A spin-flip variant of the second-order approximate coupled-cluster singles and doubles method

Supplementary Information

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1 Cartesian geometries

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C    -0.690428  0.000000   1.085671
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C    -1.397826  0.000000  -0.115266
H    -2.476058  0.000000  -0.120773
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C    -1.5516738597   -1.9174459710    0.6216855123
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C    -2.4404422951   -3.0767823055    0.9891436674
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C    -1.7884683766    1.6766996168    0.6862923408
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H    -1.8293382510   -3.9790509196    1.0248530293
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3

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O    -1.0863580177    1.5872962809    0.7045453660
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N    -2.7336423434   -1.9056433478   -0.1370361317
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H    -2.3832137993   -2.3341014358   -0.9887331535
C    -4.1779826589   -1.6063992118   -0.2812385809
H    -4.5995491335   -1.5088882249    0.7167569764
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H    -3.9509652816   -0.4827683024   -2.0904271954
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C    -3.1877799322    1.7885317544   -1.4640335437
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H     2.4357916814   -2.7001126866    0.1223649203
H     2.2456395244   -2.1388704123   -1.3807648385
C     4.0798535321   -1.6552639611   -0.5721153213
H     4.5006453777   -1.7281982560    0.4282594133
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C     4.2637661191   -0.2692572306   -1.1472915868
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H        3.8892250618   -0.2476605094   -2.1715119771
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C        3.2835211482    1.9414419703   -1.1598403187
H        2.7641842796    2.6793528630   -0.5581710474
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H        4.2450530380    2.3463113052   -1.4814884068
C        4.1992063212    1.0681887976    0.8912164078
H        3.5810602997    1.7434307266    1.4745666489
H        4.3989122355    0.1783492095    1.4853492250
H        5.1497006857    1.5522941282    0.6575385510
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2 Artificial multiplet splittings

Table 2. Artificial energy splittings $E(M_S = 0) - E(M_S = 1)$ in eV between high-spin and low-spin components of the triplet states of various molecules.

	CH_2		NH_2^+		SiH_2		PH_2^+	
	UHF	ROHF	UHF	ROHF	UHF	ROHF	UHF	ROHF
SF-CCSD	0.0129	0.0000	0.0198	0.0000	0.0044	0.0000	0.0066	0.0000
SF-CC2	0.1086	0.0431	0.1635	0.0486	0.0534	0.0342	0.0787	0.0466
SF-RI-CC2	0.1087	0.0432	0.1637	0.0488	0.0539	0.0349	0.0766	0.0469
SF-ADC(2)	0.1298	-0.1127	0.2021	-0.2121	0.0531	-0.0414	0.0825	-0.0602
SF-CIS(D_∞)	0.1357	—	0.2087	—	0.0613	—	0.0910	—

	NH		NF		OH^+		O_2	
	UHF	ROHF	UHF	ROHF	UHF	ROHF	UHF	ROHF
SF-CCSD	0.0144	0.0000	0.0224	0.0000	0.0146	0.0000	0.0339	0.0000
SF-CC2	0.1365	0.0580	0.1552	0.0741	0.1455	0.0559	0.2482	0.1901
SF-RI-CC2	0.1366	0.0582	0.1561	0.0749	0.1457	0.0559	0.2502	0.1921
SF-ADC(2)	0.1654	-0.1555	0.1108	-0.3037	0.1756	-0.1977	0.3859	-0.1736
SF-CIS(D_∞)	0.1720	—	0.2153	—	0.1813	—	0.4893	—

	o-C_6H_4	m-C_6H_4	p-C_6H_4		O_3	$^3B_1$	$^3A_2$	$^3B_2$	$^3A_1$
SF-CCSD	0.0224	0.1744	0.0217		SF-CCSD	0.0617	0.0858	0.0376	0.0612
SF-CC2	0.1187	0.3374	0.1187		SF-CC2	0.2986	0.3100	0.4753	0.3435
SF-RI-CC2	0.1188	0.3375	0.1188		SF-ADC(2)	0.2694	0.1477	0.2227	0.3702
SF-ADC(2)	0.1031	0.4202	0.1094						

3 Wave function analysis

Table 3. Largest two amplitudes obtained in EOM-SF-CCSD, SF-CC2, SF-ADC(2), and SF-CIS(D_∞) calculations on the singlet states of various molecules.

