45 7.77 6.74 6.87 8.03 1.71 6.66

File Lix_33.out

Molecule _33 Li(H2O)+
SP Lix_33 B3LYP/Def2TZVP VAC.

1 4

Dipole 0.0000 0.0000 -3.9874 3.9874

Quadrupole -6.0426 -2.3934 8.4360 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
3	0.0000	0.0000	-1.4959	0.9309	0.8205	0.7645	1.0127	0.8692	0.9849	0.9903	0.9592	0.8510
8	0.0000	0.0000	0.3321	-0.7283	-0.2369	-0.2168	-1.1163	-0.6506	-1.0854	-1.0333	-1.2296	-0.5161
1	0.0000	0.7721	0.9154	0.3987	0.2082	0.2262	0.5518	0.3907	0.5503	0.5215	0.6352	0.3326
1	0.0000	-0.7721	0.9154	0.3987	0.2082	0.2262	0.5518	0.3907	0.5503	0.5215	0.6352	0.3326

Dipole moment (in D) 3.99 (DEN) 4.34 4.44 3.85 4.20 3.85 3.97 4.18 3.27 4.01

File Lix_37.out

Molecule _37 Li+_CH3OH
SP Lix_37 B3LYP/Def2TZVP VAC.

1 7

Dipole -5.9856 1.4013 0.0005 6.1474

Quadrupole 10.7261 -2.6312 -8.0949 -4.6678 -0.0003 -0.0004

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.4101	-0.3339	-0.0000	-0.6347	-0.0955	-0.2030	-0.8728	-0.5303	-0.8668	-0.8469	-1.1756	-0.4351
6	0.9528	0.1994	-0.0000	-0.1386	-0.2818	0.0459	-0.0300	-0.0888	0.1579	-0.2487	0.3923	-0.0858
1	1.4730	-0.1295	-0.8970	0.1733	0.1235	0.0697	0.1345	0.1278	0.0801	0.2040	0.0794	0.1251
1	0.8714	1.2834	0.0008	0.1339	0.1228	0.0694	0.1218	0.1287	0.0838	0.1919	0.0562	0.1186
1	1.4732	-0.1306	0.8964	0.1733	0.1235	0.0697	0.1345	0.1278	0.0800	0.2040	0.0794	0.1251

1	-0.3598	-1.2982	0.0002	0.3746	0.2069	0.2096	0.5090	0.3803	0.5167	0.5078	0.6140	0.3147
3	-1.9648	0.5833	0.0000	0.9182	0.8006	0.7388	1.0030	0.8547	0.9483	0.9879	0.9539	0.8375
Dipole moment (in D)	6.15 (DEN)	5.94	6.90	5.64	6.55	5.91	6.09	6.20	4.79	5.93		

File Lix_38.out

Molecule_38 Li+_0(CH3)2
SP Lix_38 B3LYP/Def2TZVP VAC.

1	10											
Dipole	0.0001	-6.4618	0.0001	6.4618								
Quadrupole	-3.8620	12.4386	-8.5766	-0.0003	-0.0002	-0.0002						
	Atomic coordinates		Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP	
8	0.0000	-0.3546	-0.0000	-0.5389	0.0442	-0.1729	-0.5505	-0.3921	-0.4311	-0.6516	-1.1379	-0.3369
6	-1.2010	0.4520	-0.0000	-0.1389	-0.2863	0.0356	-0.0813	-0.0955	-0.2479	-0.2588	0.4133	-0.0926
6	1.2010	0.4521	0.0000	-0.1389	-0.2863	0.0356	-0.0813	-0.0955	-0.2437	-0.2588	0.4134	-0.0926
1	-1.2261	1.0747	-0.8947	0.1632	0.1247	0.0642	0.1267	0.1233	0.1814	0.1993	0.0681	0.1176
1	-1.2259	1.0750	0.8945	0.1632	0.1247	0.0642	0.1267	0.1233	0.1814	0.1993	0.0681	0.1176
1	-2.0563	-0.2218	0.0003	0.1263	0.1228	0.0659	0.1090	0.1253	0.1410	0.1927	0.0443	0.1126
1	1.2259	1.0750	-0.8945	0.1632	0.1247	0.0642	0.1267	0.1233	0.1810	0.1993	0.0681	0.1176
1	1.2260	1.0747	0.8947	0.1632	0.1247	0.0642	0.1267	0.1233	0.1810	0.1993	0.0681	0.1176
1	2.0563	-0.2218	-0.0002	0.1263	0.1228	0.0659	0.1090	0.1253	0.1391	0.1927	0.0443	0.1126
3	0.0000	-2.1479	0.0000	0.9113	0.7840	0.7131	0.9883	0.8395	0.9177	0.9867	0.9503	0.8264
Dipole moment (in D)	6.46 (DEN)	5.99	7.09	5.72	7.23	6.13	6.36	6.49	4.76	6.16		

File Lix_46.out

Molecule_46 Li+CH2Cl2
SP Lix_46 B3LYP/Def2TZVP VAC.

1	6											
Dipole	0.0000	0.0000	-4.6732	4.6732								
Quadrupole	-6.8782	-6.1564	13.0346	0.0000	0.0000	0.0000						
	Atomic coordinates		Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP	
6	0.0000	0.0000	0.9468	-0.0694	-0.6376	0.0797	-0.1012	-0.0232	-0.9299	-0.3620	0.2097	0.0566

1	-0.9069	0.0000	1.5399	0.2099	0.1341	0.0938	0.1713	0.1497	0.4765	0.2535	0.1634	0.1481
1	0.9069	0.0000	1.5399	0.2099	0.1341	0.0938	0.1713	0.1497	0.4774	0.2535	0.1634	0.1481
17	0.0000	1.4742	-0.0857	-0.0894	0.3960	0.0729	-0.0839	0.0290	0.0924	-0.0403	-0.2358	-0.0491
17	0.0000	-1.4742	-0.0857	-0.0894	0.3960	0.0729	-0.0839	0.0290	0.0924	-0.0403	-0.2358	-0.0491
3	0.0000	0.0000	-1.9493	0.8285	0.5773	0.5869	0.9266	0.6658	0.7912	0.9355	0.9349	0.7453

Dipole moment (in D) 4.67 (DEN) 4.89 6.65 3.80 6.53 4.15 4.66 6.62 5.19 4.49

File Lix_47.out

Molecule_47 Li+S(CH3)2

SP Lix_47 B3LYP/Def2TZVP VAC.

1 10

Dipole -0.0044 -7.1957 3.2259 7.8857

Quadrupole -5.3564 15.5778 -10.2213 0.0131 -0.0035 -6.8533

	Atomic coordinates			Mu1.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	-0.0001	-0.3379	-0.3819	-0.1849	0.4932	0.0370	-0.0706	-0.0696	-0.1975	0.0610	-0.1920	-0.1996
6	-1.4172	0.6450	0.2026	-0.3279	-0.4614	-0.0517	-0.4145	-0.1870	-0.4039	-0.7104	-0.0949	-0.1842
6	1.4177	0.6441	0.2027	-0.3278	-0.4614	-0.0517	-0.4145	-0.1870	-0.4010	-0.7104	-0.0950	-0.1842
1	-1.3831	1.6175	-0.2843	0.1749	0.1278	0.0684	0.1740	0.1216	0.2422	0.2419	0.0860	0.1294
1	-1.4045	0.7629	1.2839	0.1575	0.1170	0.0581	0.1485	0.1109	0.1510	0.2250	0.0624	0.1158
1	-2.3224	0.1272	-0.1096	0.1633	0.1268	0.0666	0.1593	0.1196	0.1864	0.2415	0.0740	0.1257
1	1.3849	1.6162	-0.2851	0.1749	0.1278	0.0684	0.1739	0.1216	0.2419	0.2419	0.0860	0.1294
1	1.4044	0.7628	1.2839	0.1575	0.1170	0.0582	0.1485	0.1109	0.1500	0.2250	0.0624	0.1158
1	2.3226	0.1251	-0.1085	0.1632	0.1268	0.0666	0.1593	0.1196	0.1859	0.2415	0.0740	0.1257
3	-0.0014	-2.4463	0.6326	0.8494	0.6863	0.6800	0.9359	0.7393	0.8451	0.9430	0.9373	0.8263

Dipole moment (in D) 7.89 (DEN) 8.44 8.81 7.20 10.04 7.48 7.69 10.40 10.03 8.27

File Lix_48.out

Molecule_48 Li+CH3F

SP Lix_48 B3LYP/Def2TZVP VAC.

1 6

Dipole 0.0016 6.2592 0.0000 6.2592

Quadrupole -7.7972 15.5944 -7.7971 0.0048 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.4200	0.0000	-0.3837	-0.0246	-0.1281	-0.4012	-0.2484	-0.3426	-0.4936	-0.6978	-0.2306
6	-0.0001	-1.0408	0.0000	-0.0693	-0.1891	0.1005	-0.0209	-0.0335	-0.0732	-0.1052	0.4003	-0.0401
1	1.0430	-1.3376	0.0000	0.1729	0.1259	0.0836	0.1427	0.1364	0.1628	0.2020	0.1114	0.1398
1	-0.5218	-1.3375	0.9034	0.1729	0.1259	0.0836	0.1427	0.1364	0.1612	0.2020	0.1114	0.1398
1	-0.5218	-1.3375	-0.9034	0.1729	0.1259	0.0836	0.1427	0.1364	0.1612	0.2020	0.1114	0.1398
3	0.0005	2.1591	0.0000	0.9343	0.8360	0.7767	0.9941	0.8728	0.9306	0.9929	0.9637	0.8515

Dipole moment (in D) 6.26 (DEN) 5.93 7.14 5.68 6.86 6.09 6.21 5.93 4.44 5.87

Keywords:

File mol197.out

Molecule 197 BeClF

SP Mol197 B3LYP/Def2TZVP VAC.

0 3

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
Dipole	0.0000	0.0000	0.2956	0.2956								
Quadrupole	2.0794	2.0794	-4.1588	0.0000	0.0000	0.0000						
9	0.0000	0.0000	-1.9742	-0.2422	-0.1027	-0.2728	-0.6380	-0.4386	-0.3649	-0.8582	-0.8773	-0.4222
4	0.0000	0.0000	-0.6034	0.4400	-0.2049	0.4419	1.1813	0.7346	0.6241	1.5989	1.7278	0.7615
17	0.0000	0.0000	1.1871	-0.1978	0.3076	-0.1691	-0.5433	-0.2960	-0.2592	-0.7407	-0.8505	-0.3393

Dipole moment (in D) 0.30 (DEN) 0.11 3.32 0.34 0.47 0.34 0.17 0.72 1.54 0.14

File mol198.out

Molecule 198 BeBrF

SP Mol198 B3LYP/Def2TZVP VAC.

0 3

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
Dipole	0.0000	0.0000	0.3674	0.3674								
Quadrupole	2.0216	2.0216	-4.0431	0.0000	0.0000	0.0000						
9	0.0000	0.0000	-2.5262	-0.2306	-0.0976	-0.2717	-0.6168	-0.4387	-0.3278	-0.8589	-0.8765	-0.4197

4	0.0000	0.0000	-1.1573	0.3802	-0.2275	0.4078	1.1015	0.6856	0.5306	1.5503	1.7042	0.7214
35	0.0000	0.0000	0.7818	-0.1496	0.3251	-0.1361	-0.4846	-0.2470	-0.2028	-0.6914	-0.8280	-0.3017
Dipole moment (in D)	0.37 (DEN)	0.12	3.67	0.52	0.46	0.58	0.27	0.79	1.95	0.05		

File mol199.out

Molecule 199 BeBrCl

SP Mol199 B3LYP/Def2TZVP VAC.

0 3

Dipole	0.0000	0.0000	0.0636	0.0636								
Quadrupole	1.1352	1.1352	-2.2704	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	-2.4522	-0.1372	0.3202	-0.1654	-0.4423	-0.2943	-0.1485	-0.7196	-0.8499	-0.3328
4	0.0000	0.0000	-0.6660	0.2295	-0.6521	0.2986	0.8480	0.5404	0.2816	1.3878	1.6794	0.6320
35	0.0000	0.0000	1.2672	-0.0923	0.3319	-0.1332	-0.4057	-0.2461	-0.1330	-0.6681	-0.8295	-0.2992
Dipole moment (in D)	0.06 (DEN)	0.32	0.33	0.18	0.03	0.24	0.04	0.03	0.41	0.08		

File mol200.out

Molecule 200 Be=CH2

SP Mol200 B3LYP/Def2TZVP VAC.

0 4

Dipole	1.2763	2.6141	0.0000	2.9090								
Quadrupole	-3.7926	3.6713	0.1213	3.4466	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0412	1.1213	0.0000	0.0675	0.2394	0.3076	0.7668	0.4399	0.4983	1.1926	1.2104	0.5005
6	0.0412	-0.4196	0.0000	-0.2653	-0.4958	-0.3388	-1.1332	-0.5624	-0.7983	-1.6164	-1.2776	-0.6315
1	-0.2060	-0.9838	0.8964	0.0989	0.1282	0.0156	0.1832	0.0613	0.1500	0.2119	0.0335	0.0655
1	-0.2060	-0.9838	-0.8964	0.0989	0.1282	0.0156	0.1832	0.0613	0.1500	0.2119	0.0335	0.0655
Dipole moment (in D)	2.91 (DEN)	0.24	1.12	2.19	4.70	2.93	2.90	7.69	8.78	3.35		

File mol202.out

Molecule 202 BeFCH3

SP Mol202 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -1.2929 1.2929

Quadrupole 1.9789 1.9789 -3.9578 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	1.5520	-0.2783	-0.1070	-0.2815	-0.6374	-0.4448	-0.4303	-0.8497	-0.8849	-0.4269
4	0.0000	0.0000	0.1746	0.4126	0.1889	0.4327	1.2173	0.6962	0.7247	1.5884	1.7080	0.7495
6	0.0000	0.0000	-1.4905	-0.4546	-0.4835	-0.2417	-1.0860	-0.4780	-0.7078	-1.4411	-0.8609	-0.5704
1	-1.0084	0.0000	-1.9077	0.1068	0.1339	0.0301	0.1687	0.0755	0.1373	0.2341	0.0125	0.0826
1	0.5042	0.8733	-1.9077	0.1068	0.1339	0.0301	0.1687	0.0755	0.1380	0.2341	0.0125	0.0826
1	0.5042	-0.8733	-1.9077	0.1068	0.1339	0.0301	0.1687	0.0755	0.1380	0.2341	0.0125	0.0826

