A New Benchmark Set for Excitation Energy of Charge Transfer States: Systematic Investigation of Coupled-Cluster Type Methods

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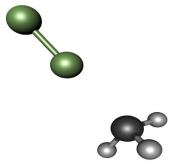
Table 1: coordinates in Angstrom (cont. 1)

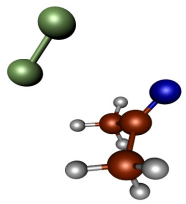
Ammonia-fluor

H	2.490675	0.939499	-0.000156
N	2.085280	0.000000	0.000003
H	2.490739	-0.469633	0.813668
H	2.490627	-0.469860	-0.813586
F	-0.222963	0.000000	0.000001
F	-1.710402	0.000000	0.000000



Aceton-fluor

H	-2.543489	0.848415	-1.328942
C	-1.483454	0.544023	-1.289081
H	-0.874751	1.463810	-1.326362
H	-1.243732	-0.093252	-2.152254
C	-1.199386	-0.211141	0.000000
O	-0.766094	-1.362999	0.000000
C	-1.483454	0.544023	1.289082
H	-1.243732	-0.093253	2.152254
H	-0.874757	1.463813	1.326367
H	-2.543491	0.848408	1.328938
F	1.631766	0.853847	0.000000
F	2.139396	-0.495631	0.000000



Pyrazine-fluor

N	0.995753	1.433963	0.000000
C	0.995753	0.702984	1.137230
C	0.995753	-0.702984	1.137230
N	0.995753	-1.433963	0.000000
C	0.995753	-0.702984	-1.137230
C	0.995753	0.702984	-1.137230
H	0.995753	1.261352	2.081529
H	0.995753	-1.261351	2.081529
H	0.995753	-1.261352	-2.081529
H	0.995753	1.261351	-2.081529
F	-2.097479	0.721626	0.000000
F	-2.097479	-0.721626	0.000000

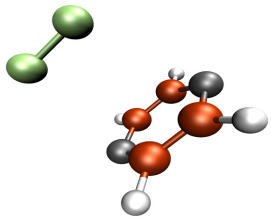
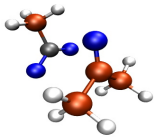


Table 2: coordinates in Angstrom (cont. 2)

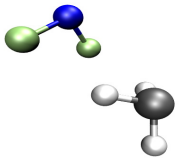
Aceton-nitromethane

H	1.811829	0.246785	1.837687
C	2.341053	0.546375	0.917315
H	3.348706	0.098100	0.941832
H	2.413351	1.642596	0.878699
C	1.569262	0.038569	-0.286392
O	1.118023	0.805512	-1.143722
C	1.383099	-1.464592	-0.377435
H	0.813573	-1.715706	-1.283526
H	2.363599	-1.969922	-0.390703
H	0.830656	-1.814945	0.510807
C	-1.970874	1.149505	-0.504785
H	-1.152760	1.388024	-1.196400
H	-2.893231	0.879281	-1.034661
H	-2.130317	1.966927	0.210009
N	-1.514242	-0.049172	0.261983
O	-0.842687	0.159540	1.295692
O	-1.782949	-1.169899	-0.222646



Ammonia-oxigen-difluorid

N	-2.420290	-0.000734	-0.132257
H	-1.815288	-0.803134	0.063560
H	-1.818726	0.804803	0.061262
H	-3.083243	0.003370	0.647931
O	0.983746	0.000141	-0.561705
F	0.656308	-1.133526	0.264727
F	0.655717	1.133681	0.264666



Ammonia-pyrazine

N	0.551070	1.435370	0.000026
C	0.551176	0.702702	1.134927
C	0.551384	-0.702642	1.134899
N	0.551493	-1.435265	-0.000032
C	0.551386	-0.702589	-1.134927
C	0.551179	0.702756	-1.134889
H	0.551093	1.259441	2.080741
H	0.551464	-1.259418	2.080691
H	0.551470	-1.259320	-2.080746
H	0.551098	1.259531	-2.080682
N	-2.516082	-0.000399	-0.000002
H	-2.940485	0.466335	-0.807243
H	-2.940280	-0.932952	0.000820
H	-2.940487	0.467759	0.806414

