aug-cc-pCVTZ / cc-pVTZ total

molecule	E[cvs]	E[full]	Δcvs	I[cvs]	I[full]
ADC(2)					
methane	290.6346	290.5669	0.0677	0.0110	0.0112
ammonia	402.7163	402.6769	0.0394	0.0053	0.0055
	404.4055	404.3760	0.0295	0.0140	0.0145
water	535.3627	535.3556	0.0071	0.0109	0.0114
	537.1964	537.1993	-0.0030	0.0206	0.0213
hydrogen fluoride	687.8359	687.8607	-0.0248	0.0159	0.0164
neon	866.6467	866.7129	-0.0661	0.0088	0.0090
ADC(1) [singles-block = full)					
methane					
ammonia					
water					
hydrogen fluoride					
neon					
ADC(3)					
methane					
ammonia					
water					
hydrogen fluoride					
neon					

ratio	singles-block E[cvs]	E[full]	Δcvs	difference
0.9752	300.1858	301.3436	-1.1578	1.2254
0.9576	416.5544	417.7278	-1.1734	1.2128
0.9650	417.1029	418.2855	-1.1826	1.2121
0.9605	551.9020	553.1004	-1.1984	1.2055
0.9672	552.7144	553.9217	-1.2073	1.2043
0.9682	706.6353	707.8626	-1.2273	1.2025
0.9784	889.2218	890.4767	-1.2549	1.1888
	299.7588	299.7715	-0.0126	
	416.1292	416.1335	-0.0043	
	416.4498	416.4636	-0.0138	
	551.2450	551.2502	-0.0052	
	551.8512	551.8649	-0.0138	
	705.7939	705.8004	-0.0066	
	888.9344	888.9376	-0.0031	
	299.3419	300.4533	-1.1114	
	415.6438	416.7116	-1.0677	
	416.2436	417.3387	-1.0952	
	551.4421	552.5171	-1.0750	
	552.2093	553.3060	-1.0967	
	706.7502	707.8539	-1.1037	
	890.4953	891.5836	-1.0883	

6-311++G**	total				
molecule	E[cvs]	E[full]	Δcvs	I[cvs]	I[full]
ADC(2)					
methane	290.8335	290.3402	0.4933	0.0120	0.0124
ammonia	402.6762	402.2601	0.4161	0.0037	0.0039
	404.1689	403.7635	0.4054	0.0101	0.0105
water	535.0816	534.7336	0.3480	0.0068	0.0072
	536.6876	536.3491	0.3385	0.0109	0.0115
hydrogen fluoride	687.6591	687.3548	0.3043	0.0101	0.0106
neon	869.1336	868.8576	0.2760	0.0126	0.0123
ADC(2)-x					
methane	288.0576	287.7118	0.3458	0.0126	0.0132
ammonia	400.1999	399.9227	0.2772	0.0048	0.0050
	401.9416	401.6654	0.2762	0.0145	0.0152
water	533.2501	533.0237	0.2264	0.0098	0.0103
	535.1090	534.8844	0.2247	0.0190	0.0199
hydrogen fluoride	686.4839	686.2924	0.1915	0.0157	0.0165
neon	868.5555	868.3881	0.1673	0.0139	0.0137
ADC(3)					
methane	290.6499	290.3390	0.3109	0.0238	0.0249
ammonia	404.4190	404.1780	0.2409	0.0088	0.0092
	406.0122	405.7647	0.2474	0.0316	0.0327
water	538.8690	538.6784	0.1906	0.0186	0.0193
	540.4488	540.2551	0.1937	0.0392	0.0405
hydrogen fluoride	692.7854	692.6353	0.1500	0.0284	0.0294
neon	874.8461	874.7284	0.1177	0.0175	0.0174