Dipole moment (in D) 1.29 (DEN) 1.41 0.86 0.83 0.59 1.39 1.32 1.12 0.65 0.74

File mol203.out

Molecule 203 BeClCH3

SP Mol203 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -1.0519 1.0519

Quadrupole 1.0171 1.0171 -2.0343 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	1.3180	-0.2021	0.3026	-0.1844	-0.4896	-0.3099	-0.2478	-0.7249	-0.8598	-0.3480
4	0.0000	0.0000	-0.4790	0.2430	-0.2138	0.3411	1.0373	0.5688	0.4156	1.4607	1.6943	0.6767
6	0.0000	0.0000	-2.1370	-0.3627	-0.4924	-0.2478	-1.0496	-0.4859	-0.3457	-1.4439	-0.8724	-0.5768
1	0.0000	1.0080	-2.5561	0.1073	0.1345	0.0304	0.1673	0.0757	0.0592	0.2360	0.0127	0.0827
1	0.8730	-0.5040	-2.5561	0.1073	0.1345	0.0304	0.1673	0.0757	0.0593	0.2360	0.0127	0.0827
1	-0.8730	-0.5040	-2.5561	0.1073	0.1345	0.0304	0.1673	0.0757	0.0594	0.2360	0.0127	0.0827

Dipole moment (in D) 1.05 (DEN) 2.07 2.51 0.53 0.87 1.07 1.16 1.82 0.86 0.88

File mol204.out

Molecule 204 BeBrCH3

SP Mol204 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -1.0461 1.0461

Quadrupole 0.4787 0.4787 -0.9574 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.0000	0.8648	-0.1556	0.3148	-0.1567	-0.4395	-0.2657	-0.2164	-0.6743	-0.8424	-0.3159
4	0.0000	0.0000	-1.0833	0.1990	-0.2273	0.3145	0.9769	0.5259	0.3867	1.4123	1.6772	0.6435
6	0.0000	0.0000	-2.7419	-0.3635	-0.4914	-0.2493	-1.0398	-0.4875	-0.4315	-1.4483	-0.8742	-0.5762
1	-1.0081	0.0000	-3.1611	0.1067	0.1346	0.0305	0.1675	0.0758	0.0866	0.2367	0.0132	0.0829
1	0.5040	0.8730	-3.1611	0.1067	0.1346	0.0305	0.1675	0.0758	0.0873	0.2367	0.0132	0.0829
1	0.5040	-0.8730	-3.1611	0.1067	0.1346	0.0305	0.1675	0.0758	0.0873	0.2367	0.0132	0.0829

Dipole moment (in D) 1.05 (DEN) 1.76 2.83 0.39 0.84 0.87 1.19 1.86 1.31 0.85

File mol190.out

Molecule 190 BeCl+

SP Mol191 B3LYP/Def2TZVP VAC.

1 2

Dipole 0.0000 0.0000 -7.8512 7.8512

Quadrupole -5.5683 -5.5683 11.1365 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	0.3241	0.2371	0.5621	0.0582	-0.4677	-0.1004	-0.1648	-0.6393	-0.7528	-0.1571
4	0.0000	0.0000	-1.3774	0.7629	0.4379	0.9418	1.4677	1.1004	1.1648	1.6393	1.7528	1.1571

Dipole moment (in D) 7.85 (DEN) 4.68 2.02 6.14 10.44 7.44 7.96 11.84 12.77 7.90

File mol192.out

Molecule 192 BeS

SP Mol192 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -5.1224 5.1224

Quadrupole -4.2318 -4.2318 8.4637 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.3442	-0.1542	0.1311	-0.3910	-0.8723	-0.5840	-0.6524	-1.2827	-1.4659	-0.6808
4	0.0000	0.0000	-1.3766	0.1542	-0.1311	0.3910	0.8723	0.5840	0.6524	1.2827	1.4659	0.6808
Dipole moment (in D)		5.12 (DEN)		1.27	1.08	3.23	7.21	4.83	5.39	10.60	12.12	5.63

File mol193.out

Molecule 193 Be=NH

SP Mol193 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 -3.8712 3.8712

Quadrupole -3.8997 -3.8997 7.7994 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0000	0.0000	-0.9708	0.0943	0.2201	0.4215	1.1616	0.7733	1.1444	1.6131	1.5954	0.7983
7	0.0000	0.0000	0.3608	-0.2870	-0.3557	-0.5067	-1.5735	-1.0460	-1.8994	-1.9699	-1.9845	-1.0304
1	0.0000	0.0000	1.3576	0.1927	0.1356	0.0852	0.4119	0.2726	0.7549	0.3567	0.3890	0.2321
Dipole moment (in D)		3.87 (DEN)		0.32	0.76	2.29	5.46	3.64	3.70	8.61	8.34	3.99

File mol195.out

Molecule 195 Be=NF

SP Mol195 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0193 5.2169 0.0000 5.2169

Quadrupole -4.8873 9.7747 -4.8875 0.0511 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	0.3385	0.0000	0.0881	-0.2402	-0.3464	-1.2077	-0.7521	-1.1248	-1.2918	-1.2066	-0.7543
4	0.0058	1.6534	0.0000	0.0535	0.1965	0.4346	1.1113	0.8058	0.9496	1.5362	1.5493	0.7979
9	-0.0026	-0.9981	0.0000	-0.1416	0.0437	-0.0882	0.0964	-0.0537	0.1753	-0.2444	-0.3426	-0.0436
Dipole moment (in D)		5.22 (DEN)		1.25	0.96	3.31	6.40	5.43	4.87	11.27	11.99	5.32

File Bex_1.out

Molecule _1 CH3BeH

SP Bex_1 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0003 0.5946 0.0000 0.5946

Quadrupole 1.9700 -3.9398 1.9699 -0.0006 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0000	-1.0706	0.0000	0.1991	0.2155	0.3466	1.0182	0.4709	0.5783	1.3280	1.6841	0.6419
6	0.0000	0.6056	0.0000	-0.4040	-0.5099	-0.2514	-1.0023	-0.4845	-0.5216	-1.4491	-0.8702	-0.5712
1	-1.0149	1.0172	0.0000	0.1029	0.1315	0.0267	0.1595	0.0716	0.0882	0.2337	0.0081	0.0784
1	0.5075	1.0173	0.8789	0.1029	0.1315	0.0267	0.1595	0.0716	0.0894	0.2337	0.0081	0.0784
1	0.5075	1.0173	-0.8789	0.1029	0.1315	0.0267	0.1595	0.0716	0.0894	0.2337	0.0081	0.0784
1	-0.0002	-2.4026	0.0000	-0.1037	-0.1001	-0.1753	-0.4944	-0.2011	-0.3237	-0.5801	-0.8383	-0.3059

Dipole moment (in D) 0.59 (DEN) 0.51 0.49 0.10 0.11 0.46 0.55 0.92 1.40 0.28

File Bex_2.out

Molecule _2 BeH(CH=CH2)

SP Bex_2 B3LYP/Def2TZVP VAC.

0 7

Dipole -0.7526 0.1944 0.0000 0.7773

Quadrupole -2.6987 2.7006 -0.0020 1.4337 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	2.8791	-0.3726	0.0000	-0.0922	-0.0978	-0.1734	-0.4890	-0.1993	-0.3286	-0.5764	-0.8379	-0.3049
4	1.6052	0.0094	0.0000	0.1535	0.2317	0.3351	0.9764	0.4646	0.6159	1.3214	1.6818	0.6140
6	0.0000	0.4699	0.0000	-0.0614	-0.3032	-0.1955	-0.7443	-0.3434	-0.4562	-0.9559	-0.8071	-0.3924
1	-0.2943	1.5209	0.0000	0.0927	0.1390	0.0280	0.1446	0.0783	0.1527	0.1991	0.0118	0.0757
6	-1.0152	-0.4043	0.0000	-0.3113	-0.2024	-0.0607	-0.0733	-0.1695	-0.2602	-0.3386	-0.0839	-0.1588
1	-0.8551	-1.4792	0.0000	0.1120	0.1189	0.0323	0.0864	0.0835	0.1340	0.1730	0.0116	0.0829
1	-2.0592	-0.1003	0.0000	0.1068	0.1138	0.0341	0.0993	0.0857	0.1425	0.1774	0.0236	0.0836

Dipole moment (in D) 0.78 (DEN) 0.52 0.39 0.05 0.47 0.37 0.73 1.15 1.49 0.08

File Bex_6.out

Molecule _6 BeH(OH)

SP Bex_6 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 1.8156 1.8156

Quadrupole 0.2209 0.2209 -0.4418 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0000	0.0000	-0.8630	0.2757	0.0991	0.3345	1.1852	0.5713	0.7082	1.4431	1.6818	0.6337
8	0.0000	0.0000	0.5220	-0.4519	-0.1739	-0.3548	-1.2100	-0.7385	-0.8726	-1.3746	-1.4971	-0.6411
1	0.0000	0.0000	-2.1904	-0.1300	-0.0990	-0.1644	-0.5253	-0.1887	-0.3266	-0.5832	-0.8243	-0.2955
1	0.0000	0.0000	1.4668	0.3061	0.1738	0.1847	0.5500	0.3559	0.4910	0.5147	0.6395	0.3030

Dipole moment (in D) 1.82 (DEN) 1.25 1.42 0.75 1.45 0.27 1.77 0.33 2.45 1.01

File Bex_7.out

Molecule _7 BeCN(OH)

SP Bex_7 B3LYP/Def2TZVP VAC.

0 5

Dipole 0.0000 0.0000 4.7504 4.7504

Quadrupole 0.8474 0.8474 -1.6949 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-1.0328	-0.2504	-0.2412	-0.0902	-0.4775	-0.0659	-0.0447	-0.4580	0.3156	-0.0860
4	0.0000	0.0000	0.6283	0.3937	0.1217	0.4362	1.3282	0.7546	0.7985	1.6172	1.7271	0.7542
8	0.0000	0.0000	2.0048	-0.4576	-0.1317	-0.3433	-1.2608	-0.7292	-0.9425	-1.3640	-1.4873	-0.6385
7	0.0000	0.0000	-2.1864	-0.0056	0.0686	-0.1974	-0.1569	-0.3250	-0.3440	-0.3166	-1.2055	-0.3426
1	0.0000	0.0000	2.9506	0.3199	0.1826	0.1947	0.5669	0.3656	0.5327	0.5214	0.6503	0.3130

Dipole moment (in D) 4.75 (DEN) 2.62 2.16 3.29 3.92 4.18 4.72 4.73 11.20 4.59

File Bex_9.out

Molecule _9 BeH(NO2)

SP Bex_9 B3LYP/Def2TZVP VAC.

0 5

Dipole 0.0000 0.0000 -2.7819 2.7819
 Quadrupole 3.4225 -1.8288 -1.5937 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.9320	-0.0592	-0.0849	-0.1427	-0.4699	-0.1681	-0.2349	-0.5594	-0.8170	-0.2741
4	0.0000	0.0000	-1.6166	0.3047	0.3159	0.4570	1.0047	0.6833	0.4822	1.3289	1.7024	0.7480
7	0.0000	0.0000	0.0077	0.3611	-0.1799	0.1040	0.1623	-0.1599	0.6334	0.0000	0.1197	-0.0350
8	0.0000	1.0876	0.5840	-0.3033	-0.0256	-0.2091	-0.3486	-0.1776	-0.4403	-0.3848	-0.5026	-0.2195
8	0.0000	-1.0876	0.5840	-0.3033	-0.0256	-0.2091	-0.3486	-0.1776	-0.4403	-0.3848	-0.5026	-0.2195

Dipole moment (in D) 2.78 (DEN) 3.22 1.41 2.71 3.13 3.94 2.88 4.60 4.53 3.18

 File Bex_10.out

Molecule _10 BeHF

SP Bex_10 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 -0.6805 0.6805
 Quadrupole 1.6112 1.6112 -3.2224 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.1131	-0.1328	-0.0951	-0.1503	-0.5017	-0.1762	-0.3069	-0.5865	-0.8103	-0.2821
4	0.0000	0.0000	-0.7886	0.3764	0.2148	0.4236	1.0988	0.6145	0.7076	1.4455	1.6905	0.6992
9	0.0000	0.0000	0.5853	-0.2435	-0.1197	-0.2732	-0.5971	-0.4383	-0.4006	-0.8590	-0.8802	-0.4171

Dipole moment (in D) 0.68 (DEN) 0.76 0.19 0.85 0.75 1.77 0.69 1.94 0.65 0.96

 File Bex_11.out

Molecule _11 CH3BeF

SP Bex_11 B3LYP/Def2TZVP VAC.

0 6

Dipole -0.0092 -1.2645 0.0000 1.2645
 Quadrupole 2.0426 -4.0843 2.0417 -0.0322 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0000	0.1777	0.0000	0.4115	0.1933	0.4326	1.2091	0.6915	0.7270	1.5842	1.7058	0.7450
6	-0.0074	-1.5022	0.0000	-0.4552	-0.4851	-0.2397	-1.0743	-0.4718	-0.7047	-1.4336	-0.8616	-0.5636

1	1.0074	-1.9098	0.0000	0.1067	0.1335	0.0297	0.1670	0.0749	0.1367	0.2332	0.0137	0.0818
1	-0.5174	-1.9040	0.8803	0.1067	0.1334	0.0297	0.1671	0.0748	0.1369	0.2332	0.0137	0.0817
1	-0.5174	-1.9040	-0.8803	0.1067	0.1334	0.0297	0.1671	0.0748	0.1369	0.2332	0.0137	0.0817
9	0.0080	1.5578	0.0000	-0.2765	-0.1086	-0.2820	-0.6360	-0.4442	-0.4329	-0.8502	-0.8856	-0.4266

Dipole moment (in D) 1.26 (DEN) 1.37 0.81 0.83 0.56 1.39 1.29 1.07 0.67 0.73

File Bex_12.out

Molecule_12 BeHCl

SP Bex_12 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 -0.3504 0.3504

Quadrupole 1.1268 1.1268 -2.2536 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.6587	-0.0999	-0.0999	-0.1564	-0.4687	-0.1827	-0.2420	-0.5653	-0.8263	-0.2884
4	0.0000	0.0000	-1.3356	0.2372	-0.1776	0.3296	0.9127	0.4789	0.4774	1.2901	1.6805	0.6198
17	0.0000	0.0000	0.4707	-0.1373	0.2775	-0.1732	-0.4440	-0.2962	-0.2353	-0.7248	-0.8540	-0.3314

Dipole moment (in D) 0.35 (DEN) 0.56 3.04 0.51 0.87 1.41 0.50 2.70 2.16 1.04

File Bex_13.out

Molecule_13 BeH(SH)

SP Bex_13 B3LYP/Def2TZVP VAC.

0 4

Dipole -0.7407 0.0700 0.0000 0.7440

Quadrupole 3.6538 -3.4385 -0.2153 0.7562 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.0602	1.4141	0.0000	0.1700	-0.1417	0.2896	0.8497	0.4404	0.4782	1.2378	1.6644	0.6270
16	0.0602	-0.4911	0.0000	-0.2037	0.1684	-0.1831	-0.5376	-0.3700	-0.3461	-0.8297	-0.8202	-0.4656
1	0.0815	2.7403	0.0000	-0.1048	-0.1034	-0.1647	-0.4592	-0.1907	-0.2675	-0.5685	-0.8352	-0.2946
1	-1.2863	-0.5389	0.0000	0.1385	0.0766	0.0582	0.1472	0.1203	0.1354	0.1605	-0.0092	0.1332

Dipole moment (in D) 0.74 (DEN) 0.91 2.96 0.40 1.17 1.31 0.92 2.70 2.27 1.44

File Bex_14.out

Molecule _14 Be(OH)(SH)

SP Bex_14 B3LYP/Def2TZVP VAC.