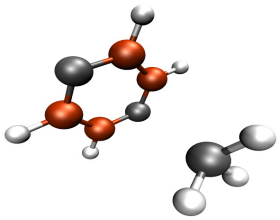
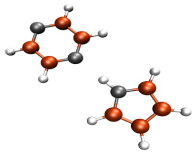


Table 3: coordinates in Angstrom (cont. 3)

Pyrrole-pyrazine (H-bond)

N	-1.116277	-0.000150	0.019717
C	-1.840966	1.141214	0.010095
C	-3.246427	1.141801	-0.008562
N	-3.972069	0.001043	-0.018193
C	-3.248391	-1.140963	-0.008585
C	-1.842932	-1.142795	0.010072
H	-1.279558	2.083082	0.017546
H	-3.807049	2.084137	-0.016006
H	-3.810634	-2.082333	-0.016048
H	-1.282199	-2.085066	0.017517
N	1.906183	-0.000072	0.015242
C	2.699989	1.126323	0.003913
C	2.700047	-1.126427	0.003917
C	4.034805	0.715035	-0.015132
C	4.034842	-0.715070	-0.015130
H	0.879481	-0.000601	0.029892
H	2.260267	2.123953	0.010185
H	2.260376	-2.124079	0.010193
H	4.904166	1.372849	-0.027538
H	4.904236	-1.372840	-0.027534



Pyrrole-pyrazine (stacked)

H	2.068365	-1.554770	-1.258236
H	-2.068564	-1.553940	-1.258236
H	2.068365	-1.554770	1.258236
H	-2.068564	-1.553940	1.258236
C	1.135821	-1.554583	-0.697884
C	-1.136020	-1.554127	-0.697884
C	1.135821	-1.554583	0.697884
C	-1.136020	-1.554127	0.697884
N	-0.000100	-1.554355	-1.417402
N	-0.000100	-1.554355	1.417402
H	-0.770304	1.855801	-2.114612
H	-0.770304	1.855801	2.114612
H	1.850809	1.855275	-1.358585
H	1.850809	1.855275	1.358585
H	-2.130086	1.856074	0.000000
C	-0.333285	1.855713	-1.125828
C	-0.333285	1.855713	1.125828
C	0.985374	1.855448	-0.709235
C	0.985374	1.855448	0.709235
N	-1.119278	1.855871	0.000000

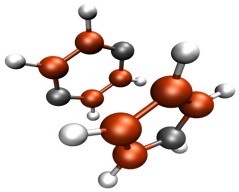
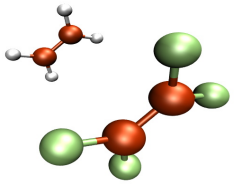


Table 4: coordinates in Angstrom (cont. 4)

Tetrafluor-ethylene-ethylene (3.5 Å)

F	-1.394866	-1.110938	-0.741831
F	-1.394866	1.110938	-0.741831
F	1.394866	-1.110938	-0.741831
F	1.394866	1.110938	-0.741831
C	-0.667784	0.000000	-0.759941
C	0.667784	0.000000	-0.759941
H	-1.244242	0.935429	2.658551
H	-1.244242	-0.935429	2.658551
H	1.244242	0.935429	2.658551
H	1.244242	-0.935429	2.658551
C	-0.674558	0.000000	2.662317
C	0.674558	0.000000	2.662317



Tetrafluor-ethylene-ethylene (5 Å)

F	-1.394866	-1.110938	-1.070259
F	-1.394866	1.110938	-1.070259
F	1.394866	-1.110938	-1.070259
F	1.394866	1.110938	-1.070259
C	-0.667784	0.000000	-1.088369
C	0.667784	0.000000	-1.088369
H	-1.244242	0.935429	3.830123
H	-1.244242	-0.935429	3.830123
H	1.244242	0.935429	3.830123
H	1.244242	-0.935429	3.830123
C	-0.674558	0.000000	3.833889
C	0.674558	0.000000	3.833889

