The Self-Associating Behavior of Acetone in Liquid Krypton

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SUPPLEMENTARY INFORMATION

Numbering the vibrational modes based on group theory

The acetone molecule has a C_{2v} symmetry point group that spans 24 fundamental vibrations. In the C_{2v} symmetry the z-axis is the axis of symmetry, but the choice of the x- and y-axes, hence the identification of the two planes in Table 1, is arbitrary. To resolve this ambiguity we followed the recommendations of Mulliken.[1] Therefore we defined the x- and y-axes as stated in Figure 1. This way the fundamental modes span the $8A_1 + 4A_2 + 5B_1 + 7B_2$ symmetries with all but four A_2 modes being active in the infrared. The modes are numbered according to descending wavenumber in each symmetry block. Because the x- and y-axes are interchanged compared to the several previous literature investigations, also the numbering of the vibrational modes disagrees with most [2-6] and agrees with only a few previous vibrational studies on acetone [7-8]. The correspondence between previous and present numbering and symmetry labels is as follows:

modes 1-7 (A_1) and 9-11 (A_2) are unchanged,
modes 13-17 (B_1) in most of the literature are now modes 20-24 (B_2),
modes 18-24 (B_2) in most of the literature are now modes 13-19 (B_1).

Table S1 Character Table of the C_{2v} symmetry point group (the x-, y- and z-axis are defined in Figure 1)

C_{2v}	E	C_2(z)	σ_v(xz)	σ_v(yz)
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

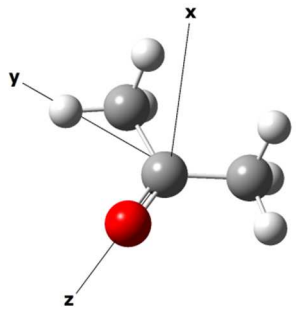


Figure S1. MP2/aug-cc-pVDZ equilibrium structure with the defined x-,y-,z-axes of the acetone monomer with C_{2v} symmetry

Coordinates of optimized geometries

Table S2: Cartesian coordinates of the optimized geometry of the acetone monomer at MP2/aug-cc-pVDZ level.

	X	Y	Z
Acetone			
C	0.000000	0.000000	0.180083
O	0.000000	0.000000	1.411068
C	0.000000	1.291622	-0.617403
H	0.887011	1.328841	-1.271370
H	-0.887011	1.328841	-1.271370
H	0.000000	2.152710	0.062635
C	0.000000	-1.291622	-0.617403
H	-0.887011	-1.328841	-1.271370
H	0.887011	-1.328841	-1.271370
H	0.000000	-2.152710	0.062635

Table S3: Cartesian coordinates of the optimized geometry of the stacked acetone dimer at MP2/aug-cc-pVDZ level.

	X	Y	Z
Stacked dimer			
C	1.589042	0.000000	0.347958
O	1.006342	0.000000	1.435801
C	1.946459	-1.289217	-0.362706
H	1.380152	-1.337897	-1.307965
H	3.019721	-1.304485	-0.613366
H	1.693918	-2.151162	0.268573
C	1.946459	1.289217	-0.362706
H	3.019721	1.304486	-0.613365
H	1.380152	1.337897	-1.307965
H	1.693918	2.151162	0.268574
C	-1.589090	0.000000	-0.347984
O	-1.006333	0.000000	-1.435797
C	-1.946450	1.289217	0.362711
H	-3.019715	1.304528	0.613349
H	-1.380164	1.337853	1.307985
H	-1.693858	2.151166	-0.268543
C	-1.946450	-1.289217	0.362711
H	-1.380164	-1.337853	1.307985
H	-3.019715	-1.304528	0.613349
H	-1.693858	-2.151166	-0.268543

Table S4: Cartesian coordinates of the optimized geometry of the planar acetone dimer at MP2/aug-cc-pVDZ level.