	Basis	EOM-SF-CCSD		SF-CC2		SF-RI-CC2		SF-ADC(2)		SF-CIS(D_∞)
		UHF	ROHF	UHF	ROHF	UHF	ROHF	UHF	ROHF	UHF
CH_2	cc-pVQZ	0.8692	-0.8723	-0.8701	-0.8726	0.8701	-0.8726	0.8697	0.9316	0.8607
		0.3160	0.3072	-0.3112	0.3033	0.3112	0.3033	-0.3123	0.3211	0.3292
NH_2^+	cc-pVQZ	-0.8134	0.8173	-0.8079	-0.8114	-0.8079	-0.8114	0.8084	0.8443	0.7897
		-0.4732	-0.4745	-0.4921	0.4934	-0.4922	0.4935	0.4912	0.5172	0.5312
SiH_2	cc-pVQZ	-0.9100	0.9102	-0.9171	0.9173	0.9171	0.9173	0.9165	-0.9592	0.9137
		-0.1991	0.1955	-0.1961	0.1927	0.1961	0.1927	-0.1958	-0.2035	0.2050
PH_2^+	cc-pVQZ	-0.9410	0.9412	-0.9465	-0.9466	0.9465	0.9466	0.9464	0.9607	0.9421
		-0.1658	0.1626	0.1776	-0.1785	-0.1777	0.1785	0.1773	0.2054	0.2274

Molecule	Basis	EOM-SF-CCSD	SF-CC2	SF-RI-CC2	SF-ADC(2)
o-C_6H_4	cc-pVQZ	0.8325	0.8429	0.8429	0.8383
		-0.2138	-0.2161	-0.2161	-0.2161
m-C_6H_4	cc-pVQZ	0.7726	-0.7852	0.7852	0.7773
		0.2778	-0.2675	0.2674	0.2774
p-C_6H_4	cc-pVQZ	0.6551	0.6786	-0.6786	0.6636
		0.4992	0.4741	-0.4741	-0.4929

Molecule / State	Basis	EOM-SF-CCSD	SF-CC2	SF-ADC(2)
O_3 / $^3A_1$	cc-pVDZ	-0.9546	-0.9164	0.9304
		-0.1034	-0.2029	0.1536
O_3 / $^3A_2$	cc-pVDZ	-0.9336	0.9408	-0.9454
		-0.0934	0.0821	-0.1172
O_3 / $^3B_1$	cc-pVDZ	0.9342	0.9288	-0.9374
		0.1155	0.1504	0.1388
O_3 / $^3B_2$	cc-pVDZ	-0.9405	0.9440	0.9517
		-0.1256	-0.0855	-0.0980

Table 4. Largest two amplitudes obtained in EOM-SF-CCSD, SF-CC2, and SF-ADC(2) calculations on the ground state of ozone at different bond lengths and a bond angle of 142.76°. The cc-pVDZ basis set was used in all calculations.

