Benchmarking the completely renormalized equation-of-motion coupled-cluster approaches for vertical excitation energies (Supplemental Data)

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This supplemental data contains the information about the symmetry unique Cartesian coordinates of the ground-state geometries of the 28 molecules comprising the benchmark set proposed in Ref. [1] resulting from the MP2/6-31G* (Table I) and CR-CC(2,3),D/TZVP (Table II) optimizations.

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[1] M. Schreiber, M. R. Silva-Junior, S. P. A. Sauer, and W. Thiel, J. Chem. Phys. **128**, 134110 (2008).

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TABLE I: Symmetry unique Cartesian coordinates of the ground-state geometries for the 28 molecules comprising the benchmark set of Ref. [1] resulting from the MP2/6-31G* optimizations (taken from Ref. [1] and recalculated in this work).

Molecule (symmetry)	Atom	X	Y	Z
Ethene (D_{2h})	H	0.000000	0.923274	1.238289
	C	0.000000	0.000000	0.668188
E-Butadiene (C_{2h})	H	-1.080977	2.558832	0.000000
	H	-2.103773	1.017723	0.000000
	H	0.973565	1.219040	0.000000
	C	0.000000	-0.728881	0.000000
	C	-1.117962	1.474815	0.000000
all-E-Hexatriene (C_{2h})	H	-0.953777	1.207691	0.000000
	H	2.155816	0.952317	0.000000
	H	2.125769	3.402692	0.000000
	H	0.275642	3.397162	0.000000
	C	0.000000	0.676808	0.000000
	C	1.204938	1.485654	0.000000
	C	1.203567	2.831663	0.000000
all-E-Octatetraene (C_{2h})	H	0.971328	1.220141	0.000000
	H	-2.098090	0.984719	0.000000
	H	-0.146884	3.418505	0.000000
	H	-2.193473	4.766086	0.000000
	H	-3.225698	3.230501	0.000000
	C	0.000000	0.721498	0.000000
	C	1.125020	-1.479523	0.000000
	C	1.121077	-2.928812	0.000000
	C	2.237388	-3.682282	0.000000
Cyclopropene (C_{2v})	H	0.912650	0.000000	1.457504
	H	0.000000	-1.585659	-1.038624
	C	0.000000	0.000000	0.859492
	C	0.000000	-0.651229	-0.499559
Cyclopentadiene (C_{2v})	H	-0.879859	0.000000	1.874608
	H	0.000000	2.211693	0.612518
	H	0.000000	1.349811	-1.886050
	C	0.000000	0.000000	1.215652
	C	0.000000	-1.177731	0.285415
	C	0.000000	-0.732372	-0.993420
Norbornadiene (C_{2v})	H	0.901419	0.000000	1.967823
	H	0.000000	2.156504	0.616597
	H	1.924341	1.340999	-1.022814
	C	0.000000	0.000000	1.346369
	C	0.000000	1.119526	0.272221
	C	1.235500	0.672374	-0.517602
Benzene (D_{6h})	H	2.151390	1.242106	0.000000
	C	1.209657	-0.698396	0.000000
Naphthalene (D_{2h})	H	1.240557	2.492735	0.000000
	H	3.377213	1.246082	0.000000
	C	0.000000	0.716253	0.000000
	C	1.241539	1.403577	0.000000
	C	2.432418	0.707325	0.000000
Furan (C_{2v})	H	0.000000	2.051058	0.851533
	H	0.000000	1.371979	-1.821224
	C	0.000000	1.095840	0.348301
	C	0.000000	0.714027	-0.963274
	O	0.000000	0.000000	1.164881