	X	Y	Z
Planar dimer			
C	-2.425872	-0.099238	-0.005140
O	-1.749819	-1.129280	-0.045976
C	3.923226	0.148672	0.240727
H	4.147580	-0.321474	1.213014
H	4.457149	-0.430643	-0.530117
H	4.271922	1.189297	0.244859
C	1.812038	-1.272376	-0.200073
H	2.173984	-1.690826	-1.155199
H	2.148311	-1.956501	0.59641
H	0.715546	-1.212528	-0.214214
C	2.425873	0.099238	-0.005145
O	1.749819	1.129281	-0.045980
C	-1.812038	1.272376	-0.200072
H	-2.14831	1.956502	0.596411
H	-0.715546	1.212528	-0.214214
H	-2.173986	1.690824	-1.155198
C	-3.923227	-0.148673	0.240727
H	-4.147583	0.321473	1.213013
H	-4.457147	0.430643	-0.530119
H	-4.271922	-1.189297	0.244857

Table S5: Calculated symmetries, wavenumbers (in cm^{-1}), infrared intensities (in km mol^{-1}) and complexation shifts (in cm^{-1}) at MP2/aug-cc-pVDZ level for the fundamental vibrational modes of the acetone monomer, and with counterpoise correction for the stacked dimer and planar dimer.

	monomer C_{2v}			stacked dimer			planar dimer		
	symmetry	$\tilde{\nu}$	intensity	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$
ν_1	A_1	3199.6	4.6	3194.3	0.0	-5.3	3196.9	16.1	-2.7
				3194.0	10.9	-5.7	3196.9	0.1	-2.7
ν_{18}	B_2	3198.8	9.8	3193.2	21.4	-5.6	3193.5	10.3	-5.3
				3192.6	0.0	-6.1	3192.6	0.3	-6.2
ν_{13}	B_1	3149.9	14.9	3153.5	0.0	3.6	3148.4	22.3	-1.5
				3152.9	19.6	3.0	3148.3	1.1	-1.6
ν_9	A_2	3144.0	0.0	3147.4	0.0	3.4	3139.9	5.1	-4.1
				3147.4	0.5	3.4	3139.8	2.4	-4.2
ν_2	A_1	3065.4	7.2	3064.1	0.0	-1.3	3063.4	0.1	-2.1
				3063.9	11.8	-1.5	3063.3	20.4	-2.2
ν_{19}	B_2	3061.0	1.5	3060.1	0.0	-0.9	3055.9	0.3	-5.1
				3059.6	3.9	-1.4	3055.9	22.5	-5.1
ν_3	A_1	1731.5	125.3	1730.5	219.0	-1.0	1732.0	272.3	0.5
				1723.2	0.0	-8.3	1726.4	0.3	-5.1
ν_{14}	B_1	1480.3	18.4	1483.4	0.0	3.1	1486.8	25.5	6.5
				1478.1	35.4	-2.2	1484.0	2.9	3.7
ν_4	A_1	1457.4	29.0	1458.3	78.9	0.9	1462.8	1.8	5.4
				1457.6	2.0	0.2	1460.8	17.7	3.4
ν_{10}	A_2	1454.2	0.0	1457.5	0.0	3.2	1456.7	0.8	2.4
				1452.8	0.0	-1.5	1455.0	35.4	0.8
ν_{20}	B_2	1448.8	0.1	1448.6	0.0	-0.3	1451.3	0.3	2.5
				1446.1	0.4	-2.7	1449.7	0.6	0.9
ν_{21}	B_2	1385.1	70.8	1386.3	145.9	1.2	1388.5	6.8	3.4
				1385.8	0.0	0.7	1387.9	114.1	2.9
ν_5	A_1	1368.6	12.6	1366.2	47.1	-2.4	1371.7	0.9	3.1
				1364.9	0.0	-3.8	1370.5	37.4	1.8
ν_{22}	B_2	1248.1	42.5	1254.2	53.9	6.1	1255.2	2.9	7.1
				1248.5	0.0	0.4	1251.8	90.1	3.7
ν_{15}	B_1	1097.3	1.2	1100.1	0.0	2.8	1099.5	2.0	2.2
				1099.0	9.6	1.7	1099.0	0.0	1.7
ν_6	A_1	1071.4	0.0	1075.5	0.0	4.0	1074.6	0.7	3.2
				1074.7	0.0	3.2	1073.1	0.0	1.7
ν_{23}	B_2	893.6	4.2	901.7	6.5	8.0	902.1	0.7	8.5
				901.4	0.0	7.7	901.8	8.4	8.2