ratio	singles-block E[cvs]	E[full]	Δcvs	difference
0.9663	300.1958	300.6505	-0.4547	0.9480
0.9441	416.4663	416.9161	-0.4498	0.8659
0.9631	417.0397	417.4933	-0.4536	0.8590
0.9531	551.7507	552.1917	-0.4410	0.7890
0.9483	552.5774	553.0212	-0.4438	0.7822
0.9478	706.4863	706.9217	-0.4354	0.7397
1.0228	890.3325	890.7591	-0.4266	0.7026
0.9519	300.1958	300.6505	-0.4547	0.8005
0.9432	416.4663	416.9161	-0.4498	0.7271
0.9584	417.0397	417.4933	-0.4536	0.7298
0.9549	551.7507	552.1917	-0.4410	0.6674
0.9533	552.5774	553.0212	-0.4438	0.6684
0.9528	706.4863	706.9217	-0.4354	0.6268
1.0148	890.3325	890.7591	-0.4266	0.5939
0.9542	299.4658	299.9463	-0.4805	0.7914
0.9542	415.7285	416.1972	-0.4687	0.7096
0.9656	416.3387	416.8116	-0.4729	0.7203
0.9652	551.4293	551.8900	-0.4607	0.6513
0.9664	552.2072	552.6701	-0.4629	0.6566
0.9646	706.6626	707.1218	-0.4592	0.6093
1.0085	890.7768	891.2335	-0.4567	0.5744

Fig_4

	Cc-pCVDZ			Cc-pCVTZ	
ADC(2)	**E[cvs]**	**E[full]**	**Δcvs**	**E[cvs]**	**E[full]**
methane	300.8302	301.7216	-0.8914	300.3238	301.4814
ammonia	416.9208	417.8118	-0.8911	416.5843	417.7564
water	551.8620	552.7573	-0.8953	551.7497	552.9464
hydrogen fluoride	706.3934	707.2936	-0.9002	706.4327	707.6583
neon	909.4386	910.3455	-0.9069	900.5682	901.8244
	Cc-pCVDZ			**Cc-pCVTZ**	
ADC(3)	**E[cvs]**	**E[full]**	**Δcvs**	**E[cvs]**	**E[full]**
methane	300.3544	301.2845	-0.9301	299.4884	300.6037
ammonia	416.3759	417.2951	-0.9192	415.5544	416.6237
water	551.7022	552.6224	-0.9201	551.0438	552.1196
hydrogen fluoride	706.7803	707.7055	-0.9252	706.1922	707.2968
neon	909.9576	910.8936	-0.9361	900.4097	901.5692

Fig_4

Δcvs	Cc-pCVQZ E[cvs]	E[full]	Δcvs	CBS E[cvs]	E[full]	Δcvs
-1.1576	300.2529	301.5158	-1.2629	300.1482	301.4469	-1.2987
-1.1721	416.5692	417.8644	-1.2953	416.4905	417.8202	-1.3297
-1.1967	551.8019	553.1383	-1.3364	551.7595	553.1307	-1.3712
-1.2256	706.5086	707.8754	-1.3668	706.4968	707.9039	-1.4071
-1.2562	896.2113	897.6087	-1.3974	895.2564	896.7000	-1.4436

Δcvs	Cc-pCVQZ E[cvs]	E[full]	Δcvs	CBS E[cvs]	E[full]	Δcvs
-1.1153						
-1.0694						
-1.0758						
-1.1046	706.3123	707.5105	-1.1982	706.1335	707.3495	-1.2160
-1.1595	896.1578	897.4094	-1.2516	895.0063	896.2869	-1.2806