Molecule (symmetry)	Atom	X	Y	Z
Pyrrole (C_{2v})	H	0.000000	2.114611	0.770889
	H	0.000000	1.358585	-1.850224
	H	0.000000	0.000000	2.130670
	C	0.000000	1.125828	0.333870
	C	0.000000	0.709235	-0.984789
	N	0.000000	0.000000	1.119862
Imidazole (C_s)	H	0.000000	2.119822	0.714354
	H	0.000000	1.202262	-1.904898
	H	0.000000	-2.104815	0.663782
	H	0.000000	-0.010302	2.116597
	C	0.000000	1.120107	0.305897
	C	0.000000	0.635508	-0.983749
	C	0.000000	-1.091835	0.283881
	N	0.000000	-0.741378	-0.994001
	N	0.000000	0.000000	1.104571
Pyridine (C_{2v})	H	0.000000	2.061947	1.308539
	H	0.000000	2.156804	-1.184054
	H	0.000000	0.000000	-2.475074
	C	0.000000	1.145417	0.721005
	C	0.000000	1.197637	-0.673735
	C	0.000000	0.000000	-1.387901
	N	0.000000	0.000000	1.426610
Pyrazine (D_{2h})	H	0.000000	2.068464	1.258236
	C	0.000000	1.135920	0.697884
	N	0.000000	0.000000	1.417402
Pyrimidine (C_{2v})	H	0.000000	2.156588	1.120200
	H	0.000000	0.000000	-2.400385
	H	0.000000	0.000000	2.440403
	C	0.000000	1.186684	0.626213
	C	0.000000	0.000000	-1.312625
	C	0.000000	0.000000	1.354949
	N	0.000000	1.203523	-0.717781
Pyridazine (C_{2v})	H	0.000000	2.409486	-0.149325
	H	0.000000	1.271234	2.102647
	C	0.000000	1.325698	-0.063084
	C	0.000000	0.693095	1.182948
	N	0.000000	0.674211	-1.238929
s-Triazine (D_{3h})	H	0.000000	0.000000	2.386083
	H	0.000000	2.066408	-1.193041
	C	0.000000	0.000000	1.298345
	C	0.000000	1.124400	-0.649173
	N	0.000000	0.000000	-1.379450
	N	0.000000	1.194639	0.689726
s-Tetrazine (D_{2h})	H	0.000000	0.000000	-2.354794
	C	0.000000	0.000000	1.269044
	N	0.000000	1.204572	0.670429
Formaldehyde (C_{2v})	H	0.000000	0.934473	-0.588078
	C	0.000000	0.000000	0.000000
	O	0.000000	0.000000	1.221104
Acetone (C_{2v})	H	0.000000	2.136732	-0.112445
	H	-0.881334	1.333733	-1.443842
	C	0.000000	0.000000	0.000000
	C	0.000000	1.287253	-0.795902
	O	0.000000	0.000000	1.227600

Molecule (symmetry)	Atom	X	Y	Z
p-Benzoquinone (D_{2h})	H	0.000000	2.182973	1.259286
	C	0.000000	0.000000	1.441079
	C	0.000000	1.266644	0.674582
	O	0.000000	0.000000	2.678518
Formamide (C_s)	H	-0.927427	-0.600301	0.000000
	H	1.070498	-1.782390	0.000000
	H	2.024514	-0.325050	0.000000
	C	0.000000	0.000000	0.000000
	O	0.000000	1.225060	0.000000
	N	1.119392	-0.775069	0.000000
Acetamide (C_s)	H	1.173209	-1.735763	0.000000
	H	2.035841	-0.226201	0.000000
	H	-2.121189	-0.156089	0.000000
	H	-1.310647	-1.472742	0.885504
	C	0.000000	0.000000	0.000000
	C	-1.267042	-0.831610	0.000000
	O	0.000000	1.229439	0.000000
	N	1.158967	-0.727718	0.000000
Propanamide (C_s)	H	1.171887	-1.734653	0.000000
	H	2.036508	-0.225526	0.000000
	H	-1.256737	-1.492368	0.877197
	H	-3.420939	-0.590421	0.000000
	H	-2.544313	0.678541	-0.880209
	C	0.000000	0.000000	0.000000
	C	-1.272727	-0.833216	0.000000
	C	-2.523376	0.033790	0.000000
	O	0.000000	1.230373	0.000000
	N	1.159100	-0.726409	0.000000
Cytosine (C_s)	H	-2.114860	-1.429678	0.000000
	H	-0.173973	-2.806186	0.000000
	H	2.073228	-1.658021	0.000000
	H	3.175240	0.564335	0.000000
	H	2.235202	2.033636	0.000000
	C	-0.060783	-1.726152	0.000000
	C	1.144884	-1.099470	0.000000
	C	1.107049	0.338190	0.000000
	C	-1.227573	0.430359	0.000000
	O	-2.315109	0.998271	0.000000
	N	0.000000	1.058130	0.000000
	N	-1.201178	-0.989148	0.000000
	N	2.278974	1.024187	0.000000
Thymine (C_s)	H	0.217481	-2.676720	0.000000
	H	2.052694	0.924773	0.000000
	H	-1.943101	-1.709021	0.000000
	H	-3.360610	0.309754	0.000000
	H	-2.616463	1.665008	0.879105
	C	1.356951	-0.994496	0.000000
	C	0.000000	1.121102	0.000000
	C	-1.214538	0.306431	0.000000
	C	-1.085764	-1.041812	0.000000
	C	-2.529824	1.020445	0.000000
	O	2.444132	-1.558490	0.000000
	O	0.023681	2.350992	0.000000
	N	0.145112	-1.666249	0.000000
	N	1.192460	0.382130	0.000000
Uracil (C_s)	H	-2.025413	-1.517742	0.000000
	H	-0.021861	1.995767	0.000000
	H	2.182391	-1.602586	0.000000