ν_{11}	A_2	873.2	0.0	873.2	0.2	0.0	875.6	0.0	2.4
				871.7	0.0	-1.4	874.1	0.2	0.9
ν_7	A_1	807.2	1.3	812.0	1.2	4.8	809.3	0.0	2.2
				811.5	0.0	4.3	807.8	4.1	0.7
ν_{24}	B_2	527.1	14.8	528.8	26.8	1.7	530.2	33.1	3.1
				527.6	0.0	0.5	529.6	0.6	2.5
ν_{16}	B_1	479.9	0.5	486.7	0.0	6.8	482.3	0.1	2.4
				479.4	1.4	-0.5	481.2	1.2	1.3
ν_8	A_1	376.4	1.3	381.1	0.0	4.8	383.2	5.0	6.9
				379.6	2.0	3.2	381.0	0.0	4.6
ν_{17}	B_1	145.7	0.1	155.3	0.0	9.6	156.6	0.2	10.9
				151.9	0.7	6.1	150.1	0.1	4.4
ν_{12}	A_2	20.6	0.0	101.3	28.1		98.5	0.0	
				94.3	0.0		95.1	0.0	
				72.6	0.0		74.3	0.0	
				66.7	0.4		67.8	13.8	
				64.1	0.0		55.0	0.1	
				52.1	0.0		24.7	11.2	
				50.3	0.4		24.6	0.3	
				20.7	5.0		12.3	1.4	

Table S6: Cartesian coordinates of the optimized geometry of the acetone monomer at MP2/ cc-pVTZ level.

	X	Y	Z
Acetone			
C	0.00000000	0.00000000	0.18355300
O	0.00000000	0.00000000	1.40092500
C	0.00000000	1.28098500	-0.61455700
H	0.87651500	1.31731400	-1.26132100
H	-0.87651500	1.31731400	-1.26132100
H	0.00000000	2.13424700	0.05562700
C	0.00000000	-1.28098500	-0.61455700
H	-0.87651500	-1.317314 -	1.26132100
H	0.87651500	-1.31731400	-1.26132100
H	0.00000000	-2.13424700	0.05562700

Table S7: Cartesian coordinates of the optimized geometry of the stacked acetone dimer at MP2/cc-pVTZ level.

	X	Y	Z
Stacked dimer			
C	1.58286500	0.00000000	-0.34469100
O	1.03282600	0.00000400	-1.43407100
C	1.92459200	1.27856400	0.37423200
H	1.34541400	1.32671100	1.29674500
H	2.97970000	1.29280800	0.64532400
H	1.68955300	2.13265300	-0.25305500
C	1.92457700	-1.27856900	0.37422900
H	2.97968600	-1.29282800	0.64531800
H	1.34540200	-1.32671200	1.29674500
H	1.68952500	-2.13265400	-0.25305900
C	-1.58286600	0.00000100	0.34469200
O	-1.03283000	0.00000300	1.43407400
C	-1.92457900	-1.27856600	-0.37423200
H	-2.97968800	-1.29282500	-0.64531800
H	-1.34540600	-1.32670300	-1.29674900
H	-1.68952500	-2.13265400	0.25305200
C	-1.92458700	1.27856500	-0.37423200
H	-1.34540300	1.32671300	-1.29674200
H	-2.97969300	1.29281100	-0.64533100
H	-1.68955100	2.13265400	0.25305700

Table S8: Cartesian coordinates of the optimized geometry of the planar acetone dimer at MP2/cc-pVTZ level.

	X	Y	Z
Planar dimer			
C	2.422333	0.103791	-0.004474
O	1.759708	1.126503	-0.040647
C	3.913235	0.138096	0.22933
H	4.138856	-0.325373	1.190158
H	4.431995	-0.440651	-0.534143
H	4.26696	1.163961	0.228456
C	1.807763	-1.258621	-0.193213
H	2.15306	-1.6733	-1.14149
H	2.144704	-1.937886	0.589381
H	0.723658	-1.196362	-0.196634
C	-2.422343	-0.103795	-0.004563
O	-1.75971	-1.126504	-0.040679
C	-1.807762	1.258622	-0.193231
H	-2.144718	1.937864	0.589379
H	-0.723658	1.196363	-0.19663
H	-2.15304	1.673331	-1.141501
C	-3.91323	-0.138095	0.229332
H	-4.138803	0.325389	1.190165
H	-4.432028	0.440641	-0.534123
H	-4.266956	-1.163959	0.228492

