Table S1. Definition of Natural Internal Coordinates for the citric acid dimer

S_1	r(33-39)	νO33-H39
S_2	r(19-21)	νO19-H21
S_3	r(3-4)	νO3-H4
S_4	r(40-42)	νO40-H42
S_5	r(13-14)	νO13-H14
S_6	r(31-35)	νO31-H35
S_7	r (25-12) - r (11- 24)	νa (O-H--O)#
S_8	r (22-24)	O22-H24
S_9	r (10-12)	O10-H12
S_{10}	r (25-12) + r (11- 24)	νs (O-H--O)#
S_{11}	r(30-34) + r(38- 41)	νs $C=O_1$
S_{12}	r(1-2) + r(18- 20)	νs $C=O_2$
S_{13}	r(30-34) - r(38- 41)	νa $C=O_1$
S_{14}	r(1-2) - r(18- 20)	νa $C=O_2$
S_{15}	r(23-25) + r(9-11)	νs $C=O_3$
S_{16}	r(23-25) - r(9-11)	νa $C=O_3$
S_{17}	r(23-22) + r(9-10)	νs C-O
S_{18}	r(23-22) - r(9-10)	νa C-O
S_{19}	r(1-3)	νC1-O3
S_{20}	r(8-13)	νC8-O13
S_{21}	r(18-19)	νC18-O19
S_{22}	r(30-33)	νC30-O33
S_{23}	r(29-31)	νC29-O31
S_{24}	r(38-40)	νC38-O40
S_{25}	r(18-15) + r(5-1)	νs $C-C_1$
S_{26}	r(18-15) - r(5-1)	νa $C-C_1$
S_{27}	r(8 -15)	νC8-C15
S_{28}	r(32 – 38)	νC32-C38
S_{29}	r(8 – 5)	νC8-C5
S_{30}	r(26 – 23) + r(8 – 9)	νs $C-C_2$
S_{31}	r(26 – 23) - r(8 – 9)	νa $C-C_2$
S_{32}	r(29 – 26)	νC29-C26
S_{33}	r(29 – 32)	νC29-C32
S_{34}	r(29 – 30)	νC29-C30
S_{35}	r(26-27) + r(32-36) – r(26- 28) – r(32-37)	νa CH_2 op
S_{36}	r(5-6) + r(15-16) – r(5-7) - r(15-17)	νa CH_2 op
S_{37}	r(26-27) + r(32-37) - r(26- 28) - r(32-36)	νa CH_2 ip
S_{38}	r(5-6) + r(15-17) - r(5-7) - r(15-16)	νa CH_2 ip
S_{39}	r(26-27) + r(26- 28) + r(32-36) + r(32-37)	νs CH_2 ip
S_{40}	r(5-6) + r(5-7) + r(15-16)+ r(15-17)	νs CH_2 ip
S_{41}	r(26-27) + r(26- 28) - r(32-36) - r(32-37)	νs CH_2 op
S_{42}	r(5-6) + r(5-7) - r(15-16) - r(15-17)	νs CH_2 op
S_{43}	α (1-3-4) + α(18-19-21)	δs COH
S_{44}	α (1-3-4) - α(18-19-21)	δa COH
S_{45}	α (23-22-24) + α(9-10-12)	δs COH
S_{46}	α (23-22-24) - α(9-10-12)	δa COH
S_{47}	α (30-33-39) + α(29-31-35)	δs COH
S_{48}	α (30-33-39) - α(29-31-35)	δa COH
S_{49}	α (8-13-14)	δC8-O13-H14
S_{50}	α (38-40-42)	δC38-O40-H42
S_{51}	5α(36-32-37) + α(27-26-28) + 5(α29-32-38) + (α23-26-29)	δCH_2 ip
S_{52}	5α(7-5-6) + α(17-15-16) + 5α(18-15-8) + α(8-5-1)	δCH_2 ip