molecule	total E[cvs]	E[full]	Δcvs	I[cvs]	I[full]
6-311++G**					
methane	290.8335	290.3402	0.4933	0.0120	0.0124
ammonia	402.6762	402.2601	0.4161	0.0037	0.0039
	404.1689	403.7635	0.4054	0.0101	0.0105
water	535.0816	534.7336	0.3480	0.0068	0.0072
	536.6876	536.3491	0.3385	0.0109	0.0115
hydrogen fluoride	687.6591	687.3548	0.3043	0.0101	0.0106
neon	869.1336	868.8576	0.2760	0.0126	0.0123
u6-311++G**					
methane	290.7306	290.1151	0.6155	0.0120	0.0125
ammonia	402.5188	401.9437	0.5751	0.0037	0.0039
	404.0176	403.4509	0.5667	0.0101	0.0105
water	534.8242	534.2791	0.5451	0.0068	0.0071
	536.4374	535.9003	0.5372	0.0109	0.0114
hydrogen fluoride	687.3120	686.7865	0.5255	0.0100	0.0105
neon	868.6848	868.1672	0.5176	0.0126	0.0126
p6-311++G**					
methane	290.7806	290.7590	0.0216	0.0120	0.0121
ammonia	402.6146	402.6583	-0.0437	0.0037	0.0039
	404.1073	404.1620	-0.0546	0.0101	0.0102
water	535.0108	535.1231	-0.1124	0.0068	0.0070
	536.6170	536.7380	-0.1210	0.0109	0.0113
hydrogen fluoride	687.5791	687.7405	-0.1614	0.0101	0.0105
neon	869.0402	869.2468	-0.2067	0.0126	0.0122
up6-311++G**					
methane	290.6781	290.5363	0.1418	0.0120	0.0122
ammonia	402.4570	402.3450	0.1120	0.0037	0.0038
	403.9560	403.8525	0.1034	0.0101	0.0103
water	534.7534	534.6737	0.0797	0.0068	0.0070
	536.3670	536.2943	0.0726	0.0109	0.0111
hydrogen fluoride	687.2323	687.1791	0.0532	0.0101	0.0103
neon	868.5918	868.5653	0.0265	0.0126	0.0125
cc-pVDZ					
methane	293.7153	293.4885	0.2268	0.0385	0.0393
ammonia	405.4118	405.1815	0.2303	0.0074	0.0076
	407.3832	407.1893	0.1939	0.0351	0.0360
water	537.8450	537.6510	0.1940	0.0129	0.0132
	539.8281	539.6602	0.1679	0.0308	0.0315
hydrogen fluoride	690.4655	690.2964	0.1691	0.0172	0.0176
neon	899.8261	899.6698	0.1563	0.0997	0.1028
cc-pCVDZ					
methane	293.3864	293.1695	0.2169	0.0383	0.0388
ammonia	404.9106	404.7099	0.2007	0.0073	0.0075
	406.8993	406.7179	0.1814	0.0351	0.0356
water	537.2284	537.0572	0.1713	0.0128	0.0131
	539.2227	539.0670	0.1557	0.0308	0.0313
hydrogen fluoride	689.7358	689.5824	0.1534	0.0172	0.0175
neon	898.9290	898.7613	0.1677	0.0984	0.1006
cc-pVTZ					
methane	292.0745	291.3890	0.6856	0.0357	0.0367
ammonia	403.3604	402.7277	0.6327	0.0058	0.0063