Table S9: Calculated symmetries, wavenumbers (in cm^{-1}), infrared intensities (in km mol^{-1}) and complexation shifts (in cm^{-1}) at MP2/cc-pVTZ level for the fundamental vibrational modes of the acetone monomer, and with counterpoise correction for the stacked dimer and planar dimer.

	monomer C_{2v}			stacked dimer			planar dimer		
	symmetry	$\tilde{\nu}$	intensity	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$
ν_1	A_1	3206.7	3.6	3202.7	0.0	-4.0	3204.8	13.1	-1.9
				3202.4	8.8	-4.3	3204.8	0.1	-1.9
ν_{18}	B_2	3205.7	7.7	3201.4	17.5	-4.3	3200.7	10.0	-4.9
				3200.9	0.0	-4.8	3199.7	0.3	-5.9
ν_{13}	B_1	3161.5	11.9	3164.9	0.0	3.4	3159.5	18.6	-2.0
				3164.4	15.2	2.9	3159.5	0.8	-2.0
ν_9	A_2	3155.6	0.0	3158.9	0.0	3.3	3151.8	3.7	-3.8
				3158.8	0.6	3.2	3151.7	2.4	-3.9
ν_2	A_1	3080.6	5.1	3079.7	0.0	-0.9	3078.5	0.0	-2.2
				3079.5	8.8	-1.1	3078.4	17.0	-2.3
ν_{19}	B_2	3076.0	1.2	3075.5	0.0	-0.5	3071.5	3.8	-4.5
				3075.0	3.1	-0.9	3071.5	13.6	-4.5
ν_3	A_1	1774.7	113.1	1773.3	193.0	-1.3	1774.8	244.7	0.1
				1766.1	0.0	-8.6	1769.1	0.2	-5.6
ν_{14}	B_1	1504.9	19.6	1507.9	0.0	3.0	1512.0	29.2	7.2
				1502.4	37.8	-2.5	1508.8	2.6	3.9
ν_4	A_1	1483.3	27.7	1484.2	76.6	1.0	1489.0	2.4	5.7
				1484.9	1.2	1.7	1487.2	9.9	4.0
ν_{10}	A_2	1481.6	0.0	1483.3	0.0	1.7	1483.5	0.7	1.9
				1479.7	0.0	-1.9	1481.4	39.4	-0.2
ν_{20}	B_2	1475.1	0.2	1474.9	0.0	-0.2	1477.5	0.2	2.3
				1472.3	0.5	-2.8	1476.1	1.3	0.9
ν_{21}	B_2	1397.0	71.4	1397.9	151.7	0.8	1402.8	5.4	5.8
				1397.3	0.0	0.3	1401.8	107.9	4.7
ν_5	A_1	1386.7	14.8	1384.4	52.2	-2.3	1389.0	1.6	2.3
				1383.5	0.0	-3.2	1388.1	51.0	1.4
ν_{22}	B_2	1253.2	53.8	1260.3	74.0	7.2	1259.8	3.5	6.6
				1253.9	0.0	0.7	1256.5	113.1	3.3
ν_{15}	B_1	1118.8	1.6	1121.9	0.0	3.0	1120.6	3.0	1.7
				1120.7	11.4	1.9	1119.9	0.0	1.1
ν_6	A_1	1084.1	0.0	1088.0	0.0	3.9	1087.3	0.5	3.1
				1087.1	0.1	3.0	1085.9	0.0	1.8
ν_{23}	B_2	901.8	5.4	907.2	7.9	5.5	907.2	0.8	5.4
				906.8	0.0	5.1	907.0	10.9	5.3

