Supplementary Material

to

Analytical Energy Gradients for Local Coupled-Cluster Methods

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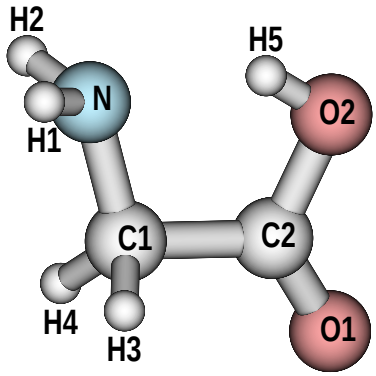
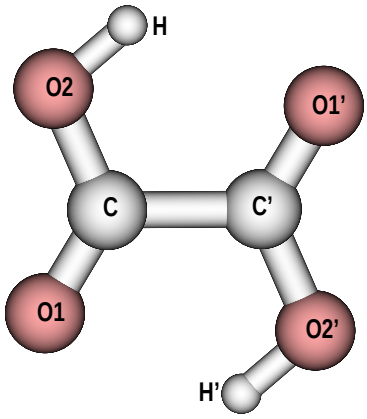
Table I: Geometrical parameters of glycine (C_1)[a].



	cc-pVDZ				cc-pVTZ			
Parameter	LMP2	QCISD	LQCISD[b]	LQCISD[c]	LMP2	QCISD	LQCISD[b]	LQCISD[c]
N-C_1	1.473	1.472	1.476	1.472	1.467	1.465	1.468	1.464
C_1-C_2	1.541	1.538	1.543	1.540	1.531	1.528	1.532	1.529
C_2-O_1	1.212	1.207	1.207	1.207	1.206	1.200	1.200	1.200
C_2-O_2	1.348	1.346	1.348	1.348	1.343	1.338	1.341	1.340
N-H_1	1.021	1.021	1.022	1.023	1.010	1.009	1.009	1.010
N-H_2	1.023	1.024	1.024	1.025	1.011	1.010	1.011	1.012
C_1-H_3	1.104	1.105	1.106	1.107	1.089	1.090	1.091	1.092
C_1-H_4	1.104	1.105	1.106	1.107	1.089	1.090	1.090	1.092
O_2-H_5	0.985	0.980	0.978	0.979	0.981	0.973	0.972	0.974
N_1-C_1-C_2	110.5	110.4	110.8	110.9	111.2	111.3	111.5	111.4
C_1-C_2-O_1	123.0	122.9	122.9	123.0	122.8	122.6	122.6	122.7
C_1-C_2-O_2	113.4	113.6	113.9	113.9	113.7	114.0	114.3	114.2
O_1-C_2-O_2	123.6	123.5	123.2	123.1	123.4	123.3	123.0	123.1
H_1-N-H_2	105.7	105.7	105.5	105.4	107.0	107.0	106.8	106.8
H_1-N-C_1	110.3	110.3	109.9	110.1	111.2	111.2	111.0	111.1
H_2-N-C_1	109.6	109.6	109.4	109.5	110.8	110.9	110.7	110.8
H_3-C_1-C_2	106.3	106.3	106.2	106.3	106.3	106.2	106.1	106.2
H_4-C_1-C_2	107.9	108.0	107.8	107.8	107.6	107.7	107.5	107.6
C_2-O_2-H_5	103.6	104.3	104.8	104.7	104.2	105.1	105.4	105.3
N-C_1-C_2-O_1	-164.1	-163.2	-162.6	-162.6	-168.4	-167.4	-166.9	-166.9
N-C_1-C_2-O_2	17.5	18.5	18.9	19.2	12.9	14.0	14.4	14.6
C_1-C_2-O_2-H_5	-3.7	-3.9	-3.7	-3.8	-2.4	-2.6	-2.5	-2.7
H_1-N-C_1-C_2	207.3	206.0	205.2	204.9	215.3	214.1	212.8	212.6
H_2-N-C_1-C_2	91.4	90.1	89.8	89.5	96.4	95.1	94.4	94.1
H_3-C_1-C_2-O_1	77.8	78.8	79.3	79.3	72.5	73.6	74.2	74.1
H_4-C_1-C_2-O_1	-37.0	-36.0	-35.4	-35.2	-42.1	-41.0	-40.4	-40.3

[a] Bond lengths in Ångström and angles in degrees. [b] Local QCISD values without specific weak pair treatment. [c] Local QCISD values with weak pairs treated at the LMP2 level.

Table II: Geometrical parameters of oxalic acid (C_{2h})[a].