0 5

Dipole 1.2750 0.7104 1.1989 1.8888

Quadrupole -0.4353 1.5072 -1.0719 -1.7371 3.7804 0.0109

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
4	0.6447	-0.0098	-0.0094	0.2652	-0.2281	0.3350	1.1546	0.6522	0.5466	1.5270	1.6962	0.7107
8	2.0563	0.0106	-0.0865	-0.4028	-0.1869	-0.3620	-1.1635	-0.7258	-0.6648	-1.3414	-1.4648	-0.6401
16	-1.2725	-0.0807	0.0072	-0.2962	0.1608	-0.1969	-0.6395	-0.3792	-0.3759	-0.8356	-0.8162	-0.4815
1	2.7238	-0.0138	0.5951	0.2994	0.1830	0.1707	0.5030	0.3369	0.3637	0.4940	0.6015	0.2822
1	-1.3923	1.2598	0.0194	0.1344	0.0713	0.0532	0.1454	0.1159	0.1304	0.1559	-0.0167	0.1286

Dipole moment (in D) 1.89 (DEN) 2.14 1.77 0.90 2.64 1.65 2.03 2.96 4.36 2.14

Keywords:

File mol276.out

Molecule 276 NaF

SP Mol276 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 7.8444 7.8444

Quadrupole -0.0068 -0.0068 0.0136 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	-1.0631	-0.7407	-0.5265	-0.6232	-0.9371	-0.7806	-0.8435	-0.9396	-0.9052	-0.7051
11	0.0000	0.0000	0.8698	0.7407	0.5265	0.6232	0.9371	0.7806	0.8435	0.9396	0.9052	0.7051

Dipole moment (in D) 7.84 (DEN) 6.88 4.89 5.79 8.70 7.25 7.83 8.72 8.40 6.55

File mol278.out

Molecule 278 NaS

SP Mol278 B3LYP/Def2TZVP VAC.

```

0 2
Dipole      0.0000  0.0000 -8.0922  8.0922
Quadrupole -0.7536 -4.1373  4.8909  0.0000  0.0000  0.0000
      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
11  0.0000  0.0000 -1.4823  0.5707  0.2062  0.4960  0.8054  0.6015  0.6760  0.8238  0.8215  0.6999
16  0.0000  0.0000  1.0191 -0.5707 -0.2062 -0.4960 -0.8054 -0.6015 -0.6760 -0.8238 -0.8214 -0.6999

Dipole moment (in D)  8.09 (DEN)  6.86  2.48  5.96  9.68  7.23  8.12  9.90  9.87  8.41

```

File mol279.out

Molecule 279 NaCl

SP Mol279 B3LYP/Def2TZVP VAC.

```

0 2
Dipole      0.0000  0.0000 -8.6220  8.6220
Quadrupole -2.8090 -2.8090  5.6180  0.0000  0.0000  0.0000
      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
17  0.0000  0.0000  0.9317 -0.6471 -0.2585 -0.5784 -0.8959 -0.6889 -0.7629 -0.9093 -0.8835 -0.7245
11  0.0000  0.0000 -1.4398  0.6471  0.2585  0.5784  0.8959  0.6889  0.7629  0.9093  0.8836  0.7245

Dipole moment (in D)  8.62 (DEN)  7.37  2.94  6.59  10.21  7.85  8.69  10.36  10.06  8.25

```

File mol280.out

Molecule 280 NaBr

SP Mol280 B3LYP/Def2TZVP VAC.

```

0 2
Dipole      0.0000  0.0000 -8.8080  8.8080
Quadrupole -5.6374 -5.6374 11.2747  0.0000  0.0000  0.0000
      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
35  0.0000  0.0000  0.6046 -0.6578 -0.2378 -0.5539 -0.8711 -0.6442 -0.7432 -0.9015 -0.8734 -0.7193
11  0.0000  0.0000 -1.9238  0.6578  0.2378  0.5539  0.8711  0.6442  0.7432  0.9015  0.8734  0.7193

Dipole moment (in D)  8.81 (DEN)  7.99  2.89  6.73  10.58  7.82  9.03  10.95  10.61  8.74

```

File mol281.out

Molecule 281 NaI

SP Mol281 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -8.9225 8.9225

Quadrupole -7.7987 -7.7987 15.5975 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
53	0.0000	0.0000	0.4737	-0.6016	-0.2087	-0.5335	-0.8323	-0.6004	-0.6959	-0.8742	-0.8553	-0.7016
11	0.0000	0.0000	-2.2823	0.6016	0.2087	0.5335	0.8323	0.6004	0.6959	0.8742	0.8553	0.7016

Dipole moment (in D) 8.92 (DEN) 7.96 2.76 7.06 11.02 7.95 9.21 11.57 11.32 9.29

File mol282.out

Molecule 282 NaOH

SP Mol282 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 6.1686 6.1686

Quadrupole -2.3173 -2.3173 4.6345 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	0.0000	0.0000	0.9196	0.7195	0.4436	0.5795	1.0287	0.7888	0.9118	0.9572	0.9114	0.7029
8	0.0000	0.0000	-1.0185	-0.9841	-0.5553	-0.6423	-1.4398	-1.0221	-1.4330	-1.3935	-1.4288	-0.8294
1	0.0000	0.0000	-1.9674	0.2646	0.1117	0.0629	0.4112	0.2334	0.5213	0.4362	0.5174	0.1266

Dipole moment (in D) 6.17 (DEN) 5.49 3.62 5.11 7.70 6.28 6.11 6.92 6.13 5.97

File mol283.out

Molecule 283 NaSH

SP Mol283 B3LYP/Def2TZVP VAC.

0 3

Dipole -0.4066 7.9872 0.0000 7.9975

Quadrupole -0.5885 5.2263 -4.6378 1.5344 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
--	--------------------	--	--	------	--------	---------	----------	-----	-----	-----	-----	-----

11	0.0476	1.5165	0.0000	0.5598	0.2365	0.5072	0.8257	0.6167	0.6774	0.8306	0.8216	0.7203
16	0.0476	-0.9736	0.0000	-0.6590	-0.2588	-0.5016	-0.9330	-0.6757	-0.7741	-0.9462	-0.7209	-0.7715
1	-1.2841	-1.1034	0.0000	0.0992	0.0223	-0.0056	0.1072	0.0590	0.0967	0.1156	-0.1007	0.0512

Dipole moment (in D) 8.00 (DEN) 6.66 2.82 6.07 9.83 7.35 8.07 9.89 9.91 8.59

File mol285.out

Molecule 285 NaCH3

SP Mol285 B3LYP/Def2TZVP VAC.

0 5

Dipole -0.0006 5.6190 0.0000 5.6190

Quadrupole -0.8535 1.7068 -0.8533 -0.0004 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	-1.1966	0.0000	-0.9521	-0.7155	-0.3559	-1.0338	-0.5691	-1.3480	-1.2422	-0.5650	-0.6356
1	1.0075	-1.6307	0.0000	0.0994	0.0968	-0.0261	0.1023	0.0197	0.2354	0.1779	-0.0488	0.0041
1	-0.5039	-1.6303	0.8726	0.0994	0.0969	-0.0261	0.1022	0.0197	0.2368	0.1779	-0.0488	0.0041
1	-0.5039	-1.6303	-0.8726	0.0994	0.0969	-0.0261	0.1022	0.0197	0.2368	0.1779	-0.0488	0.0041
11	0.0000	1.0974	0.0000	0.6538	0.4249	0.4342	0.7270	0.5099	0.6390	0.7085	0.7118	0.6234

Dipole moment (in D) 5.62 (DEN) 6.58 4.08 4.95 7.37 5.50 5.56 6.70 8.15 6.84

File mol288.out

Molecule 288 NaC2H

SP Mol288 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 7.5493 7.5493

Quadrupole -5.0706 -5.0706 10.1413 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-0.6205	-0.3032	-0.3390	-0.4005	-0.9196	-0.4875	-0.8969	-0.6568	-0.4538	-0.5500
6	0.0000	0.0000	-1.8463	-0.6960	-0.2612	-0.2112	-0.1393	-0.2658	-0.0763	-0.4450	-0.5142	-0.2570
11	0.0000	0.0000	1.6104	0.8642	0.4962	0.5620	0.9078	0.6506	0.8147	0.8995	0.8621	0.7189
1	0.0000	0.0000	-2.9134	0.1349	0.1040	0.0497	0.1511	0.1027	0.1585	0.2023	0.1059	0.0881

Dipole moment (in D) 7.55 (DEN) 11.87 5.71 6.72 8.88 7.41 7.43 10.03 11.10 8.25

File mol291.out

Molecule 291 NaC2H2F

SP Mol291 B3LYP/Def2TZVP VAC.

0 6

Dipole -6.5665 -1.1062 0.0023 6.6590

Quadrupole 10.7399 -5.9611 -4.7788 2.7783 -0.0006 -0.0008

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.5445	-0.4200	-0.0005	-0.2502	-0.2849	-0.1957	-0.4656	-0.2734	-0.7294	-0.1489	-0.1358	-0.3107
6	1.8640	-0.3174	0.0002	-0.3902	-0.3110	-0.1570	-0.3111	-0.2556	0.0862	-0.6088	-0.1230	-0.2539
11	-1.7049	-0.3731	0.0001	0.8224	0.4137	0.5529	0.9061	0.7283	0.7745	0.9031	0.8876	0.6633
9	-0.0608	1.0162	-0.0001	-0.3727	-0.0547	-0.2534	-0.3744	-0.3588	-0.2224	-0.5434	-0.6872	-0.2278
1	2.4120	0.6188	0.0008	0.0942	0.1137	0.0278	0.1264	0.0811	0.0613	0.1948	0.0359	0.0639
1	2.4372	-1.2361	0.0000	0.0964	0.1231	0.0254	0.1187	0.0785	0.0298	0.2033	0.0222	0.0653

Dipole moment (in D) 6.66 (DEN) 8.91 4.16 5.99 8.78 7.38 6.45 9.20 9.05 7.10

File mol293.out

Molecule 293 NaC2H6N

SP Mol293 B3LYP/Def2TZVP VAC.

0 10

Dipole 7.5115 0.0000 0.0000 7.5115

Quadrupole 10.2992 -4.5736 -5.7256 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	1.9247	-0.0000	-0.0000	0.7104	0.4719	0.5576	0.9033	0.7827	0.8000	0.8949	0.8589	0.7711
7	-0.1839	-0.0000	-0.0000	-0.6853	-0.2068	-0.3606	-1.0778	-0.7568	-0.9362	-0.9352	-1.2590	-0.7373
6	-1.0197	1.1607	0.0000	-0.1770	-0.3991	-0.0820	0.0387	-0.1704	0.0261	-0.3934	0.3744	-0.1423
6	-1.0198	-1.1607	0.0000	-0.1770	-0.3991	-0.0820	0.0387	-0.1704	0.0261	-0.3934	0.3742	-0.1423
1	-1.6962	-1.2276	-0.8791	0.0565	0.0847	-0.0089	0.0144	0.0487	0.0194	0.1298	-0.0560	0.0398
1	-1.6962	-1.2276	0.8791	0.0565	0.0847	-0.0089	0.0144	0.0487	0.0194	0.1298	-0.0560	0.0398
1	-0.4315	-2.0874	0.0000	0.0513	0.0971	0.0013	0.0197	0.0601	0.0033	0.1539	-0.0624	0.0460
1	-1.6962	1.2277	-0.8791	0.0565	0.0847	-0.0089	0.0144	0.0487	0.0194	0.1298	-0.0560	0.0398

1	-0.4315	2.0874	-0.0000	0.0513	0.0971	0.0013	0.0197	0.0601	0.0033	0.1539	-0.0624	0.0459
1	-1.6962	1.2277	0.8791	0.0565	0.0847	-0.0089	0.0144	0.0487	0.0194	0.1298	-0.0560	0.0398
Dipole moment (in D)	7.51 (DEN)	6.85	5.29	6.56	8.37	7.74	7.32	8.08	7.47	7.69		

File Nax_5.out

Molecule _5 (CH3)HNNa

SP Nax_5 B3LYP/Def2TZVP VAC.

0 7

Dipole 6.4715 -1.3133 0.0580 6.6037

Quadrupole 7.3859 -1.7088 -5.6771 -2.1308 -0.2374 0.3116

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-0.3358	0.4727	-0.0217	-0.8677	-0.3963	-0.4493	-1.2440	-0.9372	-1.5379	-1.2286	-1.3193	-0.8841
6	-1.5843	-0.2633	0.0047	-0.1566	-0.4255	-0.0868	0.0556	-0.1801	0.6813	-0.3797	0.3724	-0.1413
11	1.6589	-0.1537	0.0035	0.6861	0.4375	0.5280	0.8849	0.7532	0.8249	0.8871	0.8485	0.7474
1	-0.5496	1.4620	0.0629	0.1571	0.1280	0.0258	0.2511	0.2100	0.4167	0.3096	0.2666	0.1449
1	-2.1685	-0.1537	0.9381	0.0637	0.0806	-0.0098	0.0126	0.0466	-0.1562	0.1316	-0.0570	0.0415
1	-1.3938	-1.3399	-0.0983	0.0518	0.0936	0.0003	0.0227	0.0591	-0.1047	0.1462	-0.0572	0.0475
1	-2.2797	-0.0068	-0.8167	0.0654	0.0821	-0.0081	0.0171	0.0485	-0.1241	0.1339	-0.0541	0.0441

Dipole moment (in D) 6.60 (DEN) 6.12 4.68 5.82 7.75 7.06 6.57 7.54 7.16 7.05

File Nax_6.out

Molecule _6 (CH3)2NNa

SP Nax_6 B3LYP/Def2TZVP VAC.