ν_{11}	A_2	887.5	0.0	887.6	0.7	0.1	891.0	0.0	3.5
				885.8	0.0	-1.7	889.5	0.2	2.0
ν_7	A_1	805.7	1.7	810.7	1.6	5.0	808.0	0.0	2.3
				810.1	0.0	4.4	806.6	4.7	0.9
ν_{24}	B_2	530.3	14.8	531.9	27.1	1.6	533.5	33.0	3.2
				530.7	0.0	0.4	532.7	0.6	2.4
ν_{16}	B_1	484.7	0.3	491.5	0.0	6.8	487.5	0.2	2.8
				485.8	0.8	1.1	486.4	0.8	1.7
ν_8	A_1	376.1	1.0	380.7	0.0	4.6	382.7	4.2	6.6
				379.0	1.6	2.9	380.7	0.0	4.6
ν_{17}	B_1	143.2	0.0	152.8	0.0	9.6	153.6	0.1	10.3
				152.1	0.3	8.9	147.3	0.1	4.1
ν_{12}	A_2	15.7	0.0	101.0	25.2		100.6	0.0	
				90.7	0.0		97.5	0.0	
				73.9	0.0		69.6	0.0	
				66.5	0.5		64.7	12.1	
				63.0	0.0		53.8	0.1	
				54.3	0.0		27.0	0.2	
				46.7	0.7		23.2	9.5	
				22.5	4.1		13.6	1.7	

Table S10: Cartesian coordinates of the optimized geometry of the acetone monomer at MP2/aug-cc-pVTZ level.

	X	Y	Z
Acetone			
C	0.00000000	0.00000000	0.18196800
O	0.00000000	0.00000000	1.40168000
C	0.00000000	1.28144200	-0.61420700
H	0.87724600	1.31559200	-1.26145600
H	-0.87724600	1.31559200	-1.26145600
H	0.00000000	2.13592600	0.05552900
C	0.00000000	-1.28144200	-0.61420700
H	-0.87724600	-1.315592 -	1.26145600
H	0.87724600	-1.31559200	-1.26145600
H	0.00000000	-2.13592600	0.05552900

Table S11: Cartesian coordinates of the optimized geometry of the stacked acetone dimer at MP2/aug-cc-pVTZ level.

	X	Y	Z
Stacked dimer			
C	1.55841200	-0.00000100	0.34916800
O	0.98874100	-0.00000900	1.43182700
C	1.90864100	-1.27904700	-0.36274300
H	1.33325700	-1.32710000	-1.28898400
H	2.96591500	-1.28888800	-0.62849800
H	1.67197200	-2.13408900	0.26392100
C	1.90861800	1.27905800	-0.36273000
H	2.96589800	1.28894000	-0.62845700
H	1.33325500	1.32708700	-1.28898400
H	1.67190000	2.13409300	0.26392600
C	-1.55841600	-0.00000200	-0.34917000
O	-0.98874200	-0.00000400	-1.43183000
C	-1.90862200	1.27905200	0.36273600
H	-2.96590100	1.28892000	0.62847500
H	-1.33325000	1.32709600	1.28898400
H	-1.67192300	2.13408500	-0.26392800
C	-1.90863400	-1.27905100	0.36274100
H	-1.33326000	-1.32708800	1.28899000
H	-2.96591200	-1.28891700	0.62848100
H	-1.67193500	-2.13408900	-0.26391500

Table S12: Cartesian coordinates of the optimized geometry of the planar acetone dimer at MP2/cc-pVTZ level.

	X	Y	Z
Planar dimer			
C	2.396806	0.101712	-0.005143
O	1.72939	1.124278	-0.046492
C	3.884874	0.143293	0.240836
H	4.102881	-0.326818	1.201103
H	4.410481	-0.43028	-0.522987
H	4.235594	1.170872	0.248846
C	1.787523	-1.261401	-0.199606
H	2.145473	-1.673229	-1.14549
H	2.121821	-1.938899	0.586782
H	0.702223	-1.20391	-0.212863
C	-2.396807	-0.101712	-0.00514
O	-1.729391	-1.124279	-0.046493
C	-1.787521	1.261401	-0.199601
H	-2.121822	1.938901	0.586784
H	-0.702221	1.20391	-0.212855
H	-2.145468	1.673225	-1.145487
C	-3.884874	-0.143292	0.240835
H	-4.102883	0.326826	1.201099
H	-4.410481	0.430275	-0.522992
H	-4.235594	-1.170871	0.248853

Table S13: Calculated symmetries, wavenumbers (in cm^{-1}), infrared intensities (in km mol^{-1}) and complexation shifts (in cm^{-1}) at MP2/aug-cc-pVTZ level for the fundamental vibrational modes of the acetone monomer, and with counterpoise correction for the stacked dimer and planar dimer.