S_{53}	5α(36-32-37) + α(27-26-28) - 5(α29-32-38) - (α23-26-29)	δCH_2 op
S_{54}	5α(7-5-6) + α(17-15-16) - 5α(18-15-8) - α(8-5-1)	δCH_2 op
S_{55}	5α(29-32-38) + α(23-26-29) + 5α(36-32-37) + α(27-26-28)	δCCC ip
S_{56}	5α(18-15-8) + α(8-5-1)+ 5α(7-5-6) + α(17-15-16)	δCCC ip
S_{57}	5α(29-32-38) + α(23-26-29) - 5α(36-32-37) - α(27-26-28)	δCCC op
S_{58}	5α(18-15-8) + α(8-5-1) - 5α(7-5-6) - α(17-15-16)	δCCC op
S_{59}	5α(26-29-32) + α(30-29-31)	δC26-C29-C32
S_{60}	5α(5-8-15) + α(9-8-13)	δC5-C8-C15
S_{61}	5α(9-8-5) + α(15-8-13)	δC9-C8-C5
S_{62}	5α(26-29-30) + α(32-29-31)	δC26-C29-C30
S_{63}	α(2-1-3) - α(5-1-2) - α(5-1-3)	δCOO_1
S_{64}	α(11-9-10) - α(8-9-10) - α(8-9-11)	δCOO_2
S_{65}	α(19-18-20) - α(15-18-20) - α(15-18-19)	δCOO_3
S_{66}	α(25-23-22) - α(26-23-22) - α(26-23-25)	δCOO_4
S_{67}	α(34-30-33) - α(29-30-33) - α(29-30-34)	δCOO_5
S_{68}	α(40-38-41) + α(32-38-40) - α(32-38-41)	δCOO_6
S_{69}	α(5-1-2) - α(5-1-3)	ρCOO_1
S_{70}	α(8-9-10) - α(8-9-11)	ρCOO_2
S_{71}	α(15-18-20) - α(15-18-19))	ρCOO_3
S_{72}	α(26-23-22) - α(26-23-25))	ρCOO_4
S_{73}	α(29-30-33) - α(29-30-34)	ρCOO_5
S_{74}	α(32-38-40) - α(32-38-41)	ρCOO_6
S_{75}	α(7-5-1) + α(6-5-1) + α(17-15-8) + α(16-15-8) - α(7-5-8) – (6-5-8) – (17-15-18) - (16-15-18)	wag CH_2 ip
S_{76}	α(7-5-1) + α(6-5-8) + α(17-15-18) + α(16-15-8) - α(7-5-8) - (6-5-1) - (17-15-8) - (16-15-18)	wag CH_2 op
S_{77}	α(27-26-23) + α(28-26-23) + α(36-32-38) + α(37-32-38) - α(27-26-29) - α(28-26-29) - α(36-32-29) - α(37-32-29)	wag CH_2 ip
S_{78}	α(7-5-1) + α(6-5-1) + α(17-15-18) + α(16-15-18) - α(7-5-8) - α(6-5-8) - α(17-15-8) - α(16-15-8)	wag CH_2 op
S_{79}	α(27-26-23 + α(28-26-23+ α(36-32-29 + α(37-32-29 - α(27-26-29) - α(28-26-29) - α(36-32-38) - α(37-32-38)	ρCH_2 ip
S_{80}	α(27-26-23) + α(28-26-29) + α(36-32-38) + α(37-32-29) - 27-26-29) + α(28-26-23) + α(36-32-29) + α(37-32-38)	ρCH_2 op
S_{81}	α(7-5-1) + α(6-5-8) + α(17-15-8) + α(16-15-8) - α (7-5-8) + α(6-5-1) + α(17-15-18) + α(16-15-18)	ρCH_2 ip
S_{82}	α(27-26-23) + α(28-26-29) + α(36-32-29) + α(37-32-38) - α(27-26-29) + α(28-26-23) + α(36-32-38) + α(37-32-29)	ρCH_2 op
S_{83}	γ(2-1-5-3)	γCOO_1
S_{84}	γ(11-9-8-10)	γCOO_2
S_{85}	γ(20-18-15-19)	γCOO_3
S_{86}	γ(25-23-26-22)	γCOO_4
S_{87}	γ(34-30-29-33)	γCOO_5
S_{88}	γ(41-38-32-40)	γCOO_6
S_{89}	α(7-5-1) + α(7-5-8) + α(17-15-8) + α(17-15-18) - α(6-5-1) - α(6-5-8) - α(16-15-18) + α(16-15-8)	τwCH_2 ip
S_{90}	α(7-5-1) + α(7-5-8) + α(16-15-18) + α(16-15-8) - α(6-5-1) - α(6-5-8) - α(17-15-8) - α(17-15-18)	τwCH_2 op
S_{91}	α(27-26-23 + α(27-26-29) + α(36-32-29) + α(36-32-38) + α(28-26-29 + α(28-26-23) + α(37-32-38) + α(37-32-29)	τwCH_2 op
S_{92}	α(27-26-23) + α(27-26-29) + α(37-32-38) + α(37-32-29) + α(28-26-29) + α(28-26-23) + α(36-32-29) + α(36-32-38)	τwCH_2 op
S_{93}	τ(4-3-1-2) + τ(4-3-1-5)	τ(O3-H4)
S_{94}	τ(12-10-9-11 + τ(12-10-9-8)	τ(O10-H12)
S_{95}	τ(21-19-18-20) + τ(21-19-18-15)	τ(O19-H21)