R/Å	EOM-SF-CCSD		SF-CC2		SF-ADC(2)	
			reference state = $^3A_1$			
1.30	-0.9546	-0.1034	-0.9164	-0.2029	0.9304	0.1536
1.35	-0.9432	0.1444	-0.8748	0.2867	-0.9061	0.2087
1.40	0.9253	-0.2001	0.8070	-0.3867	0.8710	0.2749
1.45	-0.8999	-0.2667	-0.7091	-0.4860	0.8216	0.3459
1.50	0.8660	0.3394	-0.5884	-0.5592	-0.7595	0.4062
1.55	-0.8229	0.4136	0.5901	-0.4639	-0.6957	0.4365
1.60	-0.7709	0.4841	-0.5804	0.3781	-0.6510	0.4165
1.65	-0.8147	0.4249	0.5421	0.4286	0.6420	-0.4538
			reference state = $^3A_2$			
1.30	-0.9336	-0.0934	0.9408	0.0821	-0.9454	-0.1172
1.35	0.9231	-0.1238	0.9344	0.0937	0.9379	-0.1723
1.40	0.9096	-0.1663	0.9276	0.1397	0.9235	0.2504
1.45	0.8928	0.2231	-0.9178	0.2074	-0.8977	-0.3424
1.50	0.8725	0.2926	-0.9006	0.2936	0.8622	0.4309
1.55	0.8483	0.3681	0.8727	0.3861	0.8244	0.5033
1.60	0.8215	-0.4403	0.8376	-0.4691	0.7910	0.5567
1.65	0.7631	0.3795	0.8028	0.5336	-0.7643	0.5945
			reference state = $^3B_1$			
1.30	0.9342	0.1155	0.9288	0.1504	-0.9374	0.1388
1.35	0.9223	0.1471	-0.9134	-0.1911	-0.9288	0.1683
1.40	-0.9047	-0.1872	-0.8934	-0.2358	-0.9201	0.1944
1.45	0.8795	0.2382	-0.8703	-0.2821	0.9109	-0.2143
1.50	-0.8438	-0.3044	0.8451	0.3325	0.8969	-0.2383
1.55	0.7908	0.3905	-0.8114	-0.3991	0.8620	-0.3066
1.60	0.7142	0.4896	0.7537	0.4918	0.7725	0.4484
1.65	-0.7154	0.5429	0.6583	0.5978	0.6340	0.5875
			reference state = $^3B_2$			
1.30	-0.9405	-0.1256	0.9440	-0.0855	0.9517	-0.0980
1.35	0.9341	-0.1404	-0.9363	0.0906	0.9480	-0.1077
1.40	-0.9264	0.1574	-0.9267	0.0977	0.9445	-0.1203
1.45	0.9160	-0.1817	-0.9139	0.1124	0.9404	-0.1376
1.50	0.9012	0.2182	-0.8964	-0.1397	0.9348	-0.1599
1.55	-0.8800	0.2690	-0.8724	-0.1824	0.9270	-0.1856
1.60	0.8499	0.3328	-0.8396	-0.2401	0.9169	-0.2110
1.65	0.8609	0.2451	0.8735	0.0839	-0.8636	0.2067

4 Potential energy curves of H_2 and HF

Table 5. Potential energy curve of the ground state of H_2 computed with various spin-flip methods and the cc-pVTZ basis set. All energies in a.u. relative to the energy at 0.75Å.

R/Å	EOM-SF-CCSD	SF-CC2	SF-ADC(2)	SF-CIS(D_∞)
0.50	0.07143154	0.07502832	0.07515472	0.07510728
0.60	0.01878329	0.02064839	0.02070641	0.02067075
0.75	0.00000000	0.00000000	0.00000000	0.00000000
0.95	0.01883390	0.01722292	0.01722460	0.01729710
1.20	0.06023365	0.05707509	0.05711329	0.05726513
1.40	0.09216351	0.08777579	0.08783516	0.08800553
1.75	0.13389682	0.12741870	0.12749589	0.12757175
2.00	0.15184623	0.14421101	0.14429387	0.14425444
2.50	0.16762139	0.15885055	0.15894010	0.15875393
3.00	0.17157542	0.16253919	0.16263107	0.16240828
3.50	0.17244344	0.16335589	0.16344847	0.16321944
4.00	0.17262618	0.16352728	0.16362001	0.16339004
4.50	0.17266584	0.16356373	0.16365641	0.16342638
5.00	0.17267595	0.16357269	0.16366543	0.16343532
5.50	0.17267921	0.16357542	0.16366833	0.16343806
6.00	0.17268044	0.16357639	0.16366916	0.16343902

Table 6. Potential energy curve of the ground state of HF computed with various spin-flip methods and the 6-31G** basis set. All energies in a.u. relative to the energy at 0.90 Å. Full CI results from A. Dutta, C.D. Sherrill, J. Chem. Phys. 118, 1610 (2003).