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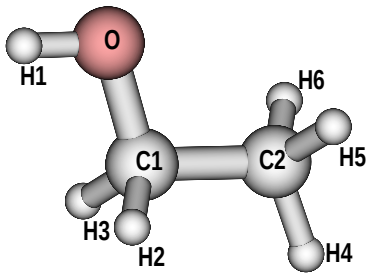
Parameter	LMP2	QCISD	LQCISD[b]	LQCISD[c]	LMP2	QCISD	LQCISD[b]	LQCISD[c]
O_1-C	1.217	1.210	1.210	1.209	1.210	1.201	1.201	1.201
O_2-C	1.330	1.330	1.332	1.332	1.327	1.323	1.325	1.325
C-C'	1.540	1.545	1.553	1.549	1.539	1.538	1.543	1.540
O_2-H	0.980	0.977	0.976	0.976	0.975	0.970	0.970	0.970
O_1-C-O_2	125.7	125.5	125.4	125.3	125.3	125.4	125.2	125.2
O_1-C-C'	121.3	121.2	121.3	121.3	121.6	121.3	121.4	121.4
O_2-C-C'	113.0	113.3	113.3	113.4	113.2	113.3	113.4	113.4
C-O_2-H	104.4	105.4	105.6	105.7	105.7	106.4	106.8	106.8

[a] Bond lengths in Ångström and angles in degrees. [b] Local QCISD values without specific weak pair treatment. [c] Local QCISD values with weak pairs treated at the LMP2 level.

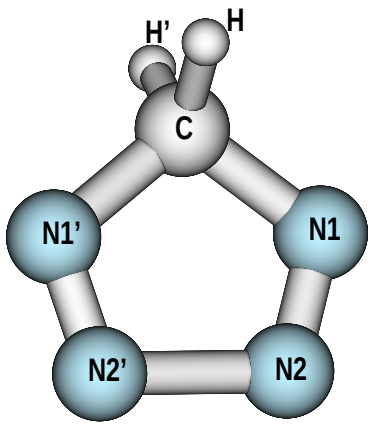
Table III: Geometrical parameters of ethanol (C_s)[a].



	cc-pVDZ				cc-pVTZ			
Parameter	LMP2	QCISD	LQCISD[b]	LQCISD[c]	LMP2	QCISD	LQCISD[b]	LQCISD[c]
C_1-C_2	1.523	1.523	1.527	1.524	1.514	1.514	1.517	1.514
C_1-O	1.426	1.423	1.427	1.425	1.426	1.422	1.424	1.421
O-H_1	0.967	0.965	0.966	0.967	0.961	0.957	0.958	0.959
C_1-H_2	1.110	1.111	1.112	1.113	1.094	1.095	1.096	1.097
C_2-H_4	1.103	1.105	1.105	1.106	1.089	1.090	1.091	1.092
C_2-H_5	1.102	1.104	1.105	1.105	1.088	1.089	1.090	1.091
C_1-O-H_1	106.4	107.0	106.7	106.8	107.6	108.0	108.0	108.1
O-C_1-C_2	107.6	107.5	107.8	107.8	107.5	107.7	107.8	107.7
H_2-C_1-H_3	107.3	107.3	107.3	107.2	107.8	107.8	107.8	107.7
C_1-C_2-H_4	110.7	110.8	110.6	110.7	110.5	110.5	110.5	110.5
H_5-C_2-H_6	108.3	108.3	108.3	108.3	108.5	108.4	108.4	108.4
C_1-C_2-H_5	110.2	110.1	110.2	110.3	110.2	110.3	110.3	110.3
H_2-C_1-C_2	109.8	109.8	109.8	109.8	110.0	110.0	110.0	110.1
H_1-O-C_1-C_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
O-C_1-C_2-H_4	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
O-C_1-C_2-H_5	59.7	59.7	59.8	59.7	59.9	59.8	59.9	59.9
H_4-C_2-C_1-H_2	58.8	58.9	58.9	58.8	59.4	59.3	59.3	59.3
H_5-C_2-C_1-H_2	-61.5	-61.5	-61.4	-61.5	-60.8	-60.9	-60.8	-60.9

[a] Bond lengths in Ångström and angles in degrees. [b] Local QCISD values without specific weak pair treatment. [c] Local QCISD values with weak pairs treated at the LMP2 level.

