Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Modeling amino-acid side chain infrared spectra: the case of carboxylic residues

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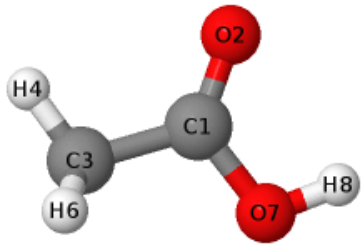
Acetic acid structure

Table 1: Structural parameters of acetic acid at the B3LYP/6-31+G(d) level of theory.



r		$\angle$		$\angle$	
C1–O2	1.2124	C1–O7–H8	107.00	O2–C1–O7–H8	0.03
C1–O7	1.3600	C3–C1–O7	111.61	O2–C1–C3–H4	0.03
O7–H8	0.9759	O2–C1–C3	126.16	O2–C1–C3–H5	121.01
C1–C3	1.5055	O2–C1–O7	122.22	O2–C1–C3–H6	-121.01
C3–H4	1.0903	C1–C3–H4	109.57	O7–C1–C3–H4	179.97
C3–H5	1.0952	C1–C3–H5	109.91	O7–C1–C3–H5	-58.99
C3–H6	1.0952	C1–C3–H6	109.91	O7–C1–C3–H6	58.99
		H4–C3–H5	110.02	C3–C1–O7–H8	58.99
		H4–C3–H6	110.02		
		H5–C3–H6	107.39		

Note r are bond lenghts in Åand $\angle$are angles and dihedrals in degrees.