R/Å	Full CI	EOM-SF-CCSD	SF-CC2	SF-ADC(2)	SF-CIS(D$_\infty$)
0.70	0.101443	0.10035112	0.09752820	0.09715801	0.09439159
0.75	0.052102	0.05124284	0.04872715	0.04845883	0.04621245
0.80	0.022353	0.02176368	0.01980438	0.01964028	0.01803618
0.85	0.006366	0.00606571	0.00493995	0.00486864	0.00401877
0.90	0.000000	0.00000000	0.00000000	0.00000000	0.00000000
0.95	0.000309	0.00062277	0.00203325	0.00207925	0.00300871
1.00	0.005195	0.00585188	0.00585188	0.00899087	0.01091500
1.10	0.023150	0.02465898	0.03156242	0.03158706	0.03561252
1.20	0.046273	0.04895138	0.05980061	0.05960304	0.06558355
1.30	0.070541	0.07471935	0.08882961	0.08811348	0.09532063
1.40	0.093800	0.09972218	0.11561932	0.11403606	0.12121307
1.60	0.133477	0.14291050	0.15632525	0.15242944	0.15630300
1.80	0.162200	0.17356837	0.17896971	0.17324800	0.17333151
2.00	0.180725	0.19098974	0.18954705	0.18295133	0.18087383
2.20	0.191535	0.19871823	0.19419053	0.18726597	0.18421451
2.40	0.197425	0.20175181	0.19626411	0.18922523	0.18576186
2.60	0.200510	0.20297782	0.19535583	0.18820083	0.18651669
2.80	0.202094	0.20351724	0.19484491	0.18768353	0.18690155
3.00	0.202904	0.20368123	0.19462321	0.18745852	0.18711014
3.20	0.203323	0.20362859	0.19454820	0.18738155	0.18723227
3.40	0.203542	0.20362388	0.19453738	0.18736958	0.18730745
3.60	0.203656	0.20363527	0.19454748	0.18737906	0.18735348
3.80	0.203714	0.20364782	0.19455981	0.18739109	0.18738023
4.00	0.203742	0.20365670	0.19456868	0.18739982	0.18739466

5   Potential energy surface of O_3

Table 7. Potential energy curve of the ground state of O_3 computed with various methods and the cc-pVDZ basis set at a bond angle of 142.76°. All values in a.u.

R(OO)/Å	CCSD	CC2	MP2
1.30	-224.84003083	-224.90745501	-224.86138149
1.35	-224.83131580	-224.91798781	-224.85322089
1.40	-224.81738882	-224.92689106	-224.83510604
1.45	-224.80001462	-224.93693093	-224.80558339
1.50	-224.78062443	-224.95179257	-224.76210807
1.55	-224.76057832	-224.98257526	-224.70425022
1.60	-224.74114908	-225.05292901	-224.63861562
1.65	-224.72314464	no convergence	-224.57662771

Table 8. Potential energy curve of the ground state of O_3 computed with various spin-flip methods and the cc-pVDZ basis set at a bond angle of 142.76°. The $^3A_1$ state is used as reference. All values in a.u.

R(OO)/Å	EOM-SF-CCSD	SF-CC2	SF-ADC(2)
1.30	-224.82905942	-224.91984306	-224.86240974
1.35	-224.81948218	-224.92983262	-224.84250170
1.40	-224.80454769	-224.93472880	-224.80620359
1.45	-224.78627773	-224.93843324	-224.77078248
1.50	-224.76598610	-224.94212315	-224.73795417
1.55	-224.74480481	-224.94585556	-224.70721442
1.60	-224.72391173	-224.94942073	-224.67795694
1.65	-224.70204970	-224.95350420	-224.65094848

Table 9. Potential energy curve of the ground state of O_3 computed with various spin-flip methods and the cc-pVDZ basis set at a bond angle of $142.76°$. The $^3B_1$ state is used as reference. All values in a.u.

R(OO)/Å	EOM-SF-CCSD	SF-CC2	SF-ADC(2)
1.30	-224.84101525	-224.87024346	-224.82660746
1.35	-224.83242849	-224.86782622	-224.80806855
1.40	-224.81865531	-224.85645635	-224.77535900
1.45	-224.80153744	-224.83485702	-224.73117411
1.50	-224.78245201	-224.80183159	-224.68152310
1.55	-224.76245205	-224.75877604	-224.63428133
1.60	-224.74241844	-224.71124350	-224.59802988
1.65	-224.71529789	-224.66640011	-224.57696800

Table 10. Potential energy curve of the ground state of O_3 computed with various spin-flip methods and the cc-pVDZ basis set at a bond angle of $142.76°$. The $^3B_2$ state is used as reference. All values in a.u.

R(OO)/Å	EOM-SF-CCSD	SF-CC2	SF-ADC(2)
1.30	-224.81013041	-224.85600234	-224.80243383
1.35	-224.80609368	-224.86195373	-224.79193622
1.40	-224.79646813	-224.86211844	-224.77181557
1.45	-224.78293448	-224.85785563	-224.74647062
1.50	-224.76674261	-224.85027252	-224.72046607
1.55	-224.74894536	-224.84001436	-224.69644394
1.60	-224.73048353	-224.82759184	-224.67564300
1.65	-224.70876342	-224.85355225	-224.65835592

Table 11. Potential energy curve of the ground state of O_3 computed with various spin-flip methods and the cc-pVDZ basis set at a bond angle of 142.76°. The $^3A_2$ state is used as reference. All values in a.u.