Molecule (symmetry)	Atom	X	Y	Z
	H	-0.026659	-2.791719	0.000000
	C	-1.239290	0.359825	0.000000
	C	1.279718	0.392094	0.000000
	C	1.243729	-1.064577	0.000000
	C	0.055755	-1.709579	0.000000
	O	-2.308803	0.954763	0.000000
	O	2.287387	1.092936	0.000000
	N	-1.139515	-1.026364	0.000000
	N	0.000000	0.978951	0.000000
Adenine (C_s)	H	0.974930	-3.075149	0.000000
	H	2.134658	2.075802	0.000000
	H	3.312010	0.776987	0.000000
	H	-3.052077	-0.334232	0.000000
	H	-2.711876	2.203052	0.000000
	C	0.662834	-2.032900	0.000000
	C	1.359313	0.172553	0.000000
	C	0.000000	0.547434	0.000000
	C	-0.924835	-0.500714	0.000000
	C	-1.906806	1.478795	0.000000
	N	-0.658577	-1.817838	0.000000
	N	1.672594	-1.133202	0.000000
	N	-2.150759	0.128726	0.000000
	N	-0.616118	1.783396	0.000000
	N	2.352763	1.090709	0.000000

TABLE II: Symmetry unique Cartesian coordinates of the ground-state geometries of the 28 molecules comprising the benchmark set of Ref. [1] resulting from the CR-CC(2,3),D/TZVP optimizations carried out in this work.

Molecule (symmetry)	Atom	X	Y	Z
Ethene (D_{2h})	H	0.000000	0.924035	1.236513
	C	0.000000	0.000000	0.668881
E-Butadiene (C_{2h})	H	-2.733502	0.488401	0.000000
	H	-1.996346	-1.209626	0.000000
	H	-0.493204	1.480741	0.000000
	C	0.613255	-0.399134	0.000000
	C	-1.846790	-0.134268	0.000000
all-E-Hexatriene (C_{2h})	H	-0.689671	-1.373825	0.000000
	H	-1.779265	1.550035	0.000000
	H	-3.983818	0.481440	0.000000
	H	-3.188581	-1.190249	0.000000
	C	-0.611506	-0.287351	0.000000
	C	-1.860731	0.465059	0.000000
	C	-3.076386	-0.110589	0.000000
all-E-Octatetraene (C_{2h})	H	-0.609354	1.435522	0.000000
	H	-1.864325	-1.371454	0.000000
	H	-3.082792	1.500066	0.000000
	H	-5.238862	0.334070	0.000000
	H	-4.370232	-1.299431	0.000000
	C	-0.638128	0.346740	0.000000
	C	1.835457	0.282916	0.000000
	C	3.116293	-0.412631	0.000000
	C	4.305668	0.215978	0.000000
Cyclopropene (C_{2v})	H	0.914476	0.000000	1.478608
	H	0.000000	-1.579439	-1.022564
	C	0.000000	0.000000	0.887272
	C	0.000000	-0.650147	-0.480853
Cyclopentadiene (C_{2v})	H	-0.884693	0.000000	1.884064
	H	0.000000	2.210781	0.627891
	H	0.000000	1.348160	-1.876762
	C	0.000000	0.000000	1.235311
	C	0.000000	-1.181911	0.294218
	C	0.000000	-0.737921	-0.982749
Norbornadiene (C_{2v})	H	0.901246	0.000000	1.976906
	H	0.000000	2.156931	0.625501
	H	1.933914	1.340614	-1.010326
	C	0.000000	0.000000	1.357782
	C	0.000000	1.123491	0.279727
	C	1.244064	0.671585	-0.512920
Benzene (D_{6h})	H	0.000000	2.482672	0.000000
	C	0.000000	1.397828	0.000000
Naphthalene (D_{2h})	H	1.241938	2.490352	0.000000
	H	3.377709	1.245631	0.000000
	C	0.000000	0.712349	0.000000
	C	1.245787	1.404252	0.000000
	C	2.434128	0.710577	0.000000
Furan (C_{2v})	H	0.000000	2.050655	0.816080
	H	0.000000	1.377422	-1.844443
	C	0.000000	1.095512	0.318614
	C	0.000000	0.720764	-0.989032
	O	0.000000	0.000000	1.138748