0 10

Dipole -0.0001 -7.4233 0.0000 7.4233

Quadrupole -5.6807 10.1946 -4.5139 0.0003 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	0.0000	0.1877	0.0000	-0.6912	-0.2121	-0.3621	-1.0786	-0.7588	-0.9804	-0.9381	-1.2516	-0.7395
11	-0.0000	-1.9153	0.0000	0.7067	0.4665	0.5533	0.9005	0.7816	0.8030	0.8935	0.8565	0.7689
6	0.0000	1.0154	1.1755	-0.1754	-0.3948	-0.0817	0.0352	-0.1711	0.0886	-0.3941	0.3661	-0.1427
6	0.0000	1.0154	-1.1755	-0.1754	-0.3948	-0.0817	0.0352	-0.1711	0.0886	-0.3941	0.3662	-0.1427

1	-0.8827	1.6871	1.2427	0.0577	0.0850	-0.0082	0.0161	0.0492	0.0070	0.1310	-0.0542	0.0406
1	0.8827	1.6871	1.2426	0.0577	0.0850	-0.0082	0.0161	0.0493	0.0067	0.1310	-0.0542	0.0406
1	0.0001	0.4108	2.0918	0.0522	0.0977	0.0025	0.0216	0.0612	-0.0137	0.1545	-0.0601	0.0469
1	-0.8827	1.6871	-1.2427	0.0577	0.0850	-0.0082	0.0161	0.0492	0.0070	0.1310	-0.0542	0.0406
1	0.8827	1.6871	-1.2426	0.0577	0.0850	-0.0082	0.0161	0.0493	0.0067	0.1310	-0.0542	0.0406
1	0.0001	0.4108	-2.0918	0.0522	0.0977	0.0025	0.0216	0.0612	-0.0137	0.1545	-0.0601	0.0469

Dipole moment (in D) 7.42 (DEN) 6.76 5.19 6.47 8.31 7.71 7.24 8.05 7.43 7.63

File Nax_7.out

Molecule_7 CH3-ONa

SP Nax_7 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0136 -7.4193 0.0000 7.4193

Quadrupole -4.1870 8.3746 -4.1875 -0.0261 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.2761	0.0000	-0.7893	-0.2408	-0.5135	-1.1941	-0.7748	-1.0885	-1.0922	-1.3496	-0.6710
6	-0.0038	1.6479	0.0000	-0.0771	-0.4649	-0.0592	0.1857	-0.1774	0.5597	-0.1923	0.6234	-0.1312
1	-0.5147	2.0821	0.8827	0.0420	0.0749	-0.0116	-0.0003	0.0445	-0.1107	0.1108	-0.0609	0.0272
1	-0.5147	2.0821	-0.8827	0.0420	0.0749	-0.0116	-0.0003	0.0445	-0.1107	0.1108	-0.0609	0.0272
1	1.0143	2.0863	0.0000	0.0420	0.0749	-0.0116	-0.0002	0.0445	-0.1128	0.1108	-0.0609	0.0272
11	0.0035	-1.6679	0.0000	0.7403	0.4810	0.6077	1.0093	0.8188	0.8629	0.9520	0.9088	0.7205

Dipole moment (in D) 7.42 (DEN) 6.33 5.60 6.37 8.21 7.66 7.27 7.27 5.96 6.88

File Nax_10.out

Molecule_10 Na(OH)

SP Nax_10 B3LYP/Def2TZVP VAC.

0 3

Dipole -0.0003 -6.1479 0.0000 6.1479

Quadrupole -2.3186 4.6372 -2.3186 -0.0017 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	0.0000	-0.9176	0.0000	0.7196	0.4420	0.5787	1.0289	0.7906	0.9115	0.9576	0.9110	0.7025

8	0.0000	1.0154	0.0000	-0.9848	-0.5572	-0.6421	-1.4386	-1.0223	-1.4306	-1.3944	-1.4244	-0.8278
1	-0.0003	1.9697	0.0000	0.2652	0.1151	0.0634	0.4097	0.2318	0.5191	0.4368	0.5135	0.1254
Dipole moment (in D)	6.15 (DEN)	5.47	3.58	5.08	7.68	6.28	6.08	6.89	6.10	5.95		

File Nax_12.out

Molecule_12 NaS

SP Nax_12 B3LYP/Def2TZVP VAC.

0 2

Dipole	0.0000	0.0000	-8.0606	8.0606								
Quadrupole	-0.7326	-4.1161	4.8487	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	0.0000	0.0000	-1.4759	0.5721	0.2024	0.4951	0.8063	0.6035	0.6762	0.8246	0.8211	0.7004
16	0.0000	0.0000	1.0147	-0.5721	-0.2024	-0.4951	-0.8062	-0.6035	-0.6762	-0.8246	-0.8211	-0.7004
Dipole moment (in D)	8.06 (DEN)	6.84	2.42	5.92	9.65	7.22	8.09	9.86	9.82	8.38		

File Nax_13.out

Molecule_13 Na+CH3

SP Nax_13 B3LYP/Def2TZVP VAC.

1 5

Dipole	0.0002	4.2673	0.0000	4.2673								
Quadrupole	-3.0235	6.0457	-3.0222	0.0008	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	-0.0000	1.2231	0.0000	0.8810	0.7786	0.8269	0.9846	0.8575	0.8987	0.9756	0.9536	0.9082
6	-0.0000	-1.4559	0.0000	-0.4409	-0.1571	-0.0328	-0.4480	-0.2065	-0.4697	-0.5516	-0.2392	-0.2577
1	1.0769	-1.5722	0.0000	0.1866	0.1262	0.0686	0.1544	0.1163	0.1896	0.1919	0.0951	0.1165
1	-0.5382	-1.5735	0.9326	0.1867	0.1262	0.0687	0.1545	0.1164	0.1907	0.1920	0.0952	0.1165
1	-0.5382	-1.5735	-0.9326	0.1867	0.1262	0.0687	0.1545	0.1164	0.1907	0.1920	0.0952	0.1165
Dipole moment (in D)	4.27 (DEN)	4.03	2.81	3.53	5.42	3.84	4.25	5.24	5.12	4.50		

File Nax_14.out

Molecule _14 Na+C2H5

SP Nax_14 B3LYP/Def2TZVP VAC.

1 8

Dipole -6.2449 -0.7222 0.0000 6.2865

Quadrupole 11.9117 -5.9236 -5.9881 1.5768 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.5995	-0.4309	0.0000	-0.2957	-0.3117	-0.0651	-0.3919	-0.2166	0.0032	-0.6940	-0.0029	-0.2340
6	0.6418	0.6996	0.0000	-0.4150	-0.1659	-0.0299	-0.2716	-0.1693	-0.3668	-0.3789	-0.2175	-0.1882
1	0.4626	1.2473	0.9219	0.1833	0.1412	0.0548	0.1125	0.1045	0.1347	0.1883	0.0573	0.0953
1	1.5248	-1.0541	-0.8930	0.1424	0.1384	0.0546	0.1398	0.1053	0.0265	0.2285	0.0394	0.1038
1	1.5249	-1.0541	0.8930	0.1424	0.1384	0.0546	0.1398	0.1053	0.0265	0.2285	0.0394	0.1038
1	2.6273	-0.0317	-0.0000	0.1830	0.1641	0.0767	0.1865	0.1267	0.1471	0.2696	0.0845	0.1280
1	0.4626	1.2473	-0.9219	0.1833	0.1412	0.0548	0.1125	0.1045	0.1347	0.1883	0.0573	0.0953
11	-1.8228	-0.1788	0.0000	0.8763	0.7541	0.7995	0.9725	0.8395	0.8942	0.9699	0.9426	0.8962

Dipole moment (in D) 6.29 (DEN) 6.07 4.79 5.61 7.53 5.97 6.13 7.45 7.16 6.72

File Nax_15.out

Molecule _15 Na+C2H3

SP Nax_15 B3LYP/Def2TZVP VAC.

1 6

Dipole -5.1297 -0.6823 0.6589 5.2167

Quadrupole 8.9916 -2.9669 -6.0247 0.1784 0.9661 1.0433

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	1.3568	-0.4831	0.0182	-0.2024	-0.1601	-0.0226	-0.2799	-0.1344	-0.1815	-0.4878	-0.0542	-0.1460
6	0.8511	0.7101	-0.1531	-0.2374	-0.0483	-0.0228	-0.2502	-0.1157	-0.2710	-0.1914	-0.2817	-0.1325
1	1.2114	-1.3005	-0.6859	0.1896	0.1590	0.0810	0.1649	0.1322	0.1700	0.2341	0.0982	0.1226
1	1.9981	-0.7085	0.8749	0.1922	0.1660	0.0912	0.1964	0.1424	0.1827	0.2530	0.1271	0.1388
1	0.9618	1.6981	0.2746	0.2159	0.1555	0.0950	0.1916	0.1458	0.2302	0.2139	0.1619	0.1389
11	-1.5835	-0.0956	0.0314	0.8421	0.7278	0.7781	0.9772	0.8297	0.8696	0.9782	0.9486	0.8782

Dipole moment (in D) 5.22 (DEN) 4.87 3.60 4.41 6.65 4.92 5.21 6.70 6.31 5.55

File Nax_18.out

Molecule _18 Na+propyne

SP Nax_18 B3LYP/Def2TZVP VAC.

1 8

Dipole 5.9023 -2.6185 0.0001 6.4571

Quadrupole 12.7175 -3.1628 -9.5547 -2.1644 -0.0001 0.0001

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0848	1.2842	-0.0000	-0.2637	-0.0588	-0.0873	-0.4965	-0.1771	-0.6325	-0.3665	-0.2090	-0.2020
6	-0.7402	0.4033	0.0000	0.0480	-0.0716	0.0156	0.1610	-0.0215	0.2662	0.0304	-0.2593	0.0042
1	0.6735	2.1749	0.0000	0.2396	0.1660	0.1149	0.2537	0.1672	0.3693	0.2681	0.2049	0.1576
6	-1.7960	-0.5996	-0.0000	-0.3772	-0.2374	-0.0366	-0.4282	-0.1820	-0.4800	-0.6970	0.0673	-0.2094
1	-1.7552	-1.2299	-0.8899	0.1685	0.1532	0.0705	0.1639	0.1219	0.1615	0.2517	0.0725	0.1193
1	-1.7541	-1.2312	0.8889	0.1684	0.1532	0.0704	0.1639	0.1219	0.1614	0.2517	0.0725	0.1193
1	-2.7623	-0.0900	0.0010	0.1932	0.1676	0.0858	0.1974	0.1377	0.2649	0.2774	0.1062	0.1372
11	1.8460	-0.5592	0.0000	0.8233	0.7278	0.7667	0.9849	0.8318	0.8893	0.9843	0.9450	0.8738

Dipole moment (in D) 6.46 (DEN) 6.07 4.86 5.50 7.92 6.18 6.32 8.06 7.43 6.75

File Nax_19.out

Molecule _19 Na(NH3)+

SP Nax_19 B3LYP/Def2TZVP VAC.

1 5

Dipole 0.0020 -2.6762 0.0000 2.6762

Quadrupole -3.4761 6.9526 -3.4766 -0.0002 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	-0.0001	-1.1756	0.0000	0.9183	0.7286	0.7874	1.0027	0.9052	0.9391	0.9816	0.9475	0.9119
7	-0.0001	1.1720	0.0000	-0.7648	-0.2514	-0.2030	-1.1526	-0.8570	-1.1455	-1.1521	-1.1183	-0.7033
1	-0.9343	1.5770	0.0000	0.2822	0.1743	0.1386	0.3834	0.3173	0.4021	0.3902	0.3903	0.2639
1	0.4678	1.5753	0.8095	0.2822	0.1742	0.1385	0.3833	0.3173	0.4022	0.3901	0.3902	0.2638
1	0.4678	1.5753	-0.8095	0.2822	0.1742	0.1385	0.3833	0.3173	0.4022	0.3901	0.3902	0.2638

Dipole moment (in D) 2.68 (DEN) 3.08 1.57 2.44 3.45 2.73 2.62 3.17 2.78 3.12

File Nax_20.out

Molecule _20 Na+N(CH3)H2

SP Nax_20 B3LYP/Def2TZVP VAC.

1 8

Dipole 4.0463 -3.1903 0.0000 5.1527

Quadrupole 2.2236 3.1408 -5.3645 -7.4413 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	1.2658	-1.1945	0.0000	0.8972	0.7195	0.7705	0.9972	0.8955	0.9175	0.9778	0.9424	0.9054
7	0.0000	0.7796	0.0000	-0.6461	-0.1348	-0.1715	-0.9654	-0.7328	-0.9798	-0.9276	-1.0787	-0.6233
6	-1.4757	0.5738	0.0000	-0.2424	-0.3144	-0.0163	-0.1156	-0.1235	0.2319	-0.4122	0.2787	-0.1165
1	0.2429	1.3560	0.8029	0.2654	0.1804	0.1284	0.3548	0.3116	0.3728	0.3768	0.3697	0.2496
1	0.2429	1.3560	-0.8029	0.2654	0.1804	0.1284	0.3548	0.3116	0.3728	0.3768	0.3697	0.2496
1	-2.0277	1.5143	0.0000	0.1658	0.1209	0.0558	0.1328	0.1142	0.0448	0.2076	0.0509	0.1174
1	-1.7640	0.0065	0.8842	0.1474	0.1240	0.0523	0.1207	0.1116	0.0200	0.2004	0.0335	0.1090
1	-1.7640	0.0065	-0.8842	0.1474	0.1240	0.0523	0.1207	0.1116	0.0200	0.2004	0.0335	0.1090

Dipole moment (in D) 5.15 (DEN) 5.12 4.38 4.76 5.97 5.23 5.09 5.75 4.98 5.42

File Nax_21.out

Molecule _21 Na+N(CH3)2H

SP Nax_21 B3LYP/Def2TZVP VAC.

1 11

Dipole 0.0453 -6.1142 0.0000 6.1144

Quadrupole -6.0273 11.5935 -5.5662 -1.6944 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	0.1144	-1.9637	0.0000	0.8822	0.7054	0.7549	0.9844	0.8884	0.9087	0.9772	0.9400	0.9004
7	-0.3906	0.3269	0.0000	-0.5140	-0.0442	-0.1358	-0.6845	-0.6061	-0.7010	-0.7160	-1.0518	-0.5319
1	-1.4019	0.4351	0.0000	0.2437	0.1916	0.1215	0.3175	0.3100	0.3711	0.3714	0.3567	0.2387
6	0.1144	0.9928	1.2232	-0.2536	-0.3005	-0.0226	-0.1657	-0.1269	-0.0918	-0.4208	0.2799	-0.1241
6	0.1144	0.9928	-1.2232	-0.2536	-0.3005	-0.0226	-0.1657	-0.1269	-0.0918	-0.4208	0.2800	-0.1241
1	-0.1034	2.0646	1.2266	0.1577	0.1226	0.0520	0.1281	0.1113	0.1279	0.2029	0.0430	0.1110
1	1.1967	0.8712	1.2875	0.1424	0.1260	0.0489	0.1139	0.1089	0.1014	0.1965	0.0254	0.1029
1	-0.3412	0.5461	2.1072	0.1476	0.1254	0.0513	0.1150	0.1106	0.0732	0.2051	0.0292	0.1066

1	-0.1034	2.0646	-1.2266	0.1577	0.1226	0.0520	0.1281	0.1113	0.1279	0.2029	0.0430	0.1110
1	1.1967	0.8712	-1.2875	0.1424	0.1260	0.0489	0.1139	0.1089	0.1014	0.1965	0.0254	0.1029
1	-0.3412	0.5461	-2.1072	0.1476	0.1254	0.0513	0.1150	0.1106	0.0732	0.2051	0.0292	0.1066

Dipole moment (in D) 6.11 (DEN) 5.97 5.05 5.59 7.19 6.20 6.00 6.84 5.91 6.41

File Nax_22.out

Molecule _22 Na+N(CH3)3

SP Nax_22 B3LYP/Def2TZVP VAC.