	monomer C_{2v}			stacked dimer			planar dimer		
	symmetry	$\tilde{\nu}$	intensity	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$	$\tilde{\nu}$	intensity	$\Delta\tilde{\nu}$
ν_1	A_1	3200.9	2.9	3196.3	0.0	-4.6	3199.1	12.0	-1.8
				3195.9	8.3	-5.0	3199.1	0.1	-1.8
ν_{18}	B_2	3199.9	7.6	3194.9	16.7	-5.0	3192.0	15.8	-7.9
				3194.5	0.0	-5.5	3190.8	0.4	-9.2
ν_{13}	B_1	3154.7	10.1	3156.9	0.0	2.2	3152.9	14.8	-1.8
				3156.3	11.8	1.6	3152.9	0.7	-1.8
ν_9	A_2	3148.9	0.0	3151.0	0.0	2.0	3144.7	3.5	-4.3
				3150.8	0.7	1.9	3144.6	2.5	-4.4
ν_2	A_1	3074.4	5.3	3072.2	0.0	-2.3	3072.2	0.0	-2.2
				3071.9	9.9	-2.5	3072.2	15.5	-2.3
ν_{19}	B_2	3070.0	0.8	3068.2	0.0	-1.8	3064.1	24.9	-5.8
				3067.6	2.5	-2.4	3064.0	0.2	-5.9
ν_3	A_1	1756.2	130.2	1752.7	222.7	-3.6	1755.3	281.8	-0.9
				1743.9	0.0	-12.4	1749.2	0.3	-7.1
ν_{14}	B_1	1509.0	19.5	1512.1	0.0	3.1	1515.9	27.0	6.9
				1506.3	37.1	-2.7	1512.9	2.6	3.9
ν_4	A_1	1486.5	31.4	1487.4	84.2	0.9	1492.7	2.7	6.2
				1488.3	1.5	1.9	1491.0	14.2	4.5
ν_{10}	A_2	1485.1	0.0	1486.6	0.0	1.5	1485.9	0.6	0.8
				1482.8	0.0	-2.3	1483.9	43.6	-1.1
ν_{20}	B_2	1478.3	0.3	1478.4	0.0	0.1	1480.8	0.1	2.6
				1475.6	0.7	-2.7	1479.3	1.0	1.1
ν_{21}	B_2	1400.5	64.4	1400.5	136.6	0.1	1406.3	4.9	5.8
				1400.2	0.0	-0.3	1405.0	91.6	4.5
ν_5	A_1	1392.2	14.9	1389.4	54.0	-2.8	1394.0	2.0	1.8
				1388.3	0.0	-3.9	1393.2	52.5	1.0
ν_{22}	B_2	1254.5	52.9	1262.2	70.6	7.6	1261.6	3.7	7.0
				1255.9	0.0	1.3	1258.3	110.9	3.8
ν_{15}	B_1	1121.2	1.6	1123.9	0.0	2.7	1123.2	2.8	2.0
				1122.8	12.2	1.6	1122.6	0.0	1.4
ν_6	A_1	1087.0	0.0	1091.0	0.0	3.9	1090.4	0.6	3.4
				1090.1	0.0	3.1	1089.1	0.0	2.0
ν_{23}	B_2	901.8	5.4	912.0	7.5	10.3	910.8	0.9	9.1
				911.6	0.0	9.9	910.6	10.6	8.9

ν_{11}	A_2	892.0	0.0	890.5	1.0	-1.4	894.6	0.0	2.6
				889.2	0.0	-2.8	893.1	0.2	1.1
ν_7	A_1	806.4	1.6	811.7	1.6	5.3	809.0	0.0	2.5
				811.1	0.0	4.7	807.4	4.8	1.0
ν_{24}	B_2	531.3	14.4	533.2	25.9	1.9	534.5	32.4	3.2
				531.8	0.0	0.5	533.9	0.6	2.6
ν_{16}	B_1	484.4	0.5	492.1	0.0	7.6	487.5	0.2	3.1
				484.2	1.3	-0.2	486.4	1.1	2.0
ν_8	A_1	377.3	1.3	382.3	0.0	5.0	384.7	5.1	7.5
				380.4	2.0	3.1	382.2	0.0	4.9
ν_{17}	B_1	140.8	0.1	153.7	0.0	12.9	153.4	0.2	12.6
				150.0	0.7	9.2	146.7	0.1	5.9
ν_{12}	A_2	24.5	0.0	109.8	28.9		98.9	0.0	
				98.3	0.0		95.5	0.0	
				80.6	0.0		76.1	0.0	
				72.8	0.5		70.2	14.2	
				66.8	0.0		54.8	0.1	
				57.7	0.0		24.5	11.1	
				55.9	0.4		23.8	0.3	
				21.3	5.1		12.1	1.6	