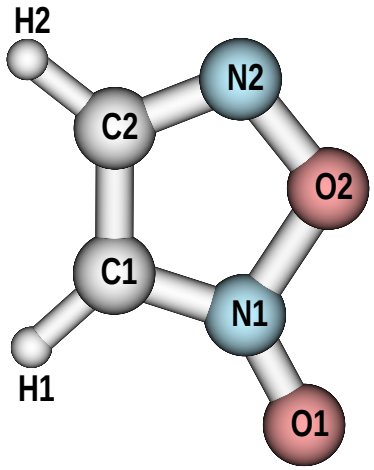
Table IV: Geometrical parameters of 5*H*-tetrazole (C_{2v})[a].



	cc-pVDZ				cc-pVTZ			
Parameter	LMP2	QCISD	LQCISD[b]	LQCISD[c]	LMP2	QCISD	LQCISD[b]	LQCISD[c]
C-N_1	1.510	1.474	1.479	1.480	1.500	1.461	1.465	1.456
N_1-N_2	1.197	1.221	1.218	1.210	1.184	1.214	1.214	1.222
N_2-N_2'	2.178	1.676	1.709	1.805	2.157	1.615	1.626	1.586
C-H	1.102	1.102	1.103	1.105	1.088	1.089	1.089	1.092
C-N_1-N_2	120.9	111.8	112.3	114.2	121.3	111.0	111.1	110.4
N_1-N_2-N_2'	95.8	105.7	105.2	103.1	95.8	106.7	106.6	107.1
N_1-C-N_1'	106.5	105.0	105.0	105.4	105.9	104.6	104.6	104.8
H-C-N_1-N_2	118.6	119.1	119.1	119.1	118.4	119.1	119.0	119.2

[a] Bond lengths in Ångström and angles in degrees. [b] Local QCISD values without specific weak pair treatment. [c] Local QCISD values with weak pairs treated at the LMP2 level.

Table V: Geometrical parameters of oxadiazole-2-oxide (C_s)[a].



		cc-pVDZ				cc-pVTZ			
Parameter	Exp.	LMP2	QCISD	LQCISD[b]	LQCISD[c]	LMP2	QCISD	LQCISD[b]	LQCISD[c]
C_1-C_2	1.401(2)	1.405	1.428	1.430	1.428	1.393	1.415	1.418	1.416
C_1-N_1	1.302(2)	1.359	1.332	1.333	1.334	1.349	1.319	1.321	1.322
C_2-N_2	1.292(2)	1.341	1.323	1.313	1.315	1.329	1.300	1.301	1.302
N_1-O_2	1.441(2)	1.564	1.442	1.441	1.445	1.486	1.416	1.416	1.418
N_2-O_2	1.379(1)	1.330	1.370	1.373	1.371	1.343	1.368	1.371	1.369
N_1-O_1	1.240(1)	1.201	1.219	1.220	1.219	1.207	1.218	1.219	1.218
C_1-H_1	0.92(2)	1.087	1.086	1.087	1.088	1.074	1.072	1.073	1.074
C_2-H_2	0.97(2)	1.089	1.090	1.091	1.091	1.076	1.075	1.076	1.077
C_1-N_1-O_1	136.4(2)	138.3	135.3	135.2	135.4	136.9	134.9	134.8	135.0
C_1-N_1-O_2	107.2(1)	102.5	106.7	106.8	106.7	104.3	107.3	107.4	107.2
C_1-C_2-N_2	111.9(1)	112.1	111.4	111.5	111.4	111.7	111.4	111.4	111.3
C_1-C_2-H_2	128(1)	128.2	128.2	128.2	128.3	128.6	128.3	128.3	128.3
C_2-N_2-O_2	106.6(1)	108.1	106.6	106.6	106.7	107.1	106.5	106.4	106.5
C_2-C_1-N_1	107.2(1)	109.0	106.5	106.4	106.5	108.0	106.4	106.3	106.4
C_2-C_1-H_1	103(1)	132.6	133.1	133.2	133.1	133.2	133.0	133.2	133.2
N_2-O_2-N_1	107.1(1)	108.4	108.7	108.7	108.7	108.8	108.6	108.5	108.6
O_1-N_1-O_2	116.4(1)	119.2	118.0	117.9	117.9	118.8	117.9	117.8	117.8
H_2-C_2-N_2	120(1)	119.8	120.4	120.3	120.3	119.7	120.4	120.3	120.3
H_1-C_1-N_1	123(1)	118.4	120.4	120.4	120.4	118.8	120.6	120.6	120.4

[a] Bond lengths in Ångström and angles in degrees. [b] Local QCISD values without specific weak pair treatment. [c] Local QCISD values with weak pairs treated at the LMP2 level.