Supplementary Material to

Tautomeric and Conformational Properties of Acetoacetamide,

$CH_3C(O)-CH_2-C(O)NH_2$: Electron Diffraction and Quantum Chemical Study.

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Contents.

Results of MP2 calculations with 6-31G(d,p) basis sets: cartesian coordinates, electronic energies, number of imaginary frequencies, zero point corrections, thermal corrections to Energies, Enthalpies and Gibbs Free Energies for enol and diketo confomers.	S2
Results of B3LYP calculations with 6-31G(d,p) basis sets: cartesian coordinates, electronic energies, number of imaginary frequencies, zero point corrections, thermal corrections to Energies, Enthalpies and Gibbs Free Energies for enol and diketo confomers.	S3
Results of MP2 calculations with 6-311++G(3df,pd) basis sets: cartesian coordinates, electronic energies, number of imaginary frequencies, zero point corrections, thermal corrections to Energies, Enthalpies and Gibbs Free Energies for enol and diketo confomers.	S4
Results of B3LYP calculations with 6-311++G(3df,pd) basis sets: cartesian coordinates, electronic energies, number of imaginary frequencies, zero point corrections, thermal corrections to Energies, Enthalpies and Gibbs Free Energies for enol and diketo confomers.	S5

*Structure of the **enol** form:*

MP2/6-31G(d,p) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007786	-0.758038	-0.006634
2	6	0	-1.269225	-0.030529	-0.002643
3	6	0	1.169698	-0.075132	0.000602
4	8	0	-1.330807	1.220818	-0.002182
5	8	0	1.240145	1.262367	0.008598
6	7	0	-2.415073	-0.772196	-0.038583
7	6	0	2.512994	-0.726806	0.000150
8	1	0	0.292453	1.572812	0.002151
9	1	0	0.003903	-1.837182	-0.022552
10	1	0	-2.395234	-1.751719	0.182058
11	1	0	-3.276488	-0.273041	0.107909
12	1	0	2.427201	-1.810243	-0.004484
13	1	0	3.070996	-0.412494	0.881321
14	1	0	3.073899	-0.405215	-0.876500

E(MP2) = -360.8232099 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.115432 (Hartree/Particle)
Thermal correction to Energy= 0.122934
Thermal correction to Enthalpy= 0.123878
Thermal correction to Gibbs Free Energy= 0.084004

*Structure of the **diketo** form:*

MP2/6-31G(d,p) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003629	-0.583276	0.670763
2	6	0	-1.334860	-0.222850	0.023937
3	6	0	1.205660	0.136315	0.077896
4	8	0	-2.116479	-1.091068	-0.357406
5	8	0	1.214080	1.359354	-0.062701
6	7	0	-1.598683	1.114348	-0.012631
7	6	0	2.386520	-0.715290	-0.305083
8	1	0	0.111005	-1.662698	0.602640
9	1	0	-0.044393	-0.306731	1.727743
10	1	0	-0.817585	1.750830	0.049982
11	1	0	-2.406470	1.389722	-0.547525
12	1	0	3.193238	-0.086353	-0.669229
13	1	0	2.087437	-1.426659	-1.075839
14	1	0	2.721043	-1.294229	0.556418

E(MP2) = -360.8264223 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.115115 (Hartree/Particle)
Thermal correction to Energy= 0.122766
Thermal correction to Enthalpy= 0.123711
Thermal correction to Gibbs Free Energy= 0.082406

*Structure of the **enol** form:*

B3LYP/6-31G(d,p) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004532	-0.764605	-0.003173
2	6	0	-1.264286	-0.038764	-0.002769
3	6	0	1.172127	-0.069779	0.000369
4	8	0	-1.317082	1.213921	-0.000157
5	8	0	1.217362	1.259247	0.003937
6	7	0	-2.419535	-0.762744	-0.022383
7	6	0	2.522832	-0.716850	0.000617
8	1	0	0.252172	1.556394	0.000706
9	1	0	0.009519	-1.847581	-0.011617
10	1	0	-2.421512	-1.761844	0.098602
11	1	0	-3.288026	-0.258880	0.066550
12	1	0	2.448715	-1.805630	0.001482
13	1	0	3.088620	-0.393616	0.880757
14	1	0	3.088177	-0.394985	-0.880310

E(RB+HF-LYP) = -361.872725490 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.112666 (Hartree/Particle)
Thermal correction to Energy= 0.120314
Thermal correction to Enthalpy= 0.121258
Thermal correction to Gibbs Free Energy= 0.081019

*Structure of the **diketo** form:*

B3LYP/6-31G(d,p) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007161	-0.674624	0.511136
2	6	0	-1.374454	-0.216309	0.009987
3	6	0	1.223139	0.126546	0.055852
4	8	0	-2.220866	-1.038097	-0.307506
5	8	0	1.198926	1.343431	-0.046231
6	7	0	-1.579578	1.127700	0.028604
7	6	0	2.477749	-0.664089	-0.240124
8	1	0	0.106067	-1.730598	0.254089
9	1	0	-0.006463	-0.613433	1.609248
10	1	0	-0.771482	1.738215	0.075998
11	1	0	-2.439024	1.460943	-0.382969
12	1	0	3.309230	0.012940	-0.438773
13	1	0	2.307148	-1.310836	-1.108988
14	1	0	2.725516	-1.322947	0.599955