	405.3644	404.7045	0.6598	0.0309	0.0320
water	535.6392	535.0551	0.5841	0.0112	0.0118
	537.5885	537.0084	0.5800	0.0276	0.0288
hydrogen fluoride	688.0196	687.4688	0.5508	0.0161	0.0169
neon	884.4902	883.9372	0.5530	0.0507	0.0511
aug-cc-pVTZ / cc-pVTZ					
methane	290.7007	290.0508	0.6499	0.0109	0.0116
ammonia	402.8187	402.1632	0.6555	0.0052	0.0048
	404.5054	403.8812	0.6242	0.0138	0.0145
water	535.5055	534.9330	0.5726	0.0109	0.0115
	537.3312	536.7661	0.5651	0.0203	0.0214
hydrogen fluoride	688.0155	687.4625	0.5530	0.0158	0.0166
neon	866.8418	866.3278	0.5140	0.0088	0.0091
cc-pCVTZ					
methane	292.0027	291.9221	0.0805	0.0359	0.0366
ammonia	403.2535	403.2054	0.0481	0.0059	0.0062
	405.2575	405.2180	0.0396	0.0311	0.0318
water	535.4835	535.4719	0.0117	0.0114	0.0118
	537.4469	537.4450	0.0020	0.0278	0.0285
hydrogen fluoride	687.8271	687.8488	-0.0218	0.0162	0.0167
neon	884.1811	884.2193	-0.0382	0.0510	0.0512
6-311++G**					
silane	1841.9234	1841.4912	0.4322	0.0035	0.0036
phosphine	2143.6123	2143.1890	0.4233	0.0055	0.0055
hydrogen sulfide	2469.2453	2468.8532	0.3921	0.0060	0.0060
	2469.4838	2469.0972	0.3866	0.0023	0.0023
hydrogen chloride	2824.8465	2824.3512	0.4953	0.0037	0.0038
argon	3202.4308	3201.9277	0.5031	0.0015	0.0016
u6-311++G**					
silane	1841.8049	1841.2264	0.5785	0.0035	0.0036
phosphine	2143.5085	2142.9534	0.5551	0.0055	0.0055
hydrogen sulfide	2469.1448	2468.6268	0.5180	0.0060	0.0061
	2469.3841	2468.8735	0.5106	0.0023	0.0023
hydrogen chloride	2824.7601	2824.1451	0.6150	0.0037	0.0038
argon	3202.3360	3201.7021	0.6339	0.0015	0.0016
p6-311++G**					
silane	1841.8756	1841.9544	-0.0787	0.0035	0.0035
phosphine	2143.5550	2143.6051	-0.0501	0.0055	0.0055
hydrogen sulfide	2469.1800	2469.2789	-0.0990	0.0060	0.0060
	2469.4213	2469.5156	-0.0943	0.0023	0.0023
hydrogen chloride	2824.1138	2824.1198	-0.0060	0.0037	0.0038
argon	3200.7330	3200.7450	-0.0120	0.0016	0.0016
up6-311++G**					
silane	1841.7571	1841.6969	0.0603	0.0035	0.0036
phosphine	2143.4550	2143.4132	0.0418	0.0055	0.0055
hydrogen sulfide	2469.0794	2469.0592	0.0202	0.0060	0.0061
	2469.3216	2469.2986	0.0230	0.0023	0.0023
hydrogen chloride	2824.0265	2823.9225	0.1040	0.0037	0.0038
argon	3200.6369	3200.5308	0.1061	0.0016	0.0016
cc-pVDZ					
silane	1857.4470	1857.4223	0.0247	0.0032	0.0032
phosphine	2158.9800	2158.9557	0.0244	0.0047	0.0048

hydrogen sulfide	2484.2080	2484.1836	0.0244	0.0053	0.0054
	2484.5856	2484.5563	0.0293	0.0030	0.0030
hydrogen chloride	2833.3684	2833.3414	0.0270	0.0042	0.0042
argon	3222.5685	3222.5433	0.0253	0.0107	0.0108
cc-pCVDZ					
silane	1843.0394	1842.6235	0.4158	0.0039	0.0039
phosphine	2144.8232	2144.4190	0.4042	0.0058	0.0058
hydrogen sulfide	2470.0857	2469.6953	0.3905	0.0064	0.0064
	2470.6922	2470.3034	0.3889	0.0036	0.0037
hydrogen chloride	2819.1132	2818.7385	0.3747	0.0051	0.0052
argon	3207.6130	3207.2440	0.3690		
cc-pVTZ					
silane	1846.4889	1846.3797	0.1092	0.0038	0.0039
phosphine	2150.3841	2150.2746	0.1095	0.0053	0.0054
hydrogen sulfide	2476.9362	2476.8300	0.1061	0.0056	0.0058
	2477.4880	2477.3778	0.1102	0.0028	0.0029
hydrogen chloride	2826.3580	2826.2524	0.1056	0.0043	0.0044
argon	3210.9476	3210.8472	0.1004	0.0060	0.0060
aug-cc-pVTZ / cc-pVTZ					
silane	1846.2879	1846.1767	0.1111	0.0034	0.0034
phosphine	2150.2332	2150.1240	0.1092	0.0050	0.0052
hydrogen sulfide	2476.7840	2476.6771	0.1069	0.0055	0.0056
	2477.1497	2477.0396	0.1101	0.0023	0.0023
hydrogen chloride	2826.2322	2826.1255	0.1067	0.0041	0.0042
argon	3203.5956	3203.4966	0.0990	0.0013	0.0014
cc-pCVTZ					
silane	1840.7313	1840.5057	0.2256	0.0040	0.0040
phosphine	2142.5548	2142.2547	0.3001	0.0057	0.0057
hydrogen sulfide	2467.8226	2467.5561	0.2664	0.0061	0.0067
	2468.6197	2468.3640	0.2557	0.0032	0.0036
hydrogen chloride	2816.9120	2816.7650	0.1470	0.0049	0.0049

