Electronic Supplementary Information (ESI) for:

Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light

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Cartesian coordinates and electronic energies of the ground and the lowest excited state equilibrium structures of formaldehyde complexes computed at the B2PLYP-D3/aug-cc-pVTZ, TD-CAMB3LYP-D3/aug-cc-pVTZ, CCSD/aug-cc-pVTZ and EOM-CCSD/aug-cc-pVTZ levels, respectively.

H_2O-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -190.66742785 au
S_1 EOM-CCSD/aug-cc-pVTZ: -190.514274578 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.268717	0.545956	-0.000338
2	8	0.921939	-0.613668	0.000199
3	1	0.534267	1.363437	-0.000701
4	1	2.333200	0.821980	-0.000439
5	8	-1.826615	0.124180	0.000671
6	1	-1.040805	-0.441473	0.000499
7	1	-2.575203	-0.476011	-0.009146

S_1 excited state equilibrium structure: TD-CAM-B3LYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -190.64628531 au
EOM-CCSD/aug-cc-pVTZ: -190.527080016 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.482600	0.550219	0.001152
2	8	0.897045	-0.589346	0.040713
3	1	1.454002	1.160937	0.908419
4	1	1.483598	1.080096	-0.956112
5	8	-1.959638	0.095258	-0.037161
6	1	-1.105324	-0.351542	-0.003169
7	1	-2.621215	-0.599319	-0.019232

COa-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -227.47190162 au
S_1 EOM-CCSD/aug-cc-pVTZ: -227.322993517

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.717048	-0.543399	-0.000005
2	8	-1.420363	0.625686	0.000005
3	1	-2.767675	-0.875036	0.000002
4	1	-0.951237	-1.335703	-0.000021
5	6	1.786852	0.593491	-0.000008
6	8	1.602319	-0.523971	0.000006

S_1 excited state equilibrium structure: TD-CAM-B3LYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -227.45468164 au
EOM-CCSD/aug-cc-pVTZ: -227.333879652 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.842613	-0.585914	-0.067958
2	8	-1.420240	0.607975	0.118585
3	1	-2.568039	-0.745382	-0.870231
4	1	-1.154155	-1.403798	0.161076
5	6	1.933853	0.568251	-0.176931
6	8	1.586320	-0.459306	0.109824

COe-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -227.47223418 au
S1 EOM-CCSD/aug-cc-pVTZ: -227.323304912 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.950844	-0.460619	-0.000046
2	8	-1.425412	0.625745	0.000039
3	1	-3.046912	-0.572233	-0.000074
4	1	-1.357854	-1.388461	-0.000100
5	6	1.378302	-0.571098	0.000085
6	8	2.132494	0.271831	-0.000057

S_1 excited state equilibrium structure: TD-CAM-B3LYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -227.4551601 au
EOM-CCSD/aug-cc-pVTZ: -227.334014413 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.129360	-0.476549	0.034515
2	8	-1.423209	0.591551	0.005441
3	1	-3.139419	-0.424529	-0.379901
4	1	-1.598981	-1.429727	-0.031254
5	6	1.431714	-0.507323	0.010168
6	8	2.245172	0.263422	-0.013058

H_2O_2-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -265.69044735 au
S_1 EOM-CCSD/aug-cc-pVTZ: -265.536790143 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.728885	-0.557578	0.178241
2	8	-1.436690	0.552473	-0.209713
3	1	-2.771948	-0.904208	0.162801
4	1	-0.966191	-1.251999	0.552941
5	8	1.347520	0.707469	0.188523
6	8	1.468630	-0.715200	-0.101113
7	1	0.400519	0.835179	-0.011613
8	1	2.030116	-0.685443	-0.885362

SO_2e-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -662.28757187 au
EOM-CCSD/aug-cc-pVTZ: -662.132690032 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.278541	-0.199649	-0.352439
2	8	-1.722309	0.606391	0.358549
3	1	-3.348846	-0.108372	-0.583176
4	1	-1.732130	-1.048313	-0.790233
5	16	0.912059	-0.026073	0.371677
6	8	0.564301	-1.331964	-0.190278
7	8	1.364499	1.000357	-0.560262

SO_2d3-HCOH

Ground electronic state equilibrium structure: B2PLYP-D3/aug-cc-pVTZ
CCSD/aug-cc-pVTZ: -662.28217334 au
EOM-CCSD/aug-cc-pVTZ: -662.135074733 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.333288	0.000384	0.000057
2	8	3.540328	-0.000618	-0.000033
3	1	1.749821	0.934985	0.000136
4	1	1.748282	-0.933257	0.000062
5	16	-1.754678	0.000280	0.000018
6	8	-1.002677	-1.249848	-0.000027
7	8	-1.001178	1.249509	-0.000030