S_{96}	τ(24-22-23-25 + τ(24-22-23-26)	τ(O22-H24)
S_{97}	τ(39-33-30-34 + τ(39-33-30-29)	τ(O33-H39)
S_{98}	τ(35-31-29-32) + τ(35-31-29-26) + τ(35-31-29-30)	τ(O31-H35)
S_{99}	τ(42-40-38-41+ τ(42-40-38-32)	τ(O40-H42)
S_{100}	τ(14-13-8-9) + τ(14-13-8-5) + τ(14-13-8-15)	τ(O13-H14)
S_{101}	τ(8-5-1-2) + τ(8-5-1-3)	τw COO_1
S_{102}	τ(8-15-18-20+ τ(8-15-18-19)	τw COO_2
S_{103}	τ(5-8-9-10) + τ(5-8-9-11)	τw COO_3
S_{104}	τ(29-26-23-25) + τ(29-26-23-22)	τw COO_4
S_{105}	τ(32-29-30-34) + τ(32-29-30-33)	τw COO_5
S_{106}	τ(29-32-38-41) + τ(29-32-38-40)	τw COO_6
S_{107}	τ(9-8-15-18) + τ(9-8-5-1)	τwCC ip
S_{108}	τ(9-8-15-18) + τ(9-8-5-1)	τwCC op
S_{109}	τ(23-26-29-30) + τ(23-26-29-32)	τCC_1
S_{110}	τ(26-29-30-33) + τ(26-29-32-38)	τCC_2
S_{111}	α(O13-C8-C9+ α(C5-C8-C15)	δC13-C8-C9
S_{112}	α(O13-C8-C5+ α(C9-C8-C15)	δC13-C8-C5
S_{113}	α(O13-C8-C15+ α(C5-C8-C9)	δC13-C8-C15
S_{114}	α(O31-C29-C30+ α(C32-C29-C26)	δC31-C29-C30
S_{115}	α(O31-C29-C26 + α(C32-C29-C30)	δC31-C29-C26
S_{116}	α(O31-C29-C32 + α(C30-C29-C26)	δC31-C29-C32
S_{117}	α(11-25-12) + α(25-11-24) - α(24-12-11) - α(12-24-25)	δ(OH---O)#
S_{118}	τ(11-24-25-12) + τ(25-12-11-24) – τ(24-25-12-11) - τ(12-11-24-25)	τwop#
S_{119}	τ(23-25-24-11) + τ(9-11-12-25) - τ(22-24-25-12) - τ(10-12-11-24)	γs (OH---O)#
S_{120}	τ(23-25-24-11) + τ(10-12-11-24) - τ(22-24-25-12) - τ(9-11-12-25)	γa (OH---O)#

Abbreviations: ν, stretching; δ, angle deformation; wag, wagging; ρ, rocking; γ, out plane deformation; τ , torsion; τw, twisting; a, antisymmetry; s, symmetry, ip, in phase; op, out phase

#Inter-monomer coordinates (See text and Table S2)

Table S2. Definition of inter-monomer coordinates for the citric acid dimer

Coordinate	Description	Definition [a,b,c,d]
$S_7 = r(25\text{-}12) + r(11\text{-}24)$	νs (O-H--O)	O---H symmetric stretching
$S_{10} = r(25\text{-}12) - r(11\text{-}24)$	νa (O-H--O)	O---H antisymmetric stretching
$S_{117} = \alpha(11\text{-}25\text{-}12) + \alpha(25\text{-}11\text{-}24) - \alpha(24\text{-}12\text{-}11) - \alpha(12\text{-}24\text{-}25)$	δ(OH---O)	O---H bending
$S_{118} = \tau(11\text{-}24\text{-}25\text{-}12) + \tau(25\text{-}12\text{-}11\text{-}24) - \tau(24\text{-}25\text{-}12\text{-}11) - \tau(12\text{-}11\text{-}24\text{-}25)$	τwop	out of plane twisting
$S_{119} = \tau(23\text{-}25\text{-}24\text{-}11) + \tau(9\text{-}11\text{-}12\text{-}25) - \tau(22\text{-}24\text{-}25\text{-}12) - \tau(10\text{-}12\text{-}11\text{-}24)$	γs (OH---O)	out of plane bending symmetric
$S_{120} = \tau(23\text{-}25\text{-}24\text{-}11) + \tau(10\text{-}12\text{-}11\text{-}24) - \tau(22\text{-}24\text{-}25\text{-}12) - \tau(9\text{-}11\text{-}12\text{-}25)$	γa (OH---O)	out of plane bending antisymmetric