ratio	singles-block E[cvs]	E[full]	Δcvs	difference
0.9663	300.1958	300.6505	-0.4547	0.9480
0.9441	416.4663	416.9161	-0.4498	0.8659
0.9631	417.0397	417.4933	-0.4536	0.8590
0.9531	551.7507	552.1917	-0.4410	0.7890
0.9483	552.5774	553.0212	-0.4438	0.7822
0.9478	706.4863	706.9217	-0.4354	0.7397
1.0228	890.3325	890.7591	-0.4266	0.7026
0.9597	300.2148	300.7189	-0.5041	1.1196
0.9531	416.4930	417.0027	-0.5097	1.0848
0.9573	417.0710	417.5838	-0.5128	1.0795
0.9560	551.7685	552.2818	-0.5134	1.0585
0.9552	552.6005	553.1160	-0.5155	1.0527
0.9584	706.4886	707.0071	-0.5185	1.0440
0.9967	890.3002	890.8190	-0.5188	1.0364
0.9932	300.1715	301.1937	-1.0223	1.0438
0.9627	416.4396	417.4612	-1.0216	0.9779
0.9885	417.0098	418.0361	-1.0263	0.9717
0.9698	551.7177	552.7364	-1.0187	0.9064
0.9718	552.5417	553.5639	-1.0223	0.9013
0.9635	706.4471	707.4630	-1.0159	0.8545
1.0270	890.2868	891.2989	-1.0121	0.8054
0.9869	300.1909	301.2645	-1.0735	1.2154
0.9697	416.4664	417.5507	-1.0843	1.1963
0.9820	417.0412	418.1295	-1.0883	1.1918
0.9716	551.7356	552.8315	-1.0959	1.1755
0.9772	552.5649	553.6637	-1.0988	1.1715
0.9727	706.4498	707.5557	-1.1060	1.1591
1.0034	890.2654	891.3774	-1.1120	1.1385
0.9777	300.8144	300.8734	-0.0590	0.2858
0.9729	416.9576	417.0063	-0.0487	0.2791
0.9761	417.3467	417.3993	-0.0525	0.2464
0.9743	551.8974	551.9401	-0.0426	0.2366
0.9764	552.5895	552.6350	-0.0455	0.2134
0.9790	706.4268	706.4659	-0.0392	0.2083
0.9700	909.4954	909.5348	-0.0393	0.1956
0.9874	300.8302	301.7216	-0.8914	1.1083
0.9764	416.9208	417.8118	-0.8911	1.0918
0.9850	417.3243	418.2233	-0.8990	1.0805
0.9786	551.8620	552.7573	-0.8953	1.0665
0.9844	552.5641	553.4666	-0.9025	1.0582
0.9845	706.3934	707.2936	-0.9002	1.0536
0.9783	909.4386	910.3455	-0.9069	1.0746
0.9745	300.3383	300.7116	-0.3732	1.0588
0.9196	416.6026	416.9341	-0.3316	0.9643

