

Supplementary Material

Tautomeric and Conformational Properties of Methyl Acetoacetate, $\text{CH}_3\text{OC(O)-CH}_2\text{-C(O)CH}_3$: Electron Diffraction and Quantum Chemical Study.

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Table S1: Optimized Geometric parameters (MP2/6-31G**) of the diketo conformers of the methyl acetoacetate $\text{C}_5\text{H}_8\text{O}_3$.^a

Table S1: Optimized Geometric parameters (MP2/6-31G) of the diketo conformers of the methyl acetoacetate C₅H₈O₃.^a**

Parameters	(ac,ac)	(ac,sp)	(sc,ac)
r(C ₁ -C ₂)	1.508	1.506	1.512
r(C ₁ -C ₃)	1.527	1.526	1.531
r(C ₃ -C ₅)	1.510	1.509	1.506
r(C ₂ -O ₁)	1.219	1.218	1.222
r(C ₃ -O ₂)	1.224	1.225	1.225
r(C ₂ -O ₃)	1.357	1.353	1.350
r(O ₃ -C ₄)	1.442	1.440	1.443
r(C ₄ -H)	1.084	1.084	1.084
	1.087	1.087	1.087
	1.087	1.087	1.087
r(C ₅ -H)	1.086	1.086	1.086
	1.090	1.090	1.091
	1.090	1.091	1.089
r(C ₁ -H)	1.089	1.091	1.086
		1.091	1.091
∠C ₂ C ₁ C ₃	112.2	110.2	109.6
∠C ₁ C ₂ O ₁	126.2	125.4	124.9
∠C ₁ C ₃ O ₂	120.9	121.4	120.3
∠C ₁ C ₂ O ₃	109.9	110.1	111.1
∠C ₁ C ₃ C ₅	116.5	116.0	116.5
∠C ₂ O ₃ C ₄	114.0	113.8	113.9
∠O ₃ C ₄ H	105.1	105.2	105.0
	110.3	110.5	110.2
	110.3	110.0	110.3
∠C ₃ C ₅ H	109.4	109.5	109.6
	110.0	110.3	109.1
	110.0	109.8	110.1
∠C ₃ C ₁ H	109.5	109.2	108.8
	107.7	109.3	109.8
∠C ₂ C ₁ H	107.7	109.0	110.5
	110.1	110.7	107.5
τ(O ₁ C ₂ O ₃ C ₄)	0.0	-3.9	0.3
τ(C ₂ O ₃ C ₄ H)	180.5	-179.8	-179.9
τ(O ₂ C ₃ C ₅ H)	10.9	-3.6	8.5
τ(C ₃ C ₁ C ₂ O ₁)	118.5	98.7	-65.1
τ(C ₂ C ₁ C ₃ O ₂)	135.2	-4.0	-105.2

^a For atom numbering see Figure 1