Table 5: all calculated excitation energies and characters

system	Assignment of the excitation		Excitation energy / eV									TheoDORE characters							
												CC2			CCSD				
	sequence #	affected molecules	CC2	CCSD	CCSD(2)	CC3	CCSD(T)(a)*	CCSDT-3	CCSDT	STEOM-CCSD	ADC(2)	POS	PR	CT	POS	PR	PRi	PRf	CT
ammonia-fluorine	1 E	2 --> 2	4.28	4.08	4.06	4.00	3.99	4.00	3.97	4.07	4.27	1.98	1.03	0.03	1.99	1.02	1.00	1.05	0.02
	2 A1	1 --> 2 (1)	5.97	6.90	6.72	6.53	6.63	6.62	6.64	6.43	5.99	1.47	1.16	0.86	1.41	1.29	1.07	1.51	0.76
	3 A1	1 --> 1 (2)	7.96	8.04	7.92	7.97	7.92	7.99	7.98	7.95	7.95	1.04	1.08	0.07	1.09	1.20	1.06	1.34	0.17
acetone-fluorine	2 A'	2 --> 2	4.43	4.27	4.23	4.20	4.19	4.20	4.18	4.20	4.45	2.00	1.01	0.01	2.00	1.00	1.00	1.00	0.00
	1 A"	2 --> 2	4.44	4.27	4.24	4.20	4.19	4.21	4.19	4.21	4.45	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	2 A"	1 --> 1	4.54	4.44	4.33	4.41	4.41	4.42	4.39	4.27	4.32	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	3 A"	1 --> 2	5.18	6.28	6.10	5.75	5.83	5.90	5.85	5.85	5.13	1.49	1.03	0.97	1.48	1.04	1.00	1.08	0.96
pyrazine-fluorine	2 A1	2 --> 2	4.41	4.25	4.22	4.18	4.17	4.19	4.16	4.17	4.43	2.00	1.01	0.01	2.00	1.01	1.01	1.00	0.01
	1 B1	2 --> 2	4.44	4.28	4.24	4.20	4.20	4.21	4.19	4.20	4.46	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	3 A1	1 --> 1	4.30	4.44	4.62	4.28	4.34	4.33	4.28	4.22	4.32	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	2 B1	1 --> 1	5.14	5.14	5.37	5.01	5.06	5.04	4.99	4.70	5.18	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	1 A2	1 --> 1	4.93	5.25	5.33	5.03	5.08	5.12	5.04	4.97	4.95	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	1 B2	1 --> 1	6.02	6.10	6.25	5.83	5.95	5.90	5.81	5.80	6.03	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	2 B2	1 --> 2	5.62	6.77	6.82	6.15	6.30	6.33	6.28	6.34	5.75	1.50	1.00	1.00	1.51	1.02	1.04	1.01	0.98
	2 A2	1,2 --> 2	6.28	6.73	6.76	6.40	6.49	6.46	6.45	6.56	6.37	1.51	1.03	0.97	1.68	1.42	1.84	1.00	0.64
ammonia-oxygen-difluoride	2 A'	2 --> 2	4.26	4.33	4.36	4.20	4.24	4.23	4.20	4.10	4.29	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	1 A"	2 --> 2	4.98	5.04	5.05	4.93	4.97	4.95	4.93	4.73	4.99	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	2 A"	2 --> 2	6.84	6.78	6.66	6.68	6.68	6.70	6.64	6.68	6.67	2.00	1.01	0.01	2.00	1.00	1.00	1.00	0.00