0.9655	417.0240	417.3493	-0.3253	0.9852
0.9442	551.7711	552.0523	-0.2812	0.8652
0.9578	552.4911	552.7744	-0.2834	0.8634
0.9519	706.4551	706.7167	-0.2616	0.8124
0.9913	900.6112	900.8577	-0.2465	0.7996
0.9428	300.2020	300.5881	-0.3861	1.0360
1.0759	416.5775	416.9293	-0.3517	1.0073
0.9502	417.1271	417.4608	-0.3336	0.9578
0.9461	551.9268	552.2177	-0.2910	0.8635
0.9458	552.7397	553.0325	-0.2928	0.8579
0.9555	706.6660	706.9440	-0.2779	0.8310
0.9572	889.2500	889.5004	-0.2503	0.7643
0.9811	300.3238	301.4814	-1.1576	1.2381
0.9583	416.5843	417.7564	-1.1721	1.2202
0.9772	417.0047	418.1871	-1.1824	1.2220
0.9656	551.7497	552.9464	-1.1967	1.2084
0.9746	552.4711	553.6780	-1.2069	1.2089
0.9696	706.4327	707.6583	-1.2256	1.2038
0.9965	900.5682	901.8245	-1.2562	1.2180
0.9906	1865.6032	1866.0201	-0.4168	0.8490
0.9924	2167.8439	2168.2658	-0.4218	0.8451
0.9939	2494.0338	2494.4699	-0.4361	0.8283
0.9909	2495.3660	2495.8031	-0.4371	0.8237
0.9728	2844.3461	2844.6834	-0.3373	0.8326
0.9777	3224.7469	3225.0567	-0.3099	0.8129
0.9832	1865.6110	1866.0683	-0.4574	1.0359
0.9886	2167.8535	2168.3151	-0.4616	1.0168
0.9911	2494.0449	2494.5217	-0.4768	0.9948
0.9873	2495.3764	2495.8531	-0.4767	0.9874
0.9704	2844.3589	2844.7303	-0.3713	0.9863
0.9776	3224.7596	3225.1016	-0.3420	0.9759
0.9983	1865.5874	1866.6030	-1.0156	0.9368
0.9978	2167.8209	2168.7982	-0.9773	0.9272
0.9981	2494.0076	2495.0205	-1.0129	0.9139
0.9986	2495.3450	2496.3578	-1.0128	0.9185
0.9855	2844.3557	2845.3227	-0.9671	0.9611
0.9869	3224.7640	3225.7331	-0.9691	0.9571
0.9915	1865.5951	1866.6593	-1.0642	1.1244
0.9943	2167.8333	2168.8964	-1.0631	1.1049
0.9953	2494.0188	2495.0796	-1.0609	1.0811
0.9950	2495.3554	2496.4152	-1.0598	1.0828
0.9832	2844.3682	2845.3802	-1.0121	1.1161
0.9874	3224.7762	3225.7921	-1.0159	1.1220
0.9827	1866.1253	1866.1259	-0.0006	0.0253
0.9805	2168.4653	2168.4659	-0.0007	0.0250

0.9811	2494.4640	2494.4646	-0.0007	0.0250
0.9856	2495.7216	2495.7223	-0.0008	0.0301
0.9852	2844.6780	2844.6786	-0.0006	0.0277
0.9888	3231.6774	3231.6779	-0.0005	0.0257
0.9877	1866.0142	1866.1622	-0.1480	0.5638
0.9880	2168.2310	2168.3961	-0.1650	0.5693
0.9873	2494.2522	2494.4311	-0.1789	0.5694
0.9839	2495.6107	2495.7902	-0.1795	0.5684
0.9838	2844.5229	2844.7136	-0.1908	0.5655
	3231.5677	3231.7688	-0.2012	0.5701
0.9733	1865.4405	1865.4510	-0.0106	0.1197
0.9727	2167.7329	2167.7404	-0.0075	0.1170
0.9724	2493.9061	2493.9121	-0.0060	0.1121
0.9695	2495.3324	2495.3387	-0.0063	0.1159
0.9689	2844.3262	2844.3319	-0.0057	0.1107
0.9980	3229.2457	3229.2508	-0.0051	0.1055
0.9767	1865.4081	1865.4191	-0.0110	0.1222
0.9744	2167.7528	2167.7606	-0.0078	0.1170
0.9728	2493.9789	2493.9853	-0.0064	0.1133
0.9708	2495.3795	2495.3862	-0.0067	0.1161
0.9717	2844.3947	2844.4006	-0.0060	0.1119
0.9577	3224.5977	3224.6029	-0.0052	0.1042
1.0004	1865.3102	1865.9651	-0.6548	0.8804
0.9969	2167.5309	2168.1847	-0.6538	0.9539
0.9160	2493.6280	2494.3003	-0.6723	0.9387
0.8864	2495.2610	2495.9219	-0.6610	0.9167
0.9903	2844.1065	2844.7915	-0.6851	0.8321