1 14

Dipole 6.6819 0.0044 0.0000 6.6819

Quadrupole 12.6719 -6.3365 -6.3354 0.0134 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	2.0917	0.0012	0.0000	0.8718	0.6882	0.7411	0.9724	0.8840	0.8994	0.9808	0.9395	0.8970
7	-0.2557	-0.0005	0.0000	-0.4130	0.0188	-0.0979	-0.3211	-0.4773	-0.2985	-0.5184	-1.0335	-0.4323
6	-0.7436	-1.3945	0.0000	-0.2575	-0.2831	-0.0268	-0.2311	-0.1285	-0.3404	-0.4255	0.2806	-0.1303
6	-0.7436	0.6968	1.2073	-0.2574	-0.2829	-0.0268	-0.2312	-0.1285	-0.2885	-0.4255	0.2803	-0.1304
6	-0.7436	0.6968	-1.2073	-0.2574	-0.2829	-0.0268	-0.2312	-0.1285	-0.2885	-0.4255	0.2804	-0.1304
1	-1.8393	-1.4377	0.0000	0.1532	0.1256	0.0493	0.1268	0.1093	0.1837	0.2001	0.0383	0.1059
1	-0.3859	-1.9180	0.8877	0.1423	0.1275	0.0482	0.1103	0.1084	0.1404	0.2023	0.0229	0.1014
1	-0.3859	-1.9180	-0.8877	0.1423	0.1275	0.0482	0.1103	0.1084	0.1404	0.2023	0.0229	0.1014
1	-1.8392	0.7194	1.2438	0.1533	0.1256	0.0493	0.1268	0.1093	0.1725	0.2002	0.0383	0.1059
1	-0.3848	1.7269	1.2171	0.1422	0.1275	0.0482	0.1102	0.1084	0.1249	0.2022	0.0228	0.1014
1	-0.3875	0.1888	2.1046	0.1424	0.1275	0.0483	0.1104	0.1085	0.1286	0.2023	0.0230	0.1015
1	-1.8392	0.7194	-1.2438	0.1533	0.1256	0.0493	0.1268	0.1093	0.1725	0.2002	0.0383	0.1059
1	-0.3875	0.1888	-2.1046	0.1424	0.1275	0.0483	0.1104	0.1085	0.1286	0.2023	0.0230	0.1015
1	-0.3848	1.7269	-1.2171	0.1422	0.1275	0.0482	0.1102	0.1084	0.1249	0.2022	0.0228	0.1014

Dipole moment (in D) 6.68 (DEN) 6.38 5.18 6.01 8.05 6.74 6.55 7.49 6.43 7.00

File Nax_23.out

Molecule _23 C5H5N-Na+

SP Nax_23 B3LYP/Def2TZVP VAC.


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1 12
Dipole      8.2869  -0.0002  -0.0012  8.2869
Quadrupole 28.3850  -8.8488 -19.5362 -0.0005 -0.0020 -0.0001

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
7      0.6434  0.0002  0.0003  -0.4657  0.1230  -0.1568  -0.6612  -0.4758  -0.7983  -0.5833  -1.2481  -0.4866
6     -0.0532  -1.1486  0.0001  0.0644  -0.1633  0.0400  0.1905  0.0541  0.4408  0.0339  0.4721  0.0813
6     -1.4374  -1.1951  -0.0000  -0.1149  -0.1079  -0.0111  -0.1444  -0.0620  -0.3630  -0.2230  -0.0016  -0.0544
6     -2.1449  -0.0002  -0.0001  -0.0844  -0.0705  0.0198  0.0132  -0.0340  0.2439  -0.1246  0.0074  -0.0247
6     -0.0534  1.1487  0.0002  0.0643  -0.1633  0.0400  0.1905  0.0541  0.4409  0.0339  0.4723  0.0813
6     -1.4377  1.1950  -0.0001  -0.1149  -0.1079  -0.0111  -0.1444  -0.0620  -0.3630  -0.2230  -0.0015  -0.0544
1      0.5193  -2.0694  0.0001  0.1343  0.1491  0.0572  0.0814  0.1223  0.0146  0.1948  0.0477  0.1036
1     -1.9448  -2.1498  -0.0001  0.1614  0.1607  0.0702  0.1385  0.1268  0.1773  0.2394  0.0855  0.1182
1     -3.2270  -0.0003  -0.0002  0.1649  0.1614  0.0744  0.1345  0.1305  0.0910  0.2365  0.0897  0.1228
1      0.5188  2.0697  0.0003  0.1344  0.1491  0.0572  0.0814  0.1223  0.0146  0.1949  0.0477  0.1036
1     -1.9453  2.1496  -0.0003  0.1614  0.1607  0.0702  0.1385  0.1268  0.1773  0.2394  0.0855  0.1182
11     2.9395  -0.0000  -0.0002  0.8948  0.7090  0.7498  0.9815  0.8968  0.9240  0.9810  0.9429  0.8911

Dipole moment (in D)  8.29 (DEN)      8.72      7.93      7.85      9.31      8.59      8.20      9.23      6.41      8.45

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File Nax_24.out

Molecule _24 HCN-Na+

SP Nax_24 B3LYP/Def2TZVP VAC.

1 4

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Dipole      0.0000  0.0000  3.0827  3.0827
Quadrupole -8.7837  -8.7837  17.5674  0.0000  0.0000  0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
1      0.0000  0.0000  -2.8604  0.2635  0.1631  0.1709  0.2509  0.2302  0.2514  0.2653  0.2906  0.2317
6      0.0000  0.0000  -1.7882  -0.0625  -0.0020  0.1778  0.2926  0.2455  0.3031  0.2523  1.0596  0.2508
7      0.0000  0.0000  -0.6457  -0.1803  0.1102  -0.1501  -0.5445  -0.4126  -0.5077  -0.5102  -1.3149  -0.3963
11     0.0000  0.0000  1.6463  0.9793  0.7287  0.8014  1.0010  0.9370  0.9532  0.9926  0.9647  0.9138

Dipole moment (in D)  3.08 (DEN)      5.22      3.20      2.93      3.64      3.42      3.06      3.62      1.39      3.12

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File Nax_25.out

Molecule _25 CH3CN-Na+

SP Nax_25 B3LYP/Def2TZVP VAC.

1 7

Dipole 5.2477 -0.0114 0.0008 5.2477

Quadrupole 25.5256 -12.7628 -12.7628 -0.0120 0.0008 0.0001

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	-0.9486	0.0007	0.0000	-0.0141	-0.0974	0.1673	0.5994	0.2706	0.6100	0.4501	1.0007	0.3165
6	-2.3969	-0.0012	0.0001	-0.2389	-0.2219	-0.0170	-0.4947	-0.1569	-0.5013	-0.7237	0.0779	-0.1859
1	-2.7664	0.9472	0.3922	0.1850	0.1670	0.0897	0.2003	0.1424	0.2107	0.2783	0.1129	0.1433
1	-2.7649	-0.1364	-1.0178	0.1850	0.1670	0.0896	0.2002	0.1423	0.2102	0.2783	0.1128	0.1432
1	-2.7642	-0.8157	0.6257	0.1850	0.1670	0.0896	0.2002	0.1423	0.2103	0.2783	0.1128	0.1432
7	0.1998	0.0027	-0.0002	-0.2660	0.1047	-0.2024	-0.7110	-0.4738	-0.6974	-0.5507	-1.3766	-0.4657
11	2.4518	-0.0011	0.0001	0.9640	0.7135	0.7833	1.0057	0.9331	0.9576	0.9893	0.9595	0.9053

Dipole moment (in D) 5.25 (DEN) 6.54 4.85 4.89 6.15 5.44 5.22 6.31 0.03 5.20

File Nax_26.out

Molecule _26 Na(H2O)+

SP Nax_26 B3LYP/Def2TZVP VAC.

1 4

Dipole 0.0000 0.0000 2.3704 2.3704

Quadrupole -5.8477 -2.2930 8.1407 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
11	0.0000	0.0000	1.1099	0.9496	0.7593	0.8208	1.0241	0.9283	0.9921	0.9951	0.9681	0.8963
8	0.0000	0.0000	-1.1036	-0.7105	-0.1660	-0.2345	-1.0791	-0.6689	-1.0163	-1.0085	-1.2035	-0.5150
1	0.0000	0.7677	-1.6902	0.3805	0.2033	0.2069	0.5276	0.3703	0.5121	0.5067	0.6177	0.3094
1	0.0000	-0.7677	-1.6902	0.3805	0.2033	0.2069	0.5276	0.3703	0.5121	0.5067	0.6177	0.3094

Dipole moment (in D) 2.37 (DEN) 2.65 1.63 2.26 2.61 2.48 2.36 2.42 1.51 2.48

File Nax_30.out

Molecule _30 Na+CH3OH

SP Nax_30 B3LYP/Def2TZVP VAC.

1 7

Dipole -4.9584 0.1275 0.0004 4.9600

Quadrupole 11.1765 -3.5665 -7.6100 -2.0339 0.0002 -0.0006

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.3836	-0.4878	-0.0000	-0.5985	-0.0224	-0.2088	-0.8134	-0.5349	-0.7842	-0.8128	-1.1477	-0.4258
6	1.5883	0.3260	0.0000	-0.1420	-0.2872	0.0298	-0.0314	-0.1052	0.1196	-0.2468	0.4150	-0.0946
1	2.1764	0.1274	-0.8948	0.1616	0.1200	0.0612	0.1213	0.1191	0.0738	0.1952	0.0643	0.1158
1	1.2732	1.3670	0.0002	0.1243	0.1210	0.0596	0.1095	0.1182	0.0802	0.1840	0.0420	0.1064
1	2.1765	0.1271	0.8947	0.1616	0.1200	0.0612	0.1213	0.1191	0.0738	0.1952	0.0643	0.1158
1	0.6509	-1.4146	0.0002	0.3567	0.2052	0.1935	0.4822	0.3627	0.4768	0.4934	0.5978	0.2937
11	-1.7159	0.1581	0.0000	0.9364	0.7435	0.8034	1.0104	0.9210	0.9600	0.9919	0.9640	0.8887

Dipole moment (in D) 4.96 (DEN) 4.68 4.48 4.54 5.36 5.04 4.92 4.82 3.44 4.86

File Nax_31.out

Molecule_31 Na+O(CH3)2

SP Nax_31 B3LYP/Def2TZVP VAC.

1 10

Dipole -6.0118 -0.0005 -0.0004 6.0118

Quadrupole 12.8904 -4.3900 -8.5004 0.0011 0.0003 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.2272	-0.0000	0.0001	-0.4817	0.1134	-0.1694	-0.4805	-0.3860	-0.3620	-0.6136	-1.1103	-0.3207
6	1.0335	1.1912	-0.0000	-0.1473	-0.2855	0.0218	-0.0852	-0.1099	-0.2309	-0.2563	0.4333	-0.0996
6	1.0341	-1.1910	-0.0000	-0.1473	-0.2855	0.0218	-0.0852	-0.1099	-0.2309	-0.2563	0.4331	-0.0996
1	1.6607	1.2222	-0.8931	0.1531	0.1222	0.0567	0.1152	0.1156	0.1623	0.1915	0.0551	0.1093
1	1.6611	1.2221	0.8927	0.1531	0.1222	0.0567	0.1152	0.1156	0.1624	0.1915	0.0551	0.1093
1	0.3637	2.0501	0.0002	0.1173	0.1222	0.0562	0.0965	0.1148	0.1199	0.1852	0.0308	0.0999
1	1.6613	-1.2217	-0.8931	0.1531	0.1222	0.0567	0.1152	0.1156	0.1623	0.1915	0.0551	0.1093
1	1.6617	-1.2217	0.8927	0.1531	0.1222	0.0567	0.1152	0.1156	0.1624	0.1915	0.0551	0.1093
1	0.3646	-2.0502	0.0002	0.1174	0.1222	0.0562	0.0965	0.1148	0.1199	0.1852	0.0309	0.0999
11	-1.9632	-0.0002	-0.0000	0.9293	0.7245	0.7863	0.9972	0.9140	0.9346	0.9899	0.9614	0.8830

Dipole moment (in D) 6.01 (DEN) 5.46 5.22 5.38 6.76 6.04 5.90 5.79 4.11 5.83

File Nax_34.out

Molecule _34 Na+OC(CH3)2

SP Nax_34 B3LYP/Def2TZVP VAC.

1 11

Dipole -6.5969 0.0003 0.0000 6.5969

Quadrupole 22.8494 -10.4004 -12.4490 0.0001 0.0000 0.1689

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	-0.4961	-0.0001	0.0000	-0.5073	0.1444	-0.2586	-0.7587	-0.4409	-0.7886	-0.7201	-1.2526	-0.4335
6	0.7337	-0.0000	0.0000	0.3181	-0.2859	0.2172	0.8305	0.2250	0.8588	0.6551	0.9432	0.3753
6	1.5032	1.2828	-0.0047	-0.3370	-0.2302	-0.0673	-0.5734	-0.2101	-0.4793	-0.7085	-0.0248	-0.2440
6	1.5034	-1.2826	0.0047	-0.3370	-0.2302	-0.0673	-0.5734	-0.2101	-0.4792	-0.7085	-0.0245	-0.2440
1	2.3279	1.2387	-0.7184	0.1575	0.1501	0.0672	0.1803	0.1198	0.1489	0.2504	0.0678	0.1200
1	1.9572	1.4192	0.9824	0.1652	0.1575	0.0713	0.1844	0.1239	0.1588	0.2593	0.0743	0.1224
1	0.8587	2.1316	-0.2198	0.1372	0.1383	0.0567	0.1659	0.1118	0.1525	0.2362	0.0553	0.1015
1	1.9574	-1.4190	-0.9825	0.1652	0.1575	0.0713	0.1844	0.1239	0.1588	0.2593	0.0743	0.1224
1	2.3282	-1.2383	0.7183	0.1575	0.1501	0.0672	0.1803	0.1198	0.1489	0.2504	0.0678	0.1200
1	0.8591	-2.1316	0.2199	0.1372	0.1383	0.0567	0.1659	0.1118	0.1525	0.2363	0.0553	0.1015
11	-2.6147	-0.0000	-0.0000	0.9436	0.7099	0.7855	1.0138	0.9251	0.9678	0.9901	0.9633	0.8583

Dipole moment (in D) 6.60 (DEN) 6.63 6.13 6.14 7.41 6.88 6.60 6.22 2.77 6.12

File Nax_37.out

Molecule _37 Na+HCON(CH3)2

SP Nax_37 B3LYP/Def2TZVP VAC.

