

The C_{2v} shape of enolic acetylacetone

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Supplementary Material: Tables (2) of frequencies and figures (2) of conformers.

Tables:

Table S1: Measured Frequencies ν and deviations $\Delta\nu$ (observed–calculated) of A_1 state rotational transitions $J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$ of Enol I-acetylacetone.

Table S2: Measured Frequencies ν and deviations $\Delta\nu$ (observed–calculated) of A_1 state rotational transitions $J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$ of the ^{13}C species of Enol I-acetylacetone.

Figures:

Figure S1: Keto I-acetylacetone

Figure S2: Keto II-acetylacetone

Table S1: Measured Frequencies ν and deviations $\Delta\nu$ (observed–calculated) of A_1 state rotational transitions $J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$ of Enol I-acetylacetone.

MB-FTMW transitions (precision: 3 kHz)			Millimeter-wave free jet transitions (precision: 100 kHz)					
$J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$	ν / MHz	$\Delta\nu$ / kHz	$J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$	ν / MHz	$\Delta\nu$ / kHz	$J'(K_{-1}') \leftarrow J''(K_{-1}'')$ ^a	ν / MHz	$\Delta\nu$ / kHz
1(1,1)-0(0,0)	7382.9020	0.6	7(5,3)-6(4,2)	61975.69	41	6(6)-5(5)	67878.86	-3
2(1,2)-1(0,1)	10084.2430	-0.2	7(5,2)-6(4,3)	61977.03	26	7(6)-6(5)	70957.58	2
2(2,1)-1(1,0)	19447.0101	1.3	8(5,4)-7(4,3)	65043.75	-2	8(6)-7(5)	74034.29	15
2(2,0)-1(1,1)	19842.7114	2.3	8(5,3)-7(4,4)	65048.75	12	8(8)-8(7)	67327.38	72
3(1,3)-2(0,2)	12608.3770	0.5	9(5,5)-8(4,4)	68099.61	-12	9(8)-9(7)	67310.18	-6
3(2,2)-2(1,1)	22148.1955	1.1	9(5,4)-8(4,5)	68114.58	-34	9(9)-9(8)	76295.47	2
3(2,2)-3(1,3)	14617.0040	3.9	9(6,4)-8(5,3)	77107.10	-175	10(8)-10(7)	67287.50	-8
3(2,1)-2(1,2)	23380.9626	-0.2	9(6,3)-8(5,4)	77107.51	-15	10(9)-10(8)	76278.27	-36
3(2,1)-3(1,2)	12497.5190	-2.4	10(4,7)-9(3,6)	61574.48	32	11(8)-11(7)	67258.16	57
3(3,1)-3(2,2)	22488.9230	5.2	10(4,6)-9(3,7)	62432.43	44	11(9)-11(8)	76256.41	0
3(3,0)-3(2,1)	22374.7590	-6.4	10(5,6)-9(4,5)	71135.40	-15	12(8)-12(7)	67220.75	74
4(1,4)-3(0,3)	14985.3620	-0.3	10(5,5)-9(4,6)	71174.53	122	12(9)-12(8)	76228.85	60
4(2,3)-3(1,2)	24659.9678	0.9	11(3,8)-10(2,9)	61398.35	-22	13(8)-13(7)	67173.86	69
4(2,3)-4(1,4)	15387.5850	0.4	11(4,8)-10(3,7)	64155.86	25	13(9)-13(8)	76195.00	151
4(3,2)-4(2,3)	22550.1890	0.1	11(4,7)-10(3,8)	65716.64	27	14(8)-14(7)	67115.79	-74
4(3,1)-4(2,2)	22215.3490	-0.7	11(5,7)-10(4,6)	74139.35	63	14(9)-14(8)	76153.01	-172
5(1,5)-4(0,4)	17261.7160	-0.7	11(5,6)-10(4,7)	74230.08	23	15(8)-15(7)	67045.19	49
5(1,4)-5(0,5)	7893.3930	-0.4	12(3,9)-11(2,10)	66724.68	-5			
5(2,4)-5(1,5)	16359.5440	1.9	12(4,9)-11(3,8)	66501.36	27			
5(2,3)-5(1,4)	11574.7740	1.6	12(4,8)-11(3,9)	69148.17	10			
5(3,3)-5(2,4)	22671.5180	-2.5	12(5,8)-11(4,7)	77093.74	75			
5(3,2)-5(2,3)	21917.7860	0.5	12(5,7)-11(4,8)	77287.12	80			
6(0,6)-5(1,5)	15387.0824	-0.9	13(3,10)-12(2,11)	72638.69	-34			
6(1,6)-5(0,5)	19494.3676	0.4	13(4,10)-12(3,9)	68569.23	23			
6(2,5)-6(1,6)	17534.5050	-1.4	13(4,9)-12(3,10)	72793.15	-17			
6(2,4)-6(1,5)	11289.4708	-1.2	14(4,11)-13(3,10)	70338.27	-27			
6(3,4)-6(2,5)	22878.1470	-2.0	14(4,10)-13(3,11)	76731.35	-5			
6(3,3)-6(2,4)	21448.2669	-1.5	15(4,12)-14(3,11)	71812.14	0			
7(0,7)-6(1,6)	18662.2057	-0.1	16(4,13)-15(3,12)	73016.43	-23			
7(1,7)-6(0,6)	21739.3834	0.5	17(4,14)-16(3,13)	73993.16	-33			

^a Transitions doubly overlapped due to near prolate degeneracy of the involved levels. Only K_a is given.

Table S2: Measured Frequencies ν and deviations $\Delta\nu$ (observed–calculated) of A_1 state rotational transitions $J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$ of the ^{13}C species of Enol I-acetylacetone.

$J'(K_{-1}', K_{+1}') \leftarrow J''(K_{-1}'', K_{+1}'')$	$^{13}\text{C}_{\text{CH}_3}$		$^{13}\text{C}_{\text{CO}}$		$^{13}\text{C}_{\text{CH}}$	
	ν / MHz	$\Delta\nu / \text{kHz}$	ν / MHz	$\Delta\nu / \text{kHz}$	ν / MHz	$\Delta\nu / \text{kHz}$
1(1,1)-0(0,0)	7311.6708	0.7	7375.6940	3.0	7334.3564	-4.2
2(1,2)-1(0,1)	9963.1503	0.2	10066.4246	1.4	10031.1482	-2.8
3(1,3)-2(0,2)	12442.7986	-0.3	12581.4137	-1.2	12549.7829	-2.0
3(2,1)-3(1,2)	12479.0692	0.1	12520.0777	-1.3	12358.0508	3.6
4(0,4)-3(1,3)	8343.3728	2.7	8526.7674	0.2	8627.1839	-1.3
4(1,4)-3(0,3)	14778.8795	-0.4	14950.1620	-0.4	14921.0116	-3.7
5(0,5)-4(1,4)	11705.1352	1.0	11938.1686	-1.1	12046.2933	0.8
5(1,5)-4(0,4)	17015.2450	0.6	17218.3513	0.6	17192.3569	3.5
6(0,6)-5(1,5)	15018.8506	-3.0	15297.5240	0.2	15408.5568	2.4

Figure S1: Keto I-acetylacetone

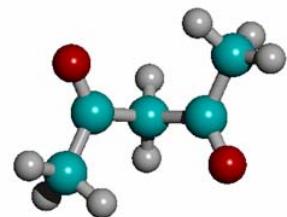


Figure S2: Keto II-acetylacetone