E(RB+HF-LYP) = -361.869812425 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.112306 (Hartree/Particle)
Thermal correction to Energy= 0.120060
Thermal correction to Enthalpy= 0.121004
Thermal correction to Gibbs Free Energy= 0.079620

*Structure of the **enol** form:*

MP2/6-311++G(3df,pd) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.006214	-0.755446	-0.003887
2	6	0	-1.264030	-0.030943	-0.002287
3	6	0	1.168955	-0.070990	0.000362
4	8	0	-1.318154	1.212343	-0.000933
5	8	0	1.222844	1.255937	0.004264
6	7	0	-2.406647	-0.764970	-0.020970
7	6	0	2.508769	-0.720351	0.000568
8	1	0	0.266411	1.555580	0.001681
9	1	0	0.008796	-1.836370	-0.011211
10	1	0	-2.387609	-1.763722	0.093619
11	1	0	-3.283608	-0.276134	0.065632
12	1	0	2.423314	-1.805017	-0.001681
13	1	0	3.067511	-0.401455	0.882125
14	1	0	3.069312	-0.397948	-0.878561

E(MP2) = -361.2086518 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.113230 (Hartree/Particle)
Thermal correction to Energy= 0.120889
Thermal correction to Enthalpy= 0.121834
Thermal correction to Gibbs Free Energy= 0.081546

*Structure of the **diketo** form:*

MP2/6-311++G(3df,pd) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011492	-0.476036	0.807606
2	6	0	-1.303529	-0.200738	0.039920
3	6	0	1.197842	0.137144	0.126102
4	8	0	-2.053722	-1.101354	-0.295282
5	8	0	1.306636	1.347128	0.022391
6	7	0	-1.548872	1.114559	-0.185576
7	6	0	2.217704	-0.815189	-0.426046
8	1	0	0.078974	-1.554500	0.914318
9	1	0	-0.099341	-0.015744	1.795675
10	1	0	-0.798835	1.782380	-0.068985
11	1	0	-2.332252	1.345549	-0.777498
12	1	0	3.021650	-0.271412	-0.916105
13	1	0	1.730395	-1.491729	-1.132990
14	1	0	2.615052	-1.433741	0.382245

E(MP2) = -361.2060445 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.112696 (Hartree/Particle)
Thermal correction to Energy= 0.120549
Thermal correction to Enthalpy= 0.121493
Thermal correction to Gibbs Free Energy= 0.079309

*Structure of the **enol** form:*

B3LYP/6-311++G(3df,pd) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.751543	0.000000
2	6	0	1.265035	0.040650	0.000000
3	6	0	-1.172330	0.062376	0.000000
4	8	0	1.330108	-1.202534	0.000000
5	8	0	-1.217134	-1.263534	0.000000
6	7	0	2.406500	0.778726	0.000000
7	6	0	-2.517517	0.707738	0.000000
8	1	0	-0.263232	-1.573500	0.000000
9	1	0	-0.018003	1.831550	0.000000
10	1	0	2.393676	1.783059	0.000000
11	1	0	3.289781	0.296433	0.000000
12	1	0	-2.440790	1.793045	0.000000
13	1	0	-3.080928	0.386514	0.878967
14	1	0	-3.080928	0.386514	-0.878967

E(RB+HF-LYP) = -362.003593562 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.112044 (Hartree/Particle)
Thermal correction to Energy= 0.119830
Thermal correction to Enthalpy= 0.120775
Thermal correction to Gibbs Free Energy= 0.079935

*Structure of the **diketo** form:*

B3LYP/6-311++G(3df,pd) *geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.008690	-0.688220	0.459317
2	6	0	-1.377022	-0.211523	0.008103
3	6	0	1.227522	0.127320	0.054354
4	8	0	-2.237323	-1.025199	-0.268275
5	8	0	1.205168	1.337674	-0.018138
6	7	0	-1.574429	1.127053	0.006197
7	6	0	2.482410	-0.657439	-0.230859
8	1	0	0.107038	-1.725271	0.144018
9	1	0	0.001261	-0.695606	1.556578
10	1	0	-0.775600	1.745005	0.063394
11	1	0	-2.455408	1.467124	-0.345938
12	1	0	3.323896	0.015415	-0.377781
13	1	0	2.331322	-1.267501	-1.125920
14	1	0	2.696144	-1.349164	0.588090

E(RB+HF-LYP) = -361.999414912 A.U.
No. of imaginary frequencies: 0
Zero-point correction= 0.111611 (Hartree/Particle)
Thermal correction to Energy= 0.119433
Thermal correction to Enthalpy= 0.120377
Thermal correction to Gibbs Free Energy= 0.078696