

IR, Raman and SERS Spectra of 2-(Methoxycarbonylmethylsulfanyl)-3,5-dinitrobenzene Carboxylic Acid

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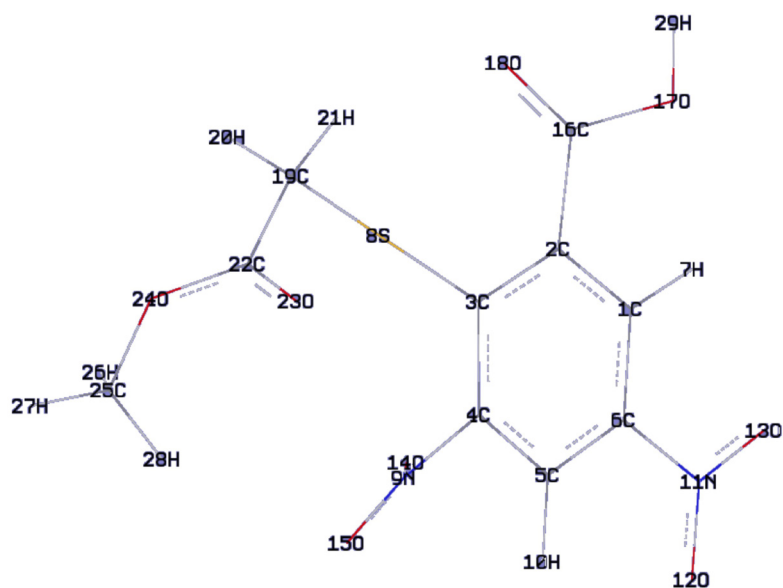


Figure S1. Optimized geometry of the molecule.

Table S1. Optimized geometrical parameters of 2-(methoxycarbonylmethylsulfanyl)-3,5-nitrobenzenecarboxylic acid, atom labeling is according to Figure 4.

Bond length/(Å)		Bond angles (°)		Dihedral angles (°)	
C ₁ -C ₂	1.4006	A(2,1,6)	120.1	D(6,1,2,3)	0.7
C ₁ -C ₆	1.3865	A(2,1,7)	120.5	D(6,1,2,16)	179.6
C ₁ -H ₇	1.0812	A(6,1,7)	119.4	D(7,1,2,3)	-179.4
C ₂ -C ₃	1.4199	A(1,2,3)	120.2	D(7,1,2,16)	-0.5
C ₂ -C ₁₆	1.4990	A(1,2,16)	116.9	D(2,1,6,5)	-1.7
C ₃ -C ₄	1.4077	A(3,2,16)	122.8	D(2,1,6,11)	178.7
C ₃ -S ₈	1.7949	A(2,3,4)	116.6	D(7,1,6,5)	178.5
C ₄ -C ₅	1.3870	A(2,3,8)	125.0	D(7,1,6,11)	-1.2
C ₄ -N ₉	1.4774	A(4,3,8)	118.4	D(1,2,3,4)	2.2
C ₅ -C ₆	1.3868	A(3,4,5)	123.8	D(1,2,3,8)	-178.7
C ₅ -H ₁₀	1.0825	A(3,4,9)	121.1	D(16,2,3,4)	-176.6
C ₆ -N ₁₁	1.4741	A(5,4,9)	115.2	D(16,2,3,8)	2.5
S ₈ -C ₁₉	1.8493	A(4,5,6)	117.5	D(1,2,16,17)	-22.4
N ₉ -O ₁₄	1.2244	A(4,5,10)	121.4	D(1,2,16,18)	157.7
N ₉ -O ₁₅	1.2292	A(6,5,10)	121.1	D(3,2,16,17)	156.4
N ₁₁ -O ₁₂	1.2287	A(1,6,5)	121.6	D(3,2,16,18)	-23.5
N ₁₁ -O ₁₃	1.2284	A(1,6,11)	119.3	D(2,3,4,5)	-4.6
C ₁₆ -O ₁₇	1.3546	A(5,6,11)	119.0	D(2,3,4,9)	176.0
C ₁₆ -O ₁₈	1.2119	A(3,8,19)	101.2	D(8,3,4,5)	176.3
O ₁₇ -H ₂₉	0.9756	A(4,9,14)	117.1	D(8,3,4,9)	-3.1
C ₁₉ -H ₂₀	1.0925	A(4,9,15)	116.7	D(2,3,8,19)	70.8
C ₁₉ -H ₂₁	1.0883	A(14,9,15)	126.1	D(4,3,8,19)	-110.1
C ₁₉ -C ₂₂	1.5131	A(6,11,12)	117.2	D(3,4,5,6)	3.7
C ₂₂ -O ₂₃	1.2139	A(6,11,13)	117.4	D(3,4,5,10)	-176.2
C ₂₂ -O ₂₄	1.3429	A(12,11,13)	125.4	D(9,4,5,6)	-176.9
O ₂₄ -C ₂₅	1.4418	A(2,16,17)	111.3	D(9,4,5,10)	3.2
C ₂₅ -H ₂₆	1.0926	A(2,16,18)	126.8	D(3,4,9,14)	-57.6
C ₂₅ -H ₂₇	1.0898	A(17,16,18)	121.9	D(3,4,9,15)	124.7
C ₂₅ -H ₂₈	1.0930	A(16,17,29)	106.0	D(5,4,9,14)	122.9
		A(8,19,20)	103.9	D(5,4,9,15)	-54.8
		A(8,19,21)	109.4	D(4,5,6,1)	-0.5
		A(8,19,22)	109.6	D(4,5,6,11)	179.2
		A(20,19,21)	110.8	D(10,5,6,1)	179.5
		A(20,19,22)	111.7	D(10,5,6,11)	-0.8
		A(21,19,22)	111.2	D(1,6,11,12)	178.3
		A(19,22,23)	123.6	D(1,6,11,13)	-1.6
		A(19,22,24)	111.8	D(5,6,11,12)	-1.3
		A(23,22,24)	124.5	D(5,6,11,13)	178.8
		A(22,24,25)	115.3	D(3,8,19,20)	178.0
		A(24,25,26)	110.5	D(3,8,19,21)	-63.6
		A(24,25,27)	105.4	D(3,8,19,22)	58.6
		A(24,25,28)	109.8	D(2,16,17,29)	178.4
		A(26,25,27)	110.8	D(18,16,17,29)	-1.7
		A(26,25,28)	109.5	D(8,19,22,23)	-83.6
		A(27,25,28)	110.7	D(8,19,22,24)	93.7
				D(20,19,22,23)	161.8
				D(20,19,22,24)	-20.9
				D(21,19,22,23)	37.5
				D(21,19,22,24)	-145.2
				D(19,22,24,25)	-173.7
				D(23,22,24,25)	3.5
				D(22,24,25,26)	-58.9
				D(22,24,25,27)	-178.7
				D(22,24,25,28)	62.0