	3 A'	2 --> 2	7.23	7.01	6.91	7.01	6.91	6.90	6.83	6.88	7.10	1.99	1.02	0.02	1.96	1.09	1.18	1.01	0.08
	4 A'	1 --> 2	6.33	7.33	7.14	6.83	7.03	7.09	7.04	7.06	6.30	1.51	1.03	0.97	1.52	1.15	1.21	1.10	0.86
	3 A"	2 --> 2	7.18	7.51	7.42	7.13	7.24	7.21	7.11	7.30	7.11	2.00	1.01	0.01	2.00	1.01	1.02	1.00	0.01
	5 A'	1 --> 1	7.98	7.98	7.87	7.96	7.93	7.98	7.96	7.93	7.99	1.00	1.01	0.01	1.02	1.05	1.01	1.09	0.04
acetone-nitromethane	2 A	2 --> 2	4.10	4.08	4.29	4.02	4.07	4.04		3.83	3.79	1.99	1.01	0.01	2.00	1.01	1.00	1.02	0.01
	3 A	1 --> 1	4.51	4.44	4.34	4.41	4.41	4.42		4.30	4.28	1.01	1.02	0.02	1.01	1.01	1.00	1.02	0.01
	4 A	2 --> 2	4.57	4.50	4.71	4.40	4.46	4.43		4.28	4.28	1.99	1.02	0.02	1.99	1.02	1.02	1.02	0.02
	5 A	1 (2) --> 2	6.06	6.75	6.77	6.28	6.42	6.42		6.33	5.75	1.47	1.07	0.94	1.55	1.23	1.36	1.11	0.80
	6 A	2 (1) --> 2	6.87	6.62	6.65	6.53	6.56	6.58		6.20	6.29	1.97	1.06	0.05	1.89	1.26	1.45	1.08	0.20
ammonia-pyrazine	2 A'	2 --> 2	4.37	4.51	4.69	4.35	4.41	4.40	4.35	4.29	4.40	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	1 A"	2 --> 2	5.14	5.14	5.37	5.01	5.06	5.03	4.99	4.70	5.18	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	2 A"	2 --> 2	4.98	5.30	5.38	5.07	5.12	5.16	5.08	5.01	4.99	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	3 A'	2 --> 2	6.09	6.17	6.32	5.90	6.02	5.98	5.88	5.87	6.10	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	3 A"	2 --> 2	6.80	7.20	7.26	6.84	6.94	6.97	6.83	6.90	6.80	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	4 A'	2 --> 2	7.05	7.13	7.19	7.02	7.06	7.04	7.04	7.14	7.01	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	5 A'	1 --> 2,1	7.31	7.93	7.90	7.46	7.73	7.53	7.49	7.38	7.28	1.45	1.26	0.78	1.38	1.45	1.15	1.74	0.63
	6 A'	1 --> 1,2	7.74	7.59	7.50	7.78	7.59	7.83	7.80	7.72	7.72	1.08	1.19	0.14	1.15	1.37	1.06	1.67	0.27
pyrrole-pyrazine (H-bond)	1 B2	2 --> 2	4.34	4.49	4.68	4.33	4.39	4.38		4.26	4.37	1.99	1.02	0.02	1.99	1.02	1.03	1.00	0.02
	1 B1	2 --> 2	5.12	5.11	5.36	4.99	5.03	5.01		4.68	5.16	1.99	1.01	0.01	2.00	1.00	1.00	1.00	0.00
	1 A2	2 --> 2	5.03	5.36	5.45	5.14	5.19	5.22		5.07	5.05	1.99	1.02	0.02	1.99	1.02	1.03	1.00	0.02