1 13

Dipole 7.2957 -0.0458 0.0002 7.2958

Quadrupole 31.4077 -13.2560 -18.1517 1.2703 0.0003 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
7	-1.1976	-0.0155	0.0000	-0.0464	0.1769	0.0046	-0.0460	-0.2784	0.0971	-0.3442	-1.1532	-0.2652
6	-0.0593	-0.6913	-0.0000	0.2253	-0.3291	0.1644	0.5617	0.2187	0.4229	0.5317	1.4443	0.3227
6	-1.2337	1.4429	0.0000	-0.2672	-0.2464	-0.0136	-0.2571	-0.1030	-0.2246	-0.4150	0.3090	-0.1126
6	-2.4851	-0.7043	0.0000	-0.2436	-0.2485	-0.0090	-0.2655	-0.0998	-0.4912	-0.3981	0.3182	-0.1059

1	-1.7603	1.7987	-0.8869	0.1536	0.1299	0.0570	0.1324	0.1185	0.1235	0.2157	0.0540	0.1162
1	-0.2203	1.8299	0.0004	0.1405	0.1300	0.0487	0.1314	0.1160	0.1211	0.2257	0.0650	0.0917
1	-1.7610	1.7986	0.8865	0.1536	0.1299	0.0570	0.1324	0.1185	0.1235	0.2157	0.0540	0.1162
1	-3.0567	-0.4276	-0.8870	0.1538	0.1284	0.0572	0.1330	0.1184	0.1908	0.2134	0.0550	0.1170
1	-2.3304	-1.7811	-0.0001	0.1346	0.1286	0.0582	0.1262	0.1204	0.1782	0.2166	0.0516	0.1186
1	-3.0566	-0.4278	0.8871	0.1538	0.1284	0.0572	0.1330	0.1184	0.1908	0.2134	0.0550	0.1170
8	1.0807	-0.1916	-0.0000	-0.6042	0.0449	-0.3145	-0.8447	-0.5044	-0.7330	-0.8050	-1.2843	-0.4770
1	-0.1894	-1.7794	0.0000	0.1184	0.1382	0.0625	0.0499	0.1373	0.0544	0.1404	0.0720	0.1103
11	3.1619	0.0315	0.0000	0.9276	0.6887	0.7702	1.0132	0.9193	0.9464	0.9899	0.9584	0.8509

Dipole moment (in D) 7.30 (DEN) 6.77 6.58 6.78 8.07 7.61 7.22 7.21 5.64 6.90

File Nax_39.out

Molecule _39 Na+CH2Cl2

SP Nax_39 B3LYP/Def2TZVP VAC.

1 6

Dipole 0.0000 0.0000 5.5266 5.5266

Quadrupole -8.1754 -8.4213 16.5968 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
6	0.0000	0.0000	-1.3224	-0.0584	-0.6336	0.0670	-0.0927	-0.0357	-0.8704	-0.3653	0.2167	0.0494
1	0.9039	0.0000	-1.9195	0.2012	0.1322	0.0867	0.1608	0.1428	0.4553	0.2475	0.1516	0.1400
1	-0.9039	0.0000	-1.9195	0.2012	0.1322	0.0867	0.1608	0.1428	0.4540	0.2475	0.1516	0.1400
17	0.0000	1.4838	-0.3136	-0.0528	0.4812	0.0331	-0.0868	-0.0142	0.0496	-0.0438	-0.2329	-0.0797
17	0.0000	-1.4838	-0.3136	-0.0528	0.4812	0.0331	-0.0868	-0.0142	0.0496	-0.0438	-0.2329	-0.0797
11	0.0000	0.0000	2.0396	0.7617	0.4069	0.6931	0.9447	0.7785	0.8618	0.9580	0.9458	0.8300

Dipole moment (in D) 5.53 (DEN) 4.28 4.12 4.67 7.14 5.26 5.44 7.27 5.79 5.48

File Nax_40.out

Molecule _40 Na+S(CH3)2

SP Nax_40 B3LYP/Def2TZVP VAC.

1 10

Dipole -7.2415 0.0001 1.7762 7.4562

Quadrupole 17.8290 -5.8600 -11.9690 -0.0001 -1.0905 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.2754	-0.0000	-0.4753	-0.0842	0.5998	0.0211	-0.0017	-0.0902	-0.2168	0.0906	-0.1403	-0.2069
6	1.1454	1.4096	0.2771	-0.3234	-0.4581	-0.0601	-0.4259	-0.1957	-0.3479	-0.7136	-0.0939	-0.1898
6	1.1454	-1.4096	0.2771	-0.3234	-0.4581	-0.0601	-0.4259	-0.1957	-0.3478	-0.7136	-0.0938	-0.1898
1	2.1929	1.3715	-0.0163	0.1697	0.1254	0.0641	0.1674	0.1172	0.2168	0.2367	0.0782	0.1247
1	1.0594	1.4013	1.3619	0.1504	0.1166	0.0530	0.1426	0.1056	0.1330	0.2206	0.0549	0.1100
1	0.7018	2.3188	-0.1250	0.1550	0.1257	0.0611	0.1522	0.1140	0.1679	0.2370	0.0656	0.1194
1	2.1928	-1.3716	-0.0164	0.1697	0.1254	0.0641	0.1674	0.1172	0.2168	0.2367	0.0782	0.1247
1	1.0595	-1.4012	1.3619	0.1504	0.1167	0.0530	0.1426	0.1056	0.1330	0.2206	0.0549	0.1100
1	0.7017	-2.3188	-0.1249	0.1550	0.1257	0.0611	0.1522	0.1139	0.1679	0.2370	0.0656	0.1194
11	-2.3690	0.0000	0.1671	0.7807	0.5809	0.7427	0.9289	0.8079	0.8770	0.9481	0.9309	0.8786

Dipole moment (in D) 7.46 (DEN) 6.63 6.23 6.86 9.34 7.32 7.26 9.77 9.28 8.05

Keywords:

File mol302.out

Molecule 302 MgClF

SP Mol302 B3LYP/Def2TZVP VAC.

0 3

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
Dipole	0.0000	0.0000	0.1218	0.1218								
Quadrupole	5.8157	5.8157	-11.6314	0.0000	0.0000	0.0000						
9	0.0000	0.0000	-2.2976	-0.5630	-0.3604	-0.4261	-0.8313	-0.5458	-0.6138	-0.9090	-0.8828	-0.4307
12	0.0000	0.0000	-0.5573	0.9888	0.3604	0.7566	1.5909	0.9551	1.1199	1.7436	1.7240	0.7888
17	0.0000	0.0000	1.6098	-0.4258	0.0001	-0.3304	-0.7596	-0.4093	-0.5061	-0.8347	-0.8413	-0.3581

Dipole moment (in D) 0.12 (DEN) 0.27 3.01 0.12 0.96 0.30 0.14 1.09 1.38 0.13

File mol303.out

Molecule 303 MgBrF

SP Mol303 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 0.2838 0.2838
 Quadrupole 5.6587 5.6587 -11.3174 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	-2.9085	-0.5605	-0.3586	-0.4261	-0.8185	-0.5459	-0.6190	-0.9074	-0.8835	-0.4290
12	0.0000	0.0000	-1.1685	0.9818	0.3168	0.7202	1.5318	0.8984	1.0968	1.7096	1.7037	0.7548
35	0.0000	0.0000	1.1485	-0.4213	0.0418	-0.2940	-0.7133	-0.3524	-0.4777	-0.8022	-0.8201	-0.3258

Dipole moment (in D) 0.28 (DEN) 0.00 3.46 0.29 1.10 0.64 0.14 1.34 1.74 0.04

 File mol304.out

Molecule 304 MgBrCl

SP Mol304 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 0.1580 0.1580
 Quadrupole 5.1768 5.1768 -10.3536 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	-2.8724	-0.4171	-0.0001	-0.3324	-0.7019	-0.4095	-0.4555	-0.8136	-0.8403	-0.3529
12	0.0000	0.0000	-0.6951	0.8356	-0.0377	0.6285	1.3712	0.7624	0.8862	1.5953	1.6586	0.6748
35	0.0000	0.0000	1.6335	-0.4186	0.0378	-0.2961	-0.6692	-0.3529	-0.4307	-0.7818	-0.8183	-0.3219

Dipole moment (in D) 0.16 (DEN) 0.32 0.42 0.16 0.14 0.33 0.05 0.24 0.36 0.09

 File mol305.out

Molecule 305 Mg=CH2

SP Mol305 B3LYP/Def2TZVP VAC.

0 4

Dipole -0.1078 -3.2510 0.0000 3.2528
 Quadrupole -1.1668 -0.1575 1.3243 3.0175 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
12	-0.0629	-0.8430	0.0000	0.4008	0.3658	0.3344	0.6061	0.3917	0.4337	0.8130	0.7950	0.3502
6	-0.0629	1.1957	0.0000	-0.6428	-0.5988	-0.3089	-0.7818	-0.4592	-0.5833	-1.1136	-0.7674	-0.4250
1	0.5665	1.4710	0.8682	0.1210	0.1165	-0.0128	0.0878	0.0337	0.0748	0.1503	-0.0139	0.0374
1	0.5665	1.4710	-0.8682	0.1210	0.1165	-0.0128	0.0878	0.0337	0.0748	0.1503	-0.0139	0.0374

Dipole moment (in D) 3.25 (DEN) 3.68 3.35 3.31 5.73 3.75 4.07 7.62 7.82 3.34

File mol307.out

Molecule 307 MgFCH3

SP Mol307 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -2.0256 2.0256

Quadrupole 4.9558 4.9558 -9.9116 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	1.8868	-0.5655	-0.3688	-0.4415	-0.8227	-0.5573	-0.6677	-0.9064	-0.8985	-0.4402
12	0.0000	0.0000	0.1331	0.9156	0.6307	0.6950	1.5142	0.8653	1.1695	1.6527	1.6330	0.7350
6	0.0000	0.0000	-1.9232	-0.7529	-0.6290	-0.2850	-1.1416	-0.4836	-1.1820	-1.3975	-0.7230	-0.4964
1	-1.0072	0.0000	-2.3463	0.1342	0.1224	0.0105	0.1500	0.0585	0.2254	0.2171	-0.0040	0.0672
1	0.5036	0.8722	-2.3463	0.1342	0.1224	0.0105	0.1500	0.0585	0.2274	0.2171	-0.0040	0.0672
1	0.5036	-0.8722	-2.3463	0.1342	0.1224	0.0105	0.1500	0.0585	0.2274	0.2171	-0.0040	0.0672

Dipole moment (in D) 2.03 (DEN) 2.12 1.27 1.28 1.01 2.01 2.05 1.59 0.29 1.21

File mol308.out

Molecule 308 MgClCH3

SP Mol308 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -2.1265 2.1265

Quadrupole 4.0048 4.0048 -8.0096 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	1.7266	-0.4414	-0.0182	-0.3611	-0.7242	-0.4367	-0.5096	-0.8246	-0.8615	-0.3795
12	0.0000	0.0000	-0.4580	0.7739	0.2808	0.6137	1.3870	0.7443	0.9014	1.5462	1.5928	0.6704
6	0.0000	0.0000	-2.5115	-0.7392	-0.6311	-0.2863	-1.1095	-0.4856	-0.7944	-1.3749	-0.7234	-0.4955
1	-1.0088	0.0000	-2.9293	0.1356	0.1228	0.0112	0.1489	0.0593	0.1333	0.2178	-0.0029	0.0682
1	0.5044	0.8736	-2.9293	0.1356	0.1228	0.0112	0.1489	0.0593	0.1347	0.2178	-0.0029	0.0682
1	0.5044	-0.8736	-2.9293	0.1356	0.1228	0.0112	0.1489	0.0593	0.1347	0.2178	-0.0029	0.0682

Dipole moment (in D) 2.13 (DEN) 2.17 1.66 1.36 1.96 1.91 2.29 2.85 1.80 1.52

File mol309.out

Molecule 309 MgBrCH3

SP Mol309 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -2.0940 2.0940

Quadrupole 2.9374 2.9374 -5.8748 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.0000	1.2281	-0.4494	0.0190	-0.3312	-0.6847	-0.3872	-0.4670	-0.7944	-0.8431	-0.3548
12	0.0000	0.0000	-1.1072	0.7725	0.2401	0.5832	1.3364	0.6941	0.8125	1.5115	1.5725	0.6430
6	0.0000	0.0000	-3.1611	-0.7315	-0.6281	-0.2862	-1.0969	-0.4855	-0.6204	-1.3705	-0.7218	-0.4938
1	0.0000	1.0095	-3.5766	0.1361	0.1230	0.0114	0.1484	0.0595	0.0912	0.2178	-0.0026	0.0686
1	0.8743	-0.5048	-3.5766	0.1361	0.1230	0.0114	0.1484	0.0595	0.0923	0.2178	-0.0026	0.0686
1	-0.8743	-0.5048	-3.5766	0.1361	0.1230	0.0114	0.1484	0.0595	0.0913	0.2178	-0.0026	0.0686

Dipole moment (in D) 2.09 (DEN) 2.67 2.03 1.30 2.14 1.67 2.38 3.14 2.25 1.55

File Mgx_1.out

Molecule _1 CH3MgH

SP Mgx_1 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0004 -0.4338 0.0000 0.4338

Quadrupole 4.3891 -8.7783 4.3892 0.0015 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
12	0.0000	0.8330	0.0000	0.4902	0.4905	0.5420	1.3278	0.5864	0.9497	1.4178	1.5181	0.6085
6	0.0000	-1.2574	0.0000	-0.7444	-0.6501	-0.2980	-1.0688	-0.4916	-0.9033	-1.3786	-0.7209	-0.4961
1	1.0161	-1.6634	0.0000	0.1267	0.1176	0.0036	0.1365	0.0514	0.1476	0.2117	-0.0135	0.0598
1	-0.5081	-1.6631	0.8800	0.1267	0.1176	0.0036	0.1364	0.0514	0.1494	0.2117	-0.0135	0.0598
1	-0.5081	-1.6631	-0.8800	0.1267	0.1176	0.0036	0.1364	0.0514	0.1494	0.2117	-0.0135	0.0598
1	-0.0003	2.5379	0.0000	-0.1258	-0.1932	-0.2548	-0.6684	-0.2489	-0.4927	-0.6742	-0.7564	-0.2919