R(OO)/Å	EOM-SF-CCSD	SF-CC2	SF-ADC(2)
1.30	-224.83833856	-224.85322174	-224.79146178
1.35	-224.82861528	-224.83827159	-224.76242696
1.40	-224.81355485	-224.81310215	-224.72801856
1.45	-224.79596092	-224.78252839	-224.69716854
1.50	-224.77854726	-224.75149353	-224.67420925
1.55	-224.76324577	-224.72356858	-224.65889924
1.60	-224.75076181	-224.70065855	-224.64930768
1.65	-224.71831906	-224.68319601	-224.64359336

Table 12. Potential energy curve of the ground state of O_3 computed with CC2 and SF-CC2 using the cc-pVDZ basis set at a bond angle of 116.78°. All values in a.u.

R(OO)/Å	CC2	SF-CC2 ($^3A_1$)	SF-CC2 ($^3B_1$)	SF-CC2 ($^3B_2$)	SF-CC2 ($^3A_2$)
1.30	-224.94116740	-224.95354322	-224.90407910	-224.84994937	-224.90041017
1.35	-224.94724247	-224.95624756	-224.89873225	-224.85799518	-224.89203945
1.40	-224.95030067	-224.95254922	-224.88391154	-224.85994699	-224.87171637
1.45	-224.95204936	-224.94592076	-224.85803426	-224.85716136	-224.83944723
1.50	-224.95297987	-224.93761663	-224.82126925	-224.85047502	-224.79954401
1.55	-224.95117249	-224.92862259	-224.77645855	-224.84066904	-224.75799859
1.60	-224.94251384	-224.92004328	-224.72873630	-224.82844599	-224.72022530

Table 13. Norms of amplitude vectors from CCSD and CC2 calculations for various states of O_3. Computed using the cc-pVDZ basis set at a bond angle of 142.76°.

R(OO)/Å	CCSD		CC2		CCSD		CC2	
	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$
	${}^1A_1$ state				${}^3A_1$ state			
1.30	0.0545	0.2187	0.1369	0.3101	0.0404	0.2302	0.0990	0.4079
1.35	0.0862	0.2386	0.2503	0.3822	0.0953	0.2543	0.2009	0.4843
1.40	0.1374	0.2612	0.4705	0.4972	0.1894	0.2879	0.3819	0.5825
1.45	0.2205	0.2887	0.9186	0.7152	0.2857	0.3266	0.6034	0.7003
1.50	0.3554	0.3258	1.9045	1.2480	0.3762	0.3697	0.8642	0.8409
1.55	0.5654	0.3820	4.5665	3.3119	0.4607	0.4174	1.1727	1.0120
1.60	0.8621	0.4723	13.3890	17.5670	0.5491	0.4699	1.5583	1.2357
1.65	1.2334	0.6165	—	—	0.2288	0.3624	2.1089	1.5784
	${}^3B_1$ state				${}^3B_2$ state			
1.30	0.0555	0.1860	0.0902	0.2277	0.0827	0.3130	0.1444	0.3362
1.35	0.0959	0.2038	0.1556	0.2583	0.1233	0.3137	0.2384	0.3924
1.40	0.1646	0.2269	0.2585	0.2922	0.1830	0.3222	0.3879	0.4682
1.45	0.2656	0.2582	0.3886	0.3243	0.2553	0.3391	0.6010	0.5731
1.50	0.3939	0.3006	0.5103	0.3436	0.3259	0.3635	0.8737	0.7171
1.55	0.5393	0.3560	0.5909	0.3410	0.3823	0.3933	1.1965	0.9079
1.60	0.6752	0.4220	0.6044	0.3141	0.4191	0.4258	1.5628	1.1540
1.65	0.1774	0.3235	0.5267	0.2642	0.3232	0.4682	1.0775	1.1464
	${}^3A_2$ state							
1.30	0.1301	0.2133	0.1610	0.2246				
1.35	0.1975	0.2286	0.2292	0.2344				
1.40	0.2719	0.2462	0.2938	0.2379				
1.45	0.3316	0.2643	0.3349	0.2344				
1.50	0.3634	0.2819	0.3399	0.2344				
1.55	0.3673	0.2988	0.3086	0.2050				
1.60	0.3482	0.3137	0.2536	0.1815				
1.65	0.4289	0.3345	0.1936	0.1574				

Table 14. Norms of amplitude vectors from CC2 calculations for various states of O_3. Computed using the cc-pVDZ basis set at a bond angle of $116.78°$.