ADC(2) diffuse cc-pCVDtotal					
molecule	**cvs**	**full**	**Δcvs**	**I[cvs]**	**I[full]**
excitation					
C-edge					
CH4	293.3864	293.1695	0.2169	0.0383	0.0388
CH3F	294.1194	293.8987	0.2207	0.0470	0.0473
	294.9943	294.7432	0.2512	0.0106	0.0111
	295.6419	295.4204	0.2214	0.0457	0.0467
CH2F2	296.9326	296.7069	0.2257	0.0445	0.0450
	297.0191	296.7912	0.2279	0.0754	0.0765
	297.9837	297.7579	0.2258	0.0527	0.0542
C2H6	291.8707	291.6430	0.2277	0.0135	0.0135
C2H4	289.2842	289.0683	0.2159	0.0989	0.1024
C2H2	290.2107	289.9960	0.2147	0.0924	0.0965
C2HF	291.1213	290.8992	0.2220	0.0457	0.0478
	293.3152	293.0891	0.2261	0.0588	0.0619
CH2O	290.4070	290.1912	0.2158	0.0667	0.0697
CHFO	293.0257	292.8026	0.2232	0.0791	0.0834
CF2O	295.6646	295.4291	0.2355	0.0929	0.0989
CO	291.4839	291.3141	0.1698	0.0829	0.0869
CS	289.3039	289.1368	0.1671	0.0735	0.0770
HCN	290.8674	290.6607	0.2067	0.0518	0.0543
mean			0.2174		
stdev			0.0202		
O-edge					
H2O	537.2284	537.0572	0.1713	0.0128	0.0131
	539.2227	539.0670	0.1557	0.0308	0.0313
HFO	537.2214	537.0513	0.1701	0.0671	0.0700
	540.8646	540.7078	0.1568	0.0223	0.0228
F2O	539.5424	539.3671	0.1753	0.0596	0.0628
	539.8369	539.6873	0.1496	0.0807	0.0844
CH2O	534.2609	534.1068	0.1542	0.0423	0.0440
CHFO	535.2697	535.1164	0.1534	0.0385	0.0401
CF2O	536.2741	536.1206	0.1535	0.0364	0.0379
CO	536.8431	536.6985	0.1447	0.0346	0.0360
HNO	534.2779	534.1262	0.1517	0.0500	0.0524
mean			0.1578		
stdev			0.0099		
ionization					
C-edge					
CH4	292.9081	292.7104	0.1977		
CH3F	295.9072	295.7067	0.2005		
CH2F2	298.9547	298.7512	0.2035		
C2H6	292.6077	292.4107	0.1970		
C2H4	292.9461	292.7588	0.1874		
C2H2	293.2760	293.0876	0.1884		
C2HF	293.6169	293.4224	0.1946		
	296.1403	295.9475	0.1929		
CH2O	297.1716	296.9791	0.1925		
CHFO	300.1439	299.9468	0.1971		
CF2O	302.9323	302.7282	0.2040		
CO	299.4052	299.2475	0.1578		
CS	296.4989	296.3558	0.1431		

HCN	295.6913	295.5027	0.1886
mean			0.1889
stdev			0.0174
O-edge			
H2O	539.3752	539.2331	0.1421
HFO	543.1643	543.0299	0.1344
F2O	546.1719	546.0466	0.1253
CH2O	538.8088	538.6733	0.1356
CHFO	539.6264	539.4896	0.1368
CF2O	540.3655	540.2271	0.1384
CO	541.4538	541.3222	0.1316
HNO	541.1990	541.0663	0.1328
mean			0.1346
stdev			0.0050