Molecule (symmetry)	Atom	X	Y	Z
Pyrrole (C_{2v})	H	0.000000	2.113533	0.765168
	H	0.000000	1.361742	-1.848823
	H	0.000000	0.000000	2.129579
	C	0.000000	1.126599	0.330605
	C	0.000000	0.714934	-0.985073
	N	0.000000	0.000000	1.123459
Imidazole (C_s)	H	-1.619793	1.573819	0.000000
	H	1.123222	1.935864	0.000000
	H	0.334319	-2.168241	0.000000
	H	-1.909946	-0.965998	0.000000
	C	-0.806312	0.867796	0.000000
	C	0.557098	1.018433	0.000000
	C	0.213535	-1.095313	0.000000
	N	1.191626	-0.213966	0.000000
	N	-1.017600	-0.499248	0.000000
Pyridine (C_{2v})	H	0.000000	2.057742	1.279370
	H	0.000000	2.157421	-1.204811
	H	0.000000	0.000000	-2.499000
	C	0.000000	1.142017	0.696089
	C	0.000000	1.198401	-0.699905
	C	0.000000	0.000000	-1.414468
	N	0.000000	0.000000	1.403713
Pyrazine (D_{2h})	H	0.000000	2.064971	1.251200
	C	0.000000	1.131290	0.698767
	N	0.000000	0.000000	1.419992
Pyrimidine (C_{2v})	H	0.000000	2.151421	1.143883
	H	0.000000	0.000000	-2.367202
	H	0.000000	0.000000	2.465179
	C	0.000000	1.185180	0.649436
	C	0.000000	0.000000	-1.282724
	C	0.000000	0.000000	1.382204
	N	0.000000	1.204114	-0.692499
Pyridazine (C_{2v})	H	0.000000	2.402231	-0.101371
	H	0.000000	1.274904	2.147804
	C	0.000000	1.321686	-0.017415
	C	0.000000	0.691188	1.234582
	N	0.000000	0.673098	-1.186891
s-Triazine (D_{3h})	H	0.000000	0.000000	2.379949
	H	0.000000	-2.061096	-1.189974
	C	0.000000	0.000000	1.295214
	C	0.000000	1.121689	-0.647607
	N	0.000000	0.000000	-1.379413
	N	0.000000	1.194607	0.689706
s-Tetrazine (D_{2h})	H	0.000000	0.000000	-2.345244
	C	0.000000	0.000000	1.263568
	N	0.000000	1.201393	0.665348
Formaldehyde (C_{2v})	H	0.000000	0.936522	-1.194669
	C	0.000000	0.000000	-0.611070
	O	0.000000	0.000000	0.601026
Acetone (C_{2v})	H	0.000000	2.146422	-0.027075
	H	-0.882224	1.327228	-1.347775
	C	0.000000	0.000000	0.101073
	C	0.000000	1.290335	-0.700873
	O	0.000000	0.000000	1.318967