R(OO)/Å	$^1A_1$ state		$^3A_1$ state		$^3B_1$ state		$^3B_2$ state		$^3A_2$ state	
	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$	$|T_1|^2$	$|T_2|^2$
1.30	0.0749	0.2921	0.1199	0.4296	0.0687	0.2208	0.1009	0.3115	0.0874	0.2194
1.35	0.1242	0.3449	0.2402	0.5066	0.1180	0.2465	0.1514	0.3511	0.1499	0.2415
1.40	0.2111	0.4153	0.4313	0.6032	0.2096	0.2743	0.2310	0.3987	0.2521	0.2623
1.45	0.3706	0.5175	0.6631	0.7185	0.3469	0.3013	0.3533	0.4579	0.3713	0.2768
1.50	0.6738	0.6838	0.9368	0.8571	0.4886	0.3198	0.5253	0.5336	0.4525	0.2786
1.55	1.2307	0.9780	1.2581	1.0277	0.5800	0.3208	0.7391	0.6296	0.4619	0.2640
1.60	2.0816	1.4641	1.6385	1.2455	0.5812	0.2979	0.9808	0.7475	0.4035	0.2344
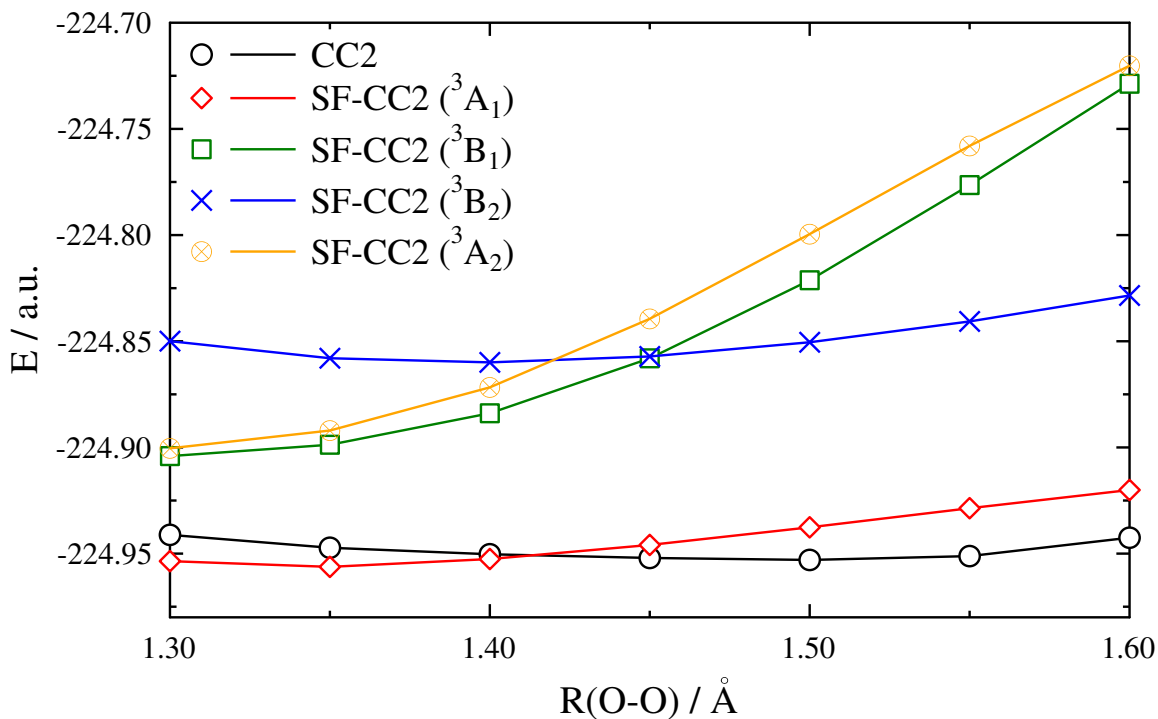
Figure 1. Potential energy curves of the ground state of ozone at a bond angle of $116.78°$ computed with conventional CC2 and SF-CC2 using the $^3A_1$, $^3B_1$, $^3B_2$, and $^3B_2$ states as reference. The cc-pVDZ basis was used for all calculations.
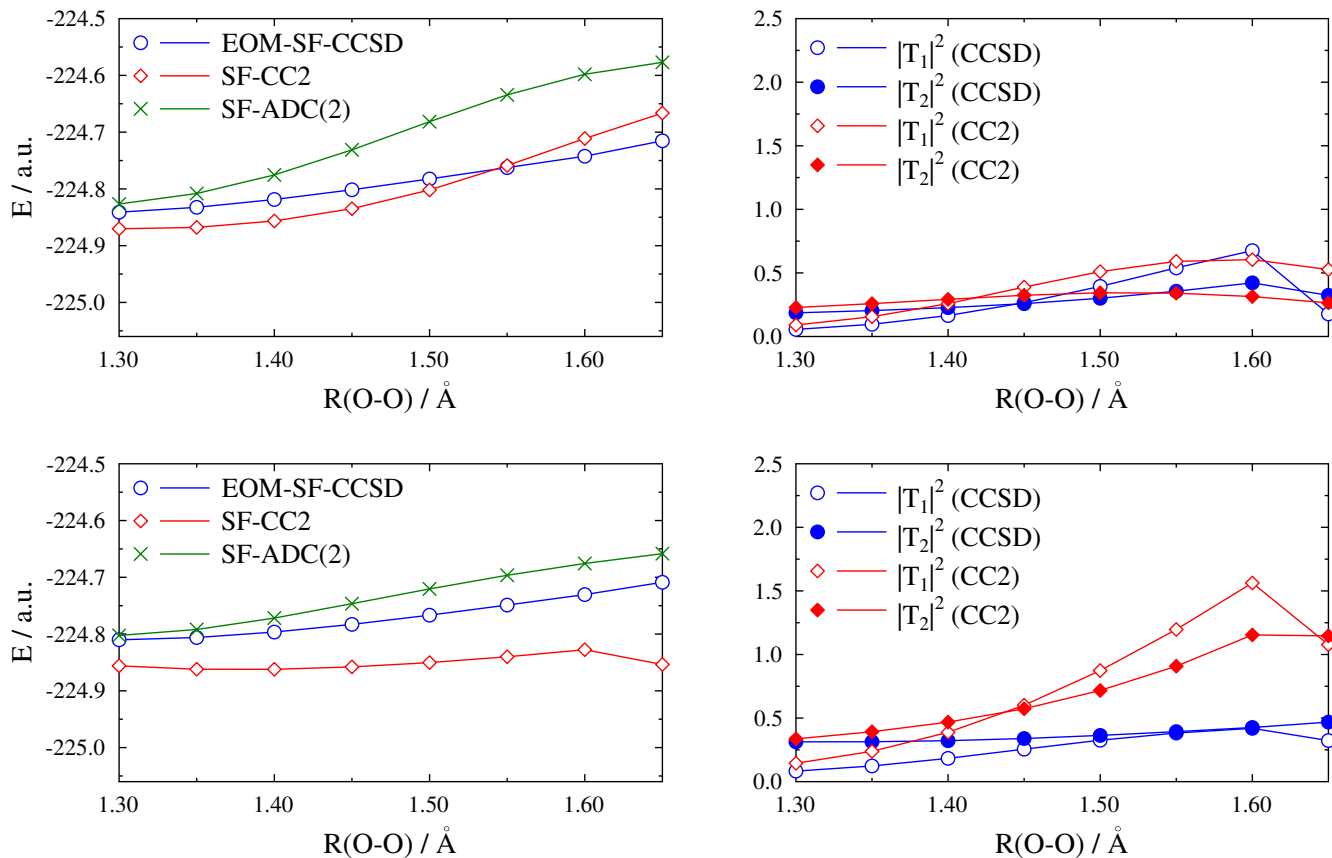
Figure 2. Left: Potential energy curves of the ground state of ozone at a bond angle of 142.76° computed with EOM-SF-CCSD, SF-CC2, and SF-ADC(2) using the $^3B_1$ state (upper panel) and the $^3B_2$ state (lower panel) as reference. Right: Norms of single and double amplitude vectors from corresponding CCSD and CC2 calculations. The cc-pVDZ basis is used in all calculations.