Dipole moment (in D) 0.43 (DEN) 1.89 0.72 0.78 0.35 1.05 0.32 0.71 1.53 0.44

File Mgx_2.out

Molecule _2 MgH(CH=CH2)
SP Mgx_2 B3LYP/Def2TZVP VAC.
0 7

Dipole -0.0887 0.3832 0.0000 0.3933

Quadrupole 3.1084 -5.3674 2.2590 -4.6388 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	-1.4338	-2.6609	0.0000	-0.1212	-0.1908	-0.2493	-0.6620	-0.2434	-0.4993	-0.6697	-0.7511	-0.2871
12	-0.8019	-1.0830	0.0000	0.4156	0.5060	0.5449	1.3280	0.5967	0.9931	1.4355	1.5333	0.5971
6	0.0000	0.8347	0.0000	-0.3151	-0.4071	-0.2479	-0.8705	-0.3558	-0.7164	-0.8675	-0.6676	-0.3207
1	-0.6276	1.7293	0.0000	0.1053	0.1293	0.0085	0.1342	0.0608	0.1811	0.1763	-0.0072	0.0575
6	1.3149	1.0871	0.0000	-0.2768	-0.2575	-0.0988	-0.0910	-0.2041	-0.1538	-0.4073	-0.1052	-0.1870
1	2.0672	0.3005	0.0000	0.0934	0.1130	0.0186	0.0690	0.0703	0.0835	0.1621	-0.0120	0.0688
1	1.7279	2.0956	0.0000	0.0987	0.1071	0.0241	0.0922	0.0755	0.1118	0.1706	0.0098	0.0714

Dipole moment (in D) 0.39 (DEN) 1.71 1.07 1.04 0.28 1.36 0.32 1.48 2.12 0.57

File Mgx_4.out

Molecule _4 MgH(CN)
SP Mgx_4 B3LYP/Def2TZVP VAC.
0 4

Dipole 0.0000 0.0000 3.5122 3.5122

Quadrupole 5.8313 5.8313 -11.6626 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	2.9532	-0.0891	-0.1762	-0.2259	-0.6476	-0.2196	-0.4543	-0.6383	-0.7253	-0.2649
12	0.0000	0.0000	1.2722	0.4888	0.5436	0.6501	1.3970	0.7080	0.9893	1.4573	1.5861	0.7037
6	0.0000	0.0000	-0.7788	-0.3443	-0.3868	-0.1879	-0.5682	-0.1272	-0.1802	-0.4364	0.3926	-0.0555
7	0.0000	0.0000	-1.9352	-0.0555	0.0193	-0.2362	-0.1811	-0.3612	-0.3548	-0.3826	-1.2535	-0.3832

Dipole moment (in D) 3.51 (DEN) 3.53 2.09 3.67 3.16 5.04 3.57 5.04 9.59 4.31

File Mgx_5.out

Molecule _5 MgH(NH2)

SP Mgx_5 B3LYP/Def2TZVP VAC.

0 5

Dipole 0.0000 0.0000 -0.7844 0.7844

Quadrupole 0.7962 5.1120 -5.9081 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	2.4460	-0.1176	-0.1899	-0.2416	-0.7063	-0.2353	-0.5321	-0.6771	-0.7464	-0.2766
12	0.0000	0.0000	0.7525	0.5468	0.4338	0.5494	1.4792	0.7251	1.1852	1.5386	1.5908	0.6948
7	0.0000	0.0000	-1.1416	-0.8598	-0.5198	-0.4330	-1.4277	-0.9828	-1.4899	-1.5756	-1.5075	-0.8318
1	0.0000	0.8127	-1.7424	0.2153	0.1380	0.0626	0.3275	0.2465	0.4184	0.3570	0.3315	0.2068
1	0.0000	-0.8127	-1.7424	0.2153	0.1380	0.0626	0.3275	0.2465	0.4184	0.3570	0.3315	0.2068

Dipole moment (in D) 0.78 (DEN) 1.70 0.12 0.47 0.60 1.12 0.80 0.27 0.30 0.36

File Mgx_6.out

Molecule _6 MgH(OH)

SP Mgx_6 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 -0.6318 0.6318

Quadrupole 2.1298 2.1298 -4.2597 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
12	0.0000	0.0000	0.6885	0.6382	0.4624	0.5946	1.6553	0.7465	1.1584	1.6028	1.6266	0.6406
8	0.0000	0.0000	-1.0763	-0.7975	-0.4242	-0.4887	-1.4131	-0.8191	-1.1376	-1.4068	-1.4761	-0.6065
1	0.0000	0.0000	2.3740	-0.1323	-0.1872	-0.2320	-0.7340	-0.2255	-0.4963	-0.6803	-0.7366	-0.2730
1	0.0000	0.0000	-2.0256	0.2916	0.1490	0.1261	0.4918	0.2981	0.4754	0.4844	0.5861	0.2388

Dipole moment (in D) 0.63 (DEN) 1.89 0.14 0.62 0.38 1.23 0.57 0.10 1.09 0.18

File Mgx_7.out

Molecule _7 MgCN(OH)

SP Mgx_7 B3LYP/Def2TZVP VAC.

0 5

```

Dipole      0.0000   0.0000   4.0839   4.0839
Quadrupole  5.1730   5.1730  -10.3460   0.0000   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
  6      0.0000   0.0000  -1.5103  -0.3435  -0.3644  -0.1780  -0.7028  -0.1192  -0.3126  -0.4632  0.3950  -0.0543
 12      0.0000   0.0000   0.5253   0.8617   0.5775   0.7538   1.7850   0.9844   1.3011   1.7685   1.7294   0.7897
   8      0.0000   0.0000   2.2749  -0.7588  -0.3950  -0.4808  -1.4543  -0.8170  -1.2293  -1.4165  -1.4762  -0.6073
   7      0.0000   0.0000  -2.6664  -0.0636   0.0252  -0.2310  -0.1368  -0.3563  -0.2898  -0.3800  -1.2461  -0.3778
   1      0.0000   0.0000   3.2241   0.3041   0.1568   0.1361   0.5089   0.3082   0.5306   0.4912   0.5979   0.2497

Dipole moment (in D)  4.08 (DEN)      1.90      1.89      3.01      3.35      3.76      4.05      4.82      10.59      4.46

```

File Mgx_8.out

```

Molecule_8      MgH(ONO)
SP Mgx_8 B3LYP/Def2TZVP VAC.
   0   5

```

```

Dipole      0.6641  -0.3462   0.0000   0.7489
Quadrupole  -5.6047  -0.8631   6.4678   3.3748   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
   1      2.5721  -1.3370   0.0000  -0.1168  -0.1808  -0.2370  -0.6869  -0.2303  -0.5243  -0.6653  -0.7374  -0.2797
  12      1.0777  -0.5603   0.0000   0.6019   0.4210   0.5735   1.4550   0.7680   1.1315   1.4757   1.6150   0.6194
   8     -0.9713  -0.6814   0.0000  -0.3805  -0.0750  -0.2168  -0.5886  -0.2518  -0.3494  -0.5776  -0.7141  -0.2267
   7     -1.1049   0.5745   0.0000   0.2758  -0.0903   0.0970   0.4092  -0.0340   0.0937   0.3449   0.5501   0.1138
   8      0.0000   1.1864   0.0000  -0.3804  -0.0750  -0.2168  -0.5887  -0.2519  -0.3515  -0.5777  -0.7141  -0.2267

Dipole moment (in D)  0.75 (DEN)      2.24      0.87      0.61      0.43      2.80      0.58      0.32      0.38      0.23

```

File Mgx_9.out

```

Molecule_9      MgH(NO2)
SP Mgx_9 B3LYP/Def2TZVP VAC.
   0   5

```

```

Dipole      0.0000   0.0000   3.7332   3.7332
Quadrupole  6.5025   0.8134  -7.3159   0.0000   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP

```

1	0.0000	0.0000	3.1886	-0.0779	-0.1729	-0.2128	-0.6197	-0.2063	-0.4064	-0.6401	-0.7060	-0.2518
12	0.0000	0.0000	1.5127	0.5778	0.5738	0.6766	1.3275	0.8239	0.8875	1.4481	1.5785	0.7492
7	0.0000	0.0000	-0.5159	0.1292	-0.2443	0.0500	0.1023	-0.1735	0.4063	0.0474	0.2293	0.0167
8	0.0000	1.0828	-1.1081	-0.3145	-0.0783	-0.2569	-0.4051	-0.2221	-0.4437	-0.4277	-0.5511	-0.2570
8	0.0000	-1.0828	-1.1081	-0.3145	-0.0783	-0.2569	-0.4051	-0.2221	-0.4437	-0.4277	-0.5511	-0.2570

Dipole moment (in D) 3.73 (DEN) 6.03 2.96 4.27 4.21 5.62 3.94 5.15 5.95 4.28

File Mgx_10.out

Molecule_10 MgHF

SP Mgx_10 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 1.5124 1.5124

Quadrupole 4.3426 4.3426 -8.6852 0.0000 0.0000 0.0000

	Atomic coordinates			Mu1.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	2.3251	-0.1303	-0.1815	-0.2238	-0.6835	-0.2175	-0.4818	-0.6737	-0.7254	-0.2669
12	0.0000	0.0000	0.6438	0.7108	0.5603	0.6643	1.4912	0.7719	1.1234	1.5798	1.6194	0.7043
9	0.0000	0.0000	-1.1168	-0.5805	-0.3787	-0.4404	-0.8076	-0.5543	-0.6416	-0.9061	-0.8940	-0.4374

Dipole moment (in D) 1.51 (DEN) 3.86 1.74 1.92 1.31 2.93 1.54 2.22 1.70 1.54

File Mgx_12.out

Molecule_12 MgHCl

SP Mgx_12 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 -1.5744 1.5744

Quadrupole 3.5964 3.5964 -7.1928 0.0000 0.0000 0.0000

	Atomic coordinates			Mu1.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
1	0.0000	0.0000	-2.8698	-0.1200	-0.1809	-0.2244	-0.6485	-0.2181	-0.4340	-0.6475	-0.7231	-0.2635
12	0.0000	0.0000	-1.1879	0.5753	0.2212	0.5818	1.3526	0.6494	0.9429	1.4667	1.5793	0.6364
17	0.0000	0.0000	1.0073	-0.4553	-0.0403	-0.3575	-0.7041	-0.4312	-0.5089	-0.8192	-0.8563	-0.3729

Dipole moment (in D) 1.57 (DEN) 3.83 1.04 1.96 2.19 2.79 1.86 3.41 3.19 1.80

File Mgx_14.out

Molecule _14 Mg(OH)(SH)

SP Mgx_14 B3LYP/Def2TZVP VAC.

0 5

Dipole 1.4494 0.5774 0.4875 1.6346

Quadrupole -4.5907 4.1798 0.4109 -2.1215 1.6460 0.0073

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
12	0.5868	-0.0123	0.0118	0.8568	0.2472	0.6323	1.6617	0.8720	1.0489	1.6969	1.6785	0.7186
8	2.3483	0.0170	-0.0396	-0.8013	-0.4120	-0.4851	-1.4229	-0.8159	-1.0324	-1.4073	-1.4714	-0.6071
16	-1.7049	-0.0774	-0.0015	-0.4914	-0.0456	-0.3086	-0.8695	-0.4541	-0.5579	-0.9197	-0.7520	-0.4649
1	3.2687	-0.0143	0.1931	0.3005	0.1517	0.1289	0.4944	0.3008	0.4282	0.4854	0.5879	0.2417
1	-1.8177	1.2640	0.0064	0.1354	0.0587	0.0325	0.1364	0.0973	0.1132	0.1448	-0.0427	0.1117

Dipole moment (in D) 1.63 (DEN) 1.37 1.75 0.67 2.63 1.16 1.89 3.07 4.01 1.99

Keywords:

File mol320.out

Molecule 320 AlH=NH

SP Mol310 B3LYP/Def2TZVP VAC.

0 4

Dipole -0.8712 -2.5436 0.0000 2.6887

Quadrupole 0.3470 -0.1162 -0.2308 -0.8458 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0018	-0.5655	0.0000	0.3904	0.2981	0.4910	1.5041	0.4805	0.9719	1.4765	2.0844	0.5222
1	0.5069	-2.0365	0.0000	-0.0283	-0.0977	-0.1007	-0.4655	-0.0206	-0.2222	-0.3591	-0.6802	-0.0462
7	0.0018	1.0683	0.0000	-0.5698	-0.3464	-0.4693	-1.4157	-0.7331	-1.0667	-1.4911	-1.7972	-0.6972
1	-0.5420	1.9099	0.0000	0.2078	0.1460	0.0789	0.3771	0.2732	0.3170	0.3737	0.3930	0.2213

Dipole moment (in D) 2.69 (DEN) 1.90 0.68 2.08 3.95 2.48 3.33 5.07 5.34 2.61

File mol317.out

Molecule 317 AlH2NH2

SP Mol317 B3LYP/Def2TZVP VAC.

0 6

Dipole 0.0000 0.0000 -1.2858 1.2858

Quadrupole 0.9678 -1.7136 0.7458 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0000	0.0000	0.6486	0.4281	0.2129	0.4563	1.6588	0.3437	1.1906	1.4047	2.2690	0.4066
7	0.0000	0.0000	-1.1136	-0.6216	-0.2742	-0.3306	-1.3314	-0.7600	-1.2510	-1.3739	-1.5267	-0.6668
1	0.0000	0.8193	-1.6978	0.2205	0.1573	0.0989	0.3654	0.2921	0.4051	0.3813	0.3653	0.2391
1	0.0000	1.3915	1.3796	-0.1237	-0.1267	-0.1617	-0.5290	-0.0839	-0.3749	-0.3967	-0.7367	-0.1090
1	0.0000	-1.3915	1.3796	-0.1237	-0.1267	-0.1617	-0.5290	-0.0839	-0.3749	-0.3967	-0.7367	-0.1090
1	0.0000	-0.8193	-1.6978	0.2205	0.1573	0.0989	0.3654	0.2921	0.4051	0.3813	0.3653	0.2391

Dipole moment (in D) 1.29 (DEN) 0.58 2.12 0.57 0.68 0.74 1.18 0.25 0.49 0.51

File mol315.out

Molecule 315 AlH2OH

SP Mol315 B3LYP/Def2TZVP VAC.