Energies of optimized geometries

Table S14: The MP2/aug-cc-pVDZ, MP2/cc-pVTZ, MP2/aug-cc-pVTZ interaction energies including BSSE corrections, for the planar and stacked acetone dimer in kJ mol^{-1}.

	Stacked Dimer	Planar Dimer
ΔE (aug-cc-pVDZ)	-25.7	-13.0
ΔE (cc-pVDZ)	-23.3	-11.5
ΔE (aug-cc-pVTZ)	-23.6	-13.8

Comparison of experimental and calculated wavenumber shifts

The calculated wavenumbers shifts of the fundamental modes of the both dimer structures can be found in the two last columns in Table S5 (MP2/aug-cc-pVDZ), Table S9 (MP2/ cc-pVTZ), Table S13 (MP2/aug-cc-pVTZ). The wavenumber shifts are being compared with the experimental shifts (Table 1) by plotting the values and calculating the linear regression line, presented in Figure S2.

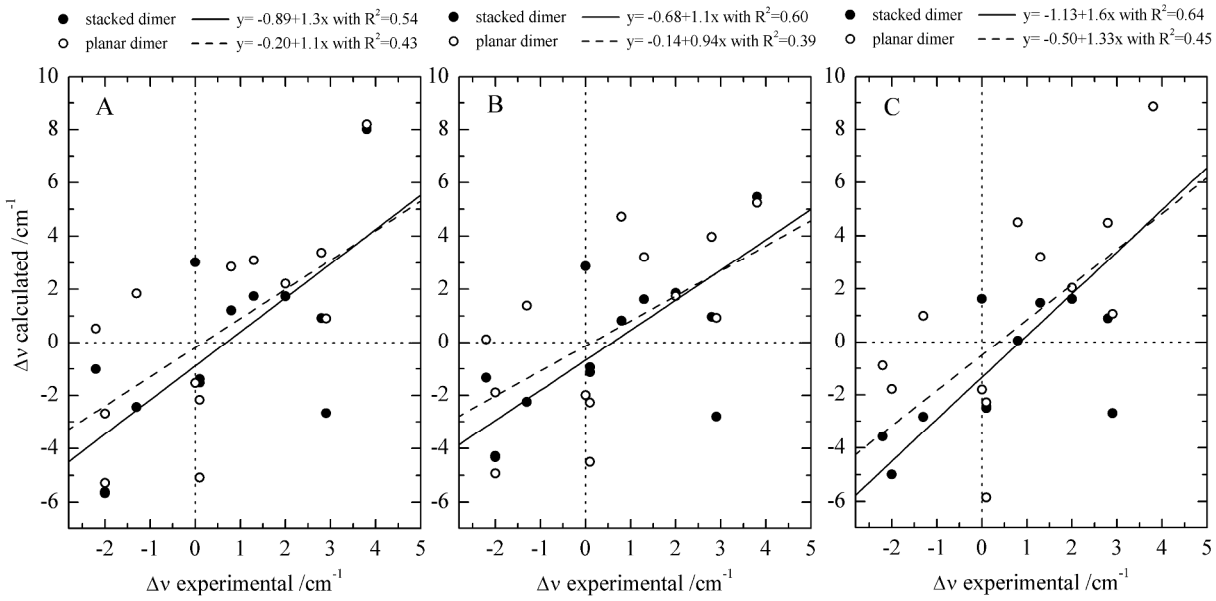


Figure S2. Linear fit of the experimental and calculated (A: MP2/aug-cc-pVDZ, B: MP2/cc-pVTZ, C: MP2/aug-cc-pVTZ) complexation shifts for the stacked (full circles) and the planar (open circles) acetone dimer with corresponding linear regression lines.

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