[a] Ref. 33

[b] Ref. 34

[c] Ref. 35

[d] Ref. 36

Table S3. Calculated total energy (*E*) and relative energy (*ΔE*) and dipolar moments for the citric acid dimer

Structures	B3LYP/6-31G*			B3LYP/6-311++G**		
	E (Hartrees)	*ΔE* kJmol^{-1}	*μ* (D)	*E* (Hartrees)	*ΔE* kJmol^{-1}	*μ* (D)
C1 x 2	-1520.10192	82.86		-1520.63060	68.64	
Dimer	-1520.13351		2.08	-1520.65677		2.25

Table S4. Analysis of the Bond Critical Point (BCP) for the citric acid dimer at different theory levels

Parameter[#]	B3LYP					
	6-31G*			6-311++G**		
	O25---H12	O11---H24	(3,+1)	O25---H12	O11---H24	(3,+1)
$\rho(r)$	0.0491	0.0452	0.0073	0.0491	0.0451	0.0077
$\nabla^2\rho(r)$	0.1522	0.1413	0.0311	0.1398	0.1347	0.0314
$\lambda 1$	-0.0869	-0.0773	-0.0064	-0.0887	-0.0787	-0.0065
$\lambda 2$	-0.0868	-0.0771	0.0105	-0.0870	-0.0772	0.0110
$\lambda 3$	0.3260	0.2957	0.0269	0.3156	0.2906	0.0269
$\lvert\lambda 1\rvert/\lambda 3$	0.2666	0.2614	0.2379	0.2810	0.2708	0.2416
O25---H12[§]		1.662			1.652	
O11---H24[§]		1.697			1.685	
O25---O10[§]		2.669			2.654	
O11---O22[§]		2.700			2.683	

[#]The quantities are in atomics units

[§]Distances in Å

Experimental values from Ref. 7: O---H: 1.550 Å; O---O: 2.618 Å

Table S5. Observed and calculated wavenumbers (cm^{-1}), potential energy distribution and assignments for the citric acid dimer

Modes	IR[a]	Raman[a]	Calculated[b]	IR intensities[c]	Raman activities[d]	Calc. SQM[e]	[a]PED (≥10%)
1		3535 vw	3689	69.4	111.5	3537	S_1 (100)
2		3535 vw	3679	24.3	236.9	3527	S_3 (84), S_2 (16)
3	3498 s		3679	77.6	72.5	3527	S_2 (84), S_3 (16)
4		3480 vw	3678	51.6	165.8	3525	S_4 (100)
5	3446 m	3446 vw	3632	95.9	35.2	3482	S_5 (100)
6	3350 sh	3342 vw	3620	86.8	29.0	3470	S_6 (100)
7	3291 s	3276 vw	3198	3358.7	100.7	3066	S_8 (77), S_9 (17)
8	3035 sh		3141	7.9	101.8	3012	S_{35} (88), S_{39} (11)
9	2994 w	2996 w	3138	16.6	99.9	3009	S_{36} (85)
10	2994 w	2996 w	3135	0.3	1.3	3006	S_{37} (87), S_{41} (11)
11	2994 w	2996 w	3132	1.2	5.5	3003	S_{38} (85), S_{42} (10)
12		2982 m	3079	4.6	178.3	2952	S_{39} (83), S_{35} (11)
13		2982 m	3078	22.5	142.5	2951	S_{40} (85), S_{36} (10)
14		2982 m	3073	29.4	33.0	2946	S_{41} (82), S_{37} (12)
15	2950 w	2961 w	3072	1.1	2.0	2945	S_{42} (88), S_{38} (11)
16	2933 w	2929 m	3068	514.1	533.2	2942	S_9 (72), S_8 (17)
17	1756 vs		1854	570.6	5.6	1786	S_{11} (74)
18	1745 sh	1750 w	1851	435.7	12.3	1783	S_{12} (71)
19		1735 s	1843	5.4	0.4	1775	S_{14} (78)
20		1735 s	1839	103.2	1.9	1771	S_{13} (78)
21	1708 vs	1708 w	1792	378.7	0.7	1726	S_{16} (67), S_{18} (11)
22	1698 sh	1693 vs	1739	15.3	22.5	1677	S_{15} (65)
23		1493 vs	1530	14.8	19.1	1483	S_{45} (17), S_{17} (16)
24		1469 w	1508	80.1	6.6	1463	S_{46} (17), S_{18} (13), S_{31} (12)
25	1430 m	1432 m,br	1497	23.2	14.6	1447	S_{51} (26), S_{48} (24), S_{34} (11)
26	1430 m	1432 m,br	1487	12.6	13.2	1430	S_{52} (40), S_{78} (22), S_{81} (17)