Molecule (symmetry)	Atom	X	Y	Z
p-Benzoquinone (D_{2h})	H	0.000000	2.186299	1.257330
	C	0.000000	0.000000	1.447657
	C	0.000000	1.272483	0.672789
	O	0.000000	0.000000	2.672016
Formamide (C_s)	H	-0.035245	-1.510395	0.000000
	H	1.985297	-0.387754	0.000000
	H	1.220829	1.174175	0.000000
	C	-0.086417	-0.408385	0.000000
	O	-1.137024	0.203772	0.000000
	N	1.148803	0.169288	0.000000
Acetamide (C_s)	H	-0.429500	1.963037	0.000000
	H	-1.825424	0.919709	0.000000
	H	1.968854	-0.768041	0.000000
	H	1.731392	0.760691	0.885868
	C	-0.048142	-0.085394	0.000000
	C	1.447136	0.186847	0.000000
	O	-0.530756	-1.207321	0.000000
	N	-0.826744	1.039291	0.000000
Propanamide (C_s)	H	-1.718718	1.621719	0.000000
	H	-2.558968	0.106405	0.000000
	H	0.700516	1.446972	0.880124
	H	2.8946227	0.629339	0.000000
	H	2.0703450	-0.674316	-0.880899
	C	-0.5133681	-0.079956	0.000000
	C	0.7402250	0.793991	0.000000
	C	2.0241565	-0.031604	0.000000
	O	-0.4793028	-1.300110	0.000000
	N	-1.6935733	0.618024	0.000000
Cytosine (C_s)	H	2.103205	1.409422	0.000000
	H	0.192912	2.827585	0.000000
	H	-2.076127	1.733417	0.000000
	H	-3.230237	-0.441208	0.000000
	H	-2.342275	-1.940394	0.000000
	C	0.057348	1.753262	0.000000
	C	-1.160876	1.158804	0.000000
	C	-1.160455	-0.287378	0.000000
	C	1.168040	-0.430384	0.000000
	O	2.229243	-1.026481	0.000000
	N	-0.075930	-1.033377	0.000000
	N	1.184394	0.990106	0.000000
	N	-2.355274	-0.933983	0.000000
Thymine (C_s)	H	-1.808790	1.976164	0.000000
	H	-0.960101	-1.978634	0.000000
	H	0.472725	2.586214	0.000000
	H	2.845328	1.936434	0.000000
	H	3.138260	0.420783	0.880445
	C	-1.629921	-0.052812	0.000000
	C	0.757392	-0.836268	0.000000
	C	1.185247	0.572789	0.000000
	C	0.232776	1.529218	0.000000
	C	2.660700	0.859484	0.000000
	O	-2.818136	-0.308378	0.000000
	O	1.510510	-1.794389	0.000000
	N	-1.122941	1.236814	0.000000
	N	-0.634602	-1.019928	0.000000
Uracil (C_s)	H	-2.017408	-1.525923	0.000000
	H	-0.037071	2.000601	0.000000
	H	2.186816	-1.597809	0.000000

Molecule (symmetry)	Atom	X	Y	Z
	H	-0.017760	-2.789145	0.000000
	C	-1.239995	0.355737	0.000000
	C	1.277990	0.401032	0.000000
	C	1.247659	-1.064625	0.000000
	C	0.063207	-1.709410	0.000000
	O	-2.304131	0.941040	0.000000
	O	2.276936	1.095016	0.000000
	N	-1.138733	-1.030829	0.000000
	N	-0.005322	0.988101	0.000000
Adenine (C_s)	H	2.011864	-2.505708	0.000000
	H	1.265984	2.708859	0.000000
	H	2.822411	1.913573	0.000000
	H	-2.721643	-1.389953	0.000000
	H	-3.312695	1.099409	0.000000
	C	1.351251	-1.644974	0.000000
	C	1.214246	0.657399	0.000000
	C	-0.188214	0.522517	0.000000
	C	-0.677566	-0.781382	0.000000
	C	-2.302961	0.717203	0.000000
	N	0.042556	-1.915431	0.000000
	N	1.976462	-0.449014	0.000000
	N	-2.048158	-0.639855	0.000000
	N	-1.219795	1.457921	0.000000
	N	1.817944	1.868950	0.000000