	2 B1	1 --> 2	5.07	5.60	5.80	5.15	5.25	5.27		5.30	5.12	1.51	1.01	0.99	1.50	1.00	1.00	1.00	1.00
	2 A1	1 --> 2	5.75	6.32	6.52	5.86	5.98	6.00		6.00	5.75	1.50	1.01	0.99	1.49	1.04	1.01	1.06	0.97
	2 B2	2 --> 2	6.10	6.20	6.36	5.93	6.05	6.01		5.87	6.10	1.98	1.04	0.04	1.98	1.03	1.06	1.00	0.03
	3 A1	1 --> 2	5.93	6.47	6.55	6.05	6.14	6.17		6.19	5.95	1.50	1.00	1.00	1.50	1.01	1.00	1.01	0.99
	4 A1	1 --> 1	6.66	6.65	6.74	6.44	6.50	6.50		6.34	6.65	1.00	1.01	0.00	1.02	1.04	1.00	1.08	0.04
pyrrole-pyrazine (stacked)	2 A'	2 --> 2	4.30	4.44	4.64	4.28	4.34	4.33		4.22	4.32	2.00	1.01	0.01	2.00	1.01	1.00	1.01	0.01
	3 A'	2 --> 2	5.05	5.08	5.33	4.95	4.99	4.98		4.64	5.07	1.92	1.18	0.13	1.95	1.11	1.19	1.04	0.08
	1 A"	2 --> 2	4.89	5.22	5.31	5.00	5.05	5.09		4.93	4.91	2.00	1.01	0.01	2.00	1.01	1.00	1.02	0.01
	2 A"	1 --> 2	5.33	5.68	5.84	5.40	5.47	5.48		5.40	5.33	1.49	1.11	0.90	1.50	1.18	1.18	1.19	0.84
	3 A"	2 --> 2	6.00	6.10	6.26	5.82	5.94	5.90		5.79	6.00	1.99	1.03	0.02	1.97	1.06	1.09	1.02	0.05
	4 A'	1 --> 2,1	5.93	6.22	6.31	6.00	6.05	6.07		5.95	5.91	1.47	1.21	0.81	1.39	1.41	1.13	1.68	0.66
	5 A'	1 --> 2,1	6.23	6.52	6.65	6.25	6.33	6.34		6.18	6.21	1.46	1.40	0.66	1.38	1.47	1.17	1.77	0.61
tetrafluor-ethylene-ethylene (5A)	1 B2	1 --> 1	7.38	7.52	7.48	7.42	7.44	7.44	7.43	7.36	7.40	1.00	1.00	0.00	1.00	1.00	1.00	1.00	0.00
	1 B1	2 --> 2	8.62	8.73	8.44	8.60	8.59	8.61	8.61	8.49	8.54	1.89	1.25	0.00	1.96	1.08	1.08	1.08	0.00
	2 B2	2 --> 2	8.92	8.83	8.53	8.79	8.77	8.80	8.77	8.80	8.92	2.00	1.00	0.00	2.00	1.00	1.00	1.00	0.00
	2 B1	1 --> 1	8.86	9.14	8.92	8.95	8.98	8.99	8.96	8.949	8.71	1.11	1.25	0.00	1.03	1.07	1.07	1.07	0.00
	5 B1	1 --> 2	10.16	10.87	10.74	10.46	10.52	10.56	10.57	10.616	10.28	1.49	1.02	0.98	1.50	1.01	1.00	1.01	0.99
tetrafluor-ethylene-ethylene (3.5A)	1 B2	1 --> 1	7.33	7.47	7.43	7.37	7.39	7.39	7.38	7.26	7.35	1.00	1.01	0.01	1.00	1.01	1.01	1.00	0.01
	1 B1	1,2 --> 2 (1)	7.99	8.24	8.02	8.05	8.08	8.09	8.08	8.00	7.97	1.58	1.81	0.37	1.68	1.75	1.91	1.59	0.24
	2 B2	2 --> 2	8.83	8.76	8.46	8.71	8.70	8.72	8.70	8.67	8.83	1.99	1.02	0.02	1.99	1.01	1.00	1.03	0.01
	2 B1	1 (2) --> 1,2	8.77	9.05	8.92	8.78	8.81	8.84	8.81	8.86	8.79	1.49	1.82	0.38	1.34	1.72	1.44	2.00	0.34
	3 B1	1 (2) --> 1,2	8.93	9.19	8.98	8.98	9.00	9.02	9.00	8.97	8.81	1.28	1.68	0.02	1.26	1.64	1.59	1.69	0.05