27		1424 sh	1480	4.6	1.7	1426	S_{51} (36), S_{53} (20)
28	1420 sh		1479	16.5	0.4	1417	S_{54} (64), S_{75} (14)
29		1413 w	1466	14.0	7.2	1412	S_{53} (52), S_{51} (11)
30	1389 m	1391 s	1439	23.4	4.1	1402	S_{81} (18), S_{78} (14), S_{46} (13), S_{52} (11)
31	1389 m		1423	82.1	9.2	1385	S_{49} (15), S_{78} (12)
32	1389 m		1419	198.2	2.2	1383	S_{49} (15)
33		1365 w	1416	164.8	1.0	1381	S_{75} (38), S_{81} (13), S_{54} (13)
34	1358 w		1383	110.2	2.0	1352	S_{79} (25), S_{46} (19), S_{77} (17)
35	1340 sh	1347 w	1369	56.1	1.5	1334	S_{47} (42), S_{22} (15), S_{67} (12), S_{73} (10)
36	1308 w		1341	168.5	0.7	1308	S_{78} (47), S_{76} (19), S_{43} (12)
37	1308 w		1331	0.6	1.2	1306	S_{77} (23), S_{50} (20), S_{79} (15)
38	1308 w	1301 vw	1331	1.1	0.8	1303	S_{75} (37), S_{44} (13)
39	1292 w	1291 vw	1329	0.7	0.6	1303	S_{81} (34), S_{75} (14)
40		1285 vw	1316	28.8	0.9	1289	S_{80} (39)
41		1256 vw	1299	97.2	0.7	1266	S_{18} (19), S_{76} (17), S_{81} (10)
42	1242 s		1292	34.9	2.9	1258	S_{76} (29), S_{17} (22), S_{81} (16)
43	1214 s	1229 w	1241	47.6	12.0	1219	S_{81} (78)
44	1214 s	1211 m	1235	28.6	12.1	1212	S_{82} (69)
45	1174 s	1179 w	1203	76.1	3.1	1169	S_{22} (22), S_{47} (16)
46		1167 w	1194	247.7	1.5	1155	S_{43} (24), S_{21} (17), S_{19} (17)
47	1140 s		1179	289.2	1.9	1145	S_{24} (36), S_{50} (22)
48	1140 s	1140 w	1173	330.6	2.0	1140	S_{44} (27), S_{21} (22), S_{19} (22)
49	1140 s	1130 w	1161	139.0	3.9	1127	S_{20} (31)
50	1081 w	1083 m	1149	277.2	4.9	1112	S_{23} (27), S_{48} (18), S_{22} (12)
51		1053 m	1087	35.5	6.6	1059	S_{29} (17), S_{75} (17), S_{27} (16), S_{81} (13)
52	1051 w		1085	15.1	7.0	1057	S_{33} (22), S_{32} (22), S_{115} (14)
53		1036 sh	1084	43.3	3.5	1039	S_{76} (11), S_{89} (10)
54		1036 sh	1083	70.3	7.1	1036	S_{91} (14), S_{34} (14)
55		966 vw	966	199.6	0.5	926	S_{30} (15), S_{31} (15), S_{28} (14), S_{59} (12)
56	945 w	943 vs	957	1.9	9.8	911	S_{25} (42), S_{60} (14)
57		914 sh	954	0.6	2.3	886	S_{92} (25), S_{90} (17)
58	904 w	904 m	951	16.6	1.7	885	S_{90} (24), S_{92} (20)
59	904 w	904 m	940	0.5	11.7	872	S_{23} (32), S_{91} (25), S_{88} (10)