0 5

Dipole -1.2915 0.1240 0.0000 1.2974

Quadrupole -1.9911 -0.7792 2.7703 -2.8590 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0305	-0.5963	0.0000	0.4847	0.2253	0.5286	1.7429	0.3771	1.2030	1.5178	2.2963	0.4070
8	0.0305	1.0963	0.0000	-0.5440	-0.1411	-0.3708	-1.1651	-0.5564	-0.8306	-1.1760	-1.4252	-0.4647
1	-0.7572	1.6329	0.0000	0.3048	0.1719	0.1550	0.4765	0.3356	0.3826	0.4850	0.5839	0.2713
1	-1.3289	-1.3872	0.0000	-0.1275	-0.1313	-0.1605	-0.5394	-0.0831	-0.4006	-0.4187	-0.7327	-0.1107
1	1.4460	-1.2646	0.0000	-0.1179	-0.1248	-0.1523	-0.5147	-0.0731	-0.3545	-0.4082	-0.7224	-0.1028

Dipole moment (in D) 1.30 (DEN) 1.16 1.72 0.63 1.90 1.28 1.24 2.38 2.35 1.01

File mol321.out

Molecule 321 AlH=PH

SP Mol310 B3LYP/Def2TZVP VAC.

```

0 4
Dipole      0.0289   2.7916   0.0000   2.7917
Quadrupole  2.8606  -1.1897  -1.6708   0.7650   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
13      0.0514   1.0598   0.0000   0.2274   0.0345   0.4202   1.1469   0.3296   0.6817   1.0680   1.8357   0.3865
1      -0.1277   2.6220   0.0000  -0.0481  -0.1083  -0.1228  -0.4184  -0.0467  -0.2023  -0.3678  -0.6930  -0.0693
15      0.0514  -1.0563   0.0000  -0.2234  -0.0091  -0.2684  -0.6630  -0.3469  -0.5081  -0.6742  -0.6309  -0.3823
1      -1.3113  -0.5550   0.0000   0.0442   0.0829  -0.0290  -0.0655   0.0641   0.0288  -0.0261  -0.5119   0.0651

Dipole moment (in D)  2.79 (DEN)      1.59      1.44      2.05      4.18      2.71      3.42      4.32      6.51      2.88

```

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File mol316.out
Molecule 316  ALH2SH
SP Mol316 B3LYP/Def2TZVP VAC.

```

```

0 5
Dipole      -0.7614   0.5439   0.0000   0.9357
Quadrupole  -0.3226  -1.7630   2.0856   1.3402   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP
13      0.0409   1.1127   0.0000   0.3825   0.0080   0.4356   1.3992   0.2561   0.9540   1.1963   2.2000   0.3409
16      0.0409  -1.0633   0.0000  -0.3063   0.1789  -0.1834  -0.5789  -0.2293  -0.4478  -0.6009  -0.7361  -0.2727
1      -1.2953  -1.1434   0.0000   0.1485   0.0646   0.0533   0.1446   0.1244   0.1442   0.1550  -0.0185   0.1334
1      -1.3318   1.8736   0.0000  -0.1104  -0.1261  -0.1532  -0.4855  -0.0762  -0.3418  -0.3759  -0.7238  -0.1011
1      1.4411   1.8179   0.0000  -0.1144  -0.1255  -0.1523  -0.4794  -0.0749  -0.3086  -0.3745  -0.7220  -0.1004

Dipole moment (in D)  0.94 (DEN)      1.28      3.48      0.44      1.44      0.95      1.11      2.22      2.80      1.11

```

```

-----
File mol319.out
Molecule 319  ALH=S
SP Mol319 B3LYP/Def2TZVP VAC.

```

```

0 3
Dipole      0.0000   0.0000  -3.7868   3.7868
Quadrupole  0.1725   0.1725  -0.3450   0.0000   0.0000   0.0000

      Atomic coordinates      Mul.      Lowdin      Hirsch.      I-Hirsch      CM5      ESP      NPA      AIM      ACP

```


13	0.0000	0.0000	-1.0102	0.3022	-0.0238	0.4877	1.3041	0.3768	0.7929	1.2402	2.0196	0.4470
16	0.0000	0.0000	0.9815	-0.2795	0.1241	-0.3834	-0.8885	-0.3508	-0.6076	-0.8842	-1.3427	-0.3966
1	0.0000	0.0000	-2.5707	-0.0227	-0.1003	-0.1044	-0.4156	-0.0260	-0.1853	-0.3560	-0.6768	-0.0504

Dipole moment (in D) 3.79 (DEN) 2.50 1.94 2.88 5.39 3.16 4.42 5.79 7.77 3.42

File mol311.out

Molecule 311 AlF

SP Mol311 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 1.4813 1.4813

Quadrupole 1.6378 1.6378 -3.2756 0.0000 0.0000 0.0000

Atomic coordinates

Mul.

Lowdin

Hirsch.

I-Hirsch

CM5

ESP

NPA

AIM

ACP

9	0.0000	0.0000	-0.9843	-0.3362	-0.0759	-0.3213	-0.5063	-0.3063	-0.3135	-0.8407	-0.9165	-0.2879
13	0.0000	0.0000	0.6814	0.3362	0.0759	0.3213	0.5063	0.3064	0.3135	0.8407	0.9165	0.2879

Dipole moment (in D) 1.48 (DEN) 2.69 0.61 2.57 4.05 2.45 2.51 6.73 7.33 2.30

File mol313.out

Molecule 313 AlCl

SP Mol313 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -1.5206 1.5206

Quadrupole 1.1124 1.1124 -2.2247 0.0000 0.0000 0.0000

Atomic coordinates

Mul.

Lowdin

Hirsch.

I-Hirsch

CM5

ESP

NPA

AIM

ACP

17	0.0000	0.0000	0.9256	-0.2705	0.1978	-0.2502	-0.3851	-0.2137	-0.2677	-0.6942	-0.8437	-0.2272
13	0.0000	0.0000	-1.2104	0.2705	-0.1978	0.2502	0.3851	0.2138	0.2677	0.6942	0.8437	0.2272

Dipole moment (in D) 1.52 (DEN) 2.77 2.03 2.57 3.95 2.19 2.75 7.12 8.66 2.33

File mol314.out

Molecule 314 AlBr

SP Mol314 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -1.7016 1.7016

Quadrupole 0.4875 0.4875 -0.9750 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
35	0.0000	0.0000	0.6243	-0.2721	0.1569	-0.2317	-0.3540	-0.1782	-0.2645	-0.6422	-0.8080	-0.2067
13	0.0000	0.0000	-1.6809	0.2721	-0.1569	0.2317	0.3540	0.1782	0.2645	0.6422	0.8080	0.2067

Dipole moment (in D) 1.70 (DEN) 3.01 1.74 2.57 3.92 1.97 2.93 7.11 8.95 2.29

File Alx_12.out

Molecule_12 ALS

SP Alx_12 B3LYP/Def2TZVP VAC.

0 2

Dipole 0.0000 0.0000 -3.7537 3.7537

Quadrupole -0.9624 -0.9624 1.9248 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
16	0.0000	0.0000	0.9169	-0.2956	0.1204	-0.3443	-0.6363	-0.3155	-0.5004	-0.8920	-1.1563	-0.3557
13	0.0000	0.0000	-1.1285	0.2956	-0.1204	0.3443	0.6363	0.3155	0.5004	0.8920	1.1563	0.3557

Dipole moment (in D) 3.75 (DEN) 2.90 1.18 3.38 6.25 3.10 4.92 8.76 11.36 3.49

File Alx_16.out

Molecule_16 ALF2

SP Alx_16 B3LYP/Def2TZVP VAC.

0 3

Dipole 0.0000 0.0000 1.8875 1.8875

Quadrupole 3.8148 -4.9871 1.1723 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0000	0.0000	0.4811	0.6496	0.0679	0.5890	1.1982	0.5582	0.7242	1.5430	1.7642	0.5340
9	0.0000	1.4305	-0.3475	-0.3248	-0.0339	-0.2945	-0.5991	-0.2791	-0.3621	-0.7715	-0.8825	-0.2670
9	0.0000	-1.4305	-0.3475	-0.3248	-0.0339	-0.2945	-0.5991	-0.2791	-0.3621	-0.7715	-0.8825	-0.2670

Dipole moment (in D) 1.89 (DEN) 2.59 0.27 2.34 4.77 2.22 2.88 6.14 7.02 2.13

File Alx_19.out

Molecule_19 ALF20

SP Alx_19 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 -0.1593 0.1593

Quadrupole 5.6875 -2.4086 -3.2789 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
8	0.0000	0.0000	1.7412	-0.2746	0.0136	-0.2202	-0.6756	-0.2318	-0.4689	-0.6596	-0.8168	-0.1935
13	0.0000	0.0000	0.0115	0.9180	-0.0195	0.7718	2.1107	0.7507	1.4488	2.1338	2.5240	0.7082
9	0.0000	1.4306	-0.7822	-0.3217	0.0029	-0.2758	-0.7176	-0.2595	-0.4899	-0.7371	-0.8536	-0.2573
9	0.0000	-1.4306	-0.7822	-0.3217	0.0029	-0.2758	-0.7176	-0.2595	-0.4899	-0.7371	-0.8536	-0.2573

Dipole moment (in D) 0.16 (DEN) 0.17 0.09 0.27 0.14 0.05 0.16 0.14 0.28 0.35

File Alx_21.out

Molecule_21 AlCl+

SP Alx_21 B3LYP/Def2TZVP VAC.

1 2

Dipole 0.0000 0.0000 -5.6238 5.6238

Quadrupole -2.8550 -2.8550 5.7100 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0000	0.0000	-1.1541	0.9195	0.4780	0.9622	1.2450	0.9156	1.0653	1.4548	1.6253	0.9525
17	0.0000	0.0000	0.8825	0.0805	0.5220	0.0378	-0.2450	0.0844	-0.0653	-0.4548	-0.6253	0.0475

Dipole moment (in D) 5.62 (DEN) 4.76 0.44 5.17 7.94 4.72 6.18 9.99 11.66 5.08

File Alx_24.out

Molecule_24 AlCl2

SP Alx_24 B3LYP/Def2TZVP VAC.

0 3

Dipole	0.0000	0.0000	1.5279	1.5279								
Quadrupole	2.7376	-4.1723	1.4347	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0000	0.0000	0.7692	0.4442	-0.5295	0.3986	0.8656	0.3219	0.4980	1.1169	1.6009	0.3559
17	0.0000	1.8291	-0.2941	-0.2221	0.2648	-0.1993	-0.4328	-0.1609	-0.2490	-0.5585	-0.8006	-0.1779
17	0.0000	-1.8291	-0.2941	-0.2221	0.2648	-0.1993	-0.4328	-0.1609	-0.2490	-0.5585	-0.8006	-0.1779
Dipole moment (in D)	1.53 (DEN)		2.27	2.70	2.04	4.42	1.64	2.54	5.70	8.18	1.82	

File Alx_25.out

Molecule_25 AlCl2-

SP Alx_25 B3LYP/Def2TZVP VAC.

-1 3

Dipole	0.0000	0.0000	-0.8492	0.8492								
Quadrupole	8.4556	-7.4572	-0.9984	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
13	0.0000	0.0000	1.0781	0.0185	-0.8263	-0.1174	0.0612	-0.1645	-0.1259	0.4795	0.8193	-0.1789
17	0.0000	1.7681	-0.4122	-0.5093	-0.0869	-0.4413	-0.5306	-0.4177	-0.4370	-0.7397	-0.9098	-0.4105
17	0.0000	-1.7681	-0.4122	-0.5093	-0.0869	-0.4413	-0.5306	-0.4177	-0.4370	-0.7397	-0.9098	-0.4105
Dipole moment (in D)	0.85 (DEN)		2.11	3.93	1.14	2.42	0.80	1.08	5.41	7.85	0.70	

File Alx_27.out

Molecule_27 AlClF+

SP Alx_27 B3LYP/Def2TZVP VAC.

1 3

Dipole	0.0000	0.0000	-0.2439	0.2439								
Quadrupole	0.6224	0.6224	-1.2448	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	-2.0987	-0.1412	0.0929	-0.1835	-0.6153	-0.1660	-0.3037	-0.6937	-0.8019	-0.1749
13	0.0000	0.0000	-0.5015	0.9879	0.3119	1.1134	2.0217	1.0442	1.3582	2.1006	2.4587	1.1039
17	0.0000	0.0000	1.4946	0.1533	0.5952	0.0701	-0.4064	0.1218	-0.0545	-0.4069	-0.6568	0.0710

Dipole moment (in D) 0.24 (DEN) 0.14 2.59 0.33 1.58 0.03 0.60 0.99 2.55 0.39

File Alx_28.out

Molecule_28 AlClF

SP Alx_28 B3LYP/Def2TZVP VAC.

0 3

Dipole -1.1330 1.2989 0.0000 1.7236

Quadrupole -3.8657 0.6050 3.2607 -2.4730 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	1.6483	0.9486	0.0000	-0.3178	-0.0375	-0.2965	-0.5776	-0.2814	-0.3418	-0.7634	-0.8847	-0.2673
13	0.0000	0.8064	0.0000	0.5461	-0.2312	0.4916	1.0451	0.4377	0.6211	1.3460	1.6828	0.4428
17	-0.8726	-1.1188	0.0000	-0.2284	0.2687	-0.1951	-0.4676	-0.1562	-0.2793	-0.5826	-0.7977	-0.1754

Dipole moment (in D) 1.72 (DEN) 2.45 2.89 2.21 4.72 2.01 2.81 6.05 7.70 2.00

File Alx_29.out

Molecule_29 AlF2Cl

SP Alx_29 B3LYP/Def2TZVP VAC.

0 4

Dipole 0.0000 0.0000 0.5061 0.5061

Quadrupole 5.6128 -3.5355 -2.0772 0.0000 0.0000 0.0000

	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
17	0.0000	0.0000	1.6489	-0.2094	0.3434	-0.1578	-0.6064	-0.1142	-0.3352	-0.5547	-0.7863	-0.1474
13	0.0000	0.0000	-0.4203	0.8447	-0.3403	0.7177	2.0459	0.6426	1.2565	2.0249	2.5018	0.6664
9	0.0000	1.4082	-1.2537	-0.3176	-0.0016	-0.2799	-0.7197	-0.2642	-0.4606	-0.7351	-0.8576	-0.2595
9	0.0000	-1.4082	-1.2537	-0.3176	-0.0016	-0.2799	-0.7197	-0.2642	-0.4606	-0.7351	-0.8576	-0.2595

Dipole moment (in D) 0.51 (DEN) 0.46 3.43 0.67 0.27 0.98 0.36 0.37 0.95 0.61

File Alx_30.out

Molecule_30 AlFC12

SP Alx_30 B3LYP/Def2TZVP VAC.

0	4											
Dipole	0.0000	0.0000	-0.4859	0.4859								
Quadrupole	4.8745	-1.3553	-3.5192	0.0000	0.0000	0.0000						
	Atomic coordinates			Mul.	Lowdin	Hirsch.	I-Hirsch	CM5	ESP	NPA	AIM	ACP
9	0.0000	0.0000	1.9867	-0.3119	-0.0063	-0.2832	-0.6880	-0.2680	-0.4356	-0.7252	-0.8619	-0.2610
13	0.0000	0.0000	0.3479	0.7221	-0.6653	0.6133	1.8329	0.5123	1.0736	1.7706	2.4414	0.5657
17	0.0000	1.8133	-0.6589	-0.2051	0.3358	-0.1650	-0.5724	-0.1221	-0.3190	-0.5227	-0.7896	-0.1523
17	0.0000	-1.8133	-0.6589	-0.2051	0.3358	-0.1650	-0.5724	-0.1221	-0.3190	-0.5227	-0.7896	-0.1523
Dipole moment (in D)	0.49 (DEN)		0.47	3.30	0.63	0.12	0.93	0.34	0.65	0.85	0.58	