ratio	singles-block cvs	full	difference
0.9874	300.8302	301.7216	-0.8914
0.9937	300.2362	301.1310	-0.8949
0.9587	310.9836	311.8712	-0.8875
0.9797	302.5600	303.4483	-0.8883
0.9896	302.3160	303.2104	-0.8944
0.9854	303.0391	303.9302	-0.8911
0.9726	304.4709	305.3568	-0.8858
1.0034	300.7880	301.6778	-0.8898
0.9663	296.2681	297.1618	-0.8937
0.9581	297.6629	298.5543	-0.8914
0.9569	298.7422	299.6335	-0.8913
0.9506	300.1141	301.0031	-0.8890
0.9579	296.1692	297.0594	-0.8902
0.9488	298.2171	299.1060	-0.8889
0.9400	300.4188	301.3065	-0.8877
0.9537	296.0955	296.9812	-0.8857
0.9550	294.5158	295.3982	-0.8824
0.9529	297.8966	298.7826	-0.8861
0.9673			-0.8894
0.0183			0.0033
0.9786	551.8620	552.7573	-0.8953
0.9844	552.5641	553.4666	-0.9025
0.9593	546.9549	547.8629	-0.9080
0.9770	554.6933	555.5874	-0.8941
0.9492	549.0299	549.9381	-0.9083
0.9567	550.1248	551.0253	-0.9005
0.9621	547.6325	548.5334	-0.9010
0.9603	547.6325	548.5334	-0.9010
0.9584	549.2747	550.1758	-0.9011
0.9619	551.8548	552.7534	-0.8986
0.9547	546.8279	547.7289	-0.9010
0.9639			-0.9010
0.0111			0.0044
	300.9686	301.8539	-0.8853
	303.3511	304.2335	-0.8824
	310.3849	311.2650	-0.8801
	305.2302	306.1153	-0.8850
	305.6951	306.5770	-0.8820
	306.0829	306.9626	-0.8797
	306.1165	306.9987	-0.8823
	311.0523	311.9292	-0.8770
	308.7131	309.5916	-0.8784
	311.2979	312.1745	-0.8766
	313.9525	314.8280	-0.8755
	309.3953	310.2647	-0.8693
	309.1256	309.9938	-0.8682

		Fig_6
307.5594	308.4354	-0.8760
		-0.8784
		0.0052
559.2044	560.1010	-0.8966
562.9942	563.8872	-0.8930
566.5275	567.4176	-0.8901
559.8849	560.7796	-0.8947
560.5936	561.4887	-0.8951
561.1527	562.0480	-0.8953
562.4312	563.3254	-0.8942
561.8658	562.7587	-0.8930
		-0.8940
		0.0020

ADC(2), aug-cc-pCVTZ / total

molecule	E[cvs]	E[full]	Δcvs	I[cvs]	I[full]
excitation					
methane	290.6346	290.5669	0.0677	0.0110	0.0112
ammonia	402.7163	402.6769	0.0394	0.0053	0.0055
	404.4055	404.3760	0.0295	0.0140	0.0145
water	535.3627	535.3556	0.0071	0.0109	0.0114
	537.1964	537.1993	-0.0030	0.0206	0.0213
hydrogen fluoride	687.8359	687.8607	-0.0248	0.0159	0.0164
neon	866.6467	866.7129	-0.0661	0.0088	0.0090
ionization					
methane	292.1484	292.0814	0.0670		
ammonia	405.5983	405.5721	0.0262		
water	538.3327	538.3413	-0.0086		
hydrogen fluoride	691.3235	691.3617	-0.0382		
neon	866.3275	866.3912	-0.0637		

ratio	singles-block E[cvs]	E[full]	Δcvs	difference
0.9752	300.1858	301.3436	-1.1578	1.2254
0.9576	416.5544	417.7278	-1.1734	1.2128
0.9650	417.1029	418.2855	-1.1826	1.2121
0.9605	551.9020	553.1004	-1.1984	1.2055
0.9672	552.7144	553.9217	-1.2073	1.2043
0.9682	706.6353	707.8626	-1.2273	1.2025
0.9784	889.2218	890.4767	-1.2549	1.1888
	304.8877	306.0376	-1.1499	1.2169
	422.8930	424.0669	-1.1739	1.2001
	559.6487	560.8476	-1.1989	1.1903
	715.6125	716.8392	-1.2266	1.1884
	891.9352	893.1890	-1.2538	1.1901