60	881 w	886 w	923	0.4	0.3	871	S_{20} (32), S_{89} (26)
61		867 vw	921	4.0	3.2	865	S_{96} (28), S_{94} (23), S_{118} (13), S_{119} (12)
62		850 vw	921	1.8	2.5	857	S_{28} (34), S_{57} (10)
63		842 vw	886	7.7	1.4	842	S_{26} (47), S_{58} (14)
64		842 vw	871	7.9	1.3	827	S_{120} (42), S_{96} (25), S_{94} (19)
65		807 vw	816	39.1	2.0	800	S_{87} (20), S_{57} (14), S_{62} (10)
66		795 sh	810	3.9	3.3	792	S_{84} (18), S_{58} (11)
67	781 s	784 vs	804	11.0	6.4	783	S_{64} (36), S_{30} (15)
68	729 sh	723 w	758	23.2	6.5	735	S_{34} (29), S_{67} (24)
69		700 w	715	69.5	3.6	685	S_{66} (35), S_{87} (11)
70	686 w		714	126.0	2.6	674	S_{88} (15), S_{87} (15), S_{99} (13)
71		666 vw	702	9.1	4.0	672	S_{85} (14), S_{95} (11)
72		656 sh	702	48.5	2.7	655	S_{84} (25), S_{93} (11), S_{90} (11)
73	640 w	642 w	668	74.9	4.0	637	S_{99} (20), S_{68} (16)
74		627 vw	655	60.9	1.4	631	S_{93} (17), S_{63} (14), S_{65} (10)
75		627 vw	653	2.5	1.2	625	S_{95} (25), S_{93} (16), S_{65} (10)
76		627 vw	633	22.2	3.0	621	S_{111} (15), S_{64} (13), S_{63} (11), S_{65} (11)
77	599 s	597 w	630	33.3	6.5	616	S_{99} (18), S_{67} (17), S_{114} (17), S_{73} (13)
78		574 w	597	163.3	1.2	574	S_{68} (22), S_{86} (13), S_{66} (12)
79		571 w	585	17.6	1.8	566	S_{86} (23), S_{115} (19), S_{97} (13)
80	550 w	559 m	563	21.4	1.9	544	S_{70} (15), S_{95} (11), S_{93} (11)
81		541 w	549	10.8	2.4	537	S_{63} (22), S_{65} (22), S_{26} (10)
82	520 sh	528 vw	548	134.9	5.6	519	S_{99} (23), S_{88} (19), S_{97} (17)
83		514 w	521	33.2	2.8	499	S_{85} (14), S_{89} (12), S_{95} (11)
84	504 w	509 sh	518	6.2	3.0	496	S_{83} (20), S_{93} (15), S_{112} (11), S_{85} (11)
85		492 vw	508	8.6	3.5	490	S_{97} (20)
86	477 sh	476 vw	500	5.0	1.6	485	S_{88} (13), S_{114} (11), S_{91} (10)
87	438 vvw	453 w	452	54.4	1.9	412	S_{98} (37), S_{115} (12), S_{72} (12)
88		415 w	427	65.9	1.3	398	S_{111} (21), S_{98} (13)
89		397 w	408	78.8	3.0	390	S_{115} (13)
90		382 m	398	9.5	0.2	387	S_{100} (40), S_{112} (19)
91		367 w	382	4.0	1.2	373	S_{71} (11), S_{112} (10), S_{69} (9)#
92		367 w	373	21.7	0.9	368	S_{114} (17), S_{73} (16)

93	348 w	356	39.5	0.5	345	S_{115} (25), S_{116} (24), S_{98} (17), S_{74} (14)
94	323 vw	341	22.1	0.3	329	S_{112} (34), S_{113} (21)
95	306 w	300	14.7	1.4	294	S_{111} (14), S_{10} (10)
96	306 w	275	2.8	0.3	271	S_{59} (25)
97	266 w	255	1.2	0.6	251	S_{62} (24), S_{114} (13), S_{115} (13)
98	254 sh	240	0.6	0.7	236	S_{60} (31), S_{61} (13), S_{111} (12)
99	247 vw	226	0.5	1.0	222	S_{61} (28), S_{112} (27), S_{113} (17)
100	237 vw	224	2.5	1.4	221	S_{115} (28), S_{116} (14)
101	217 w	183	2.3	0.5	180	S_{62} (35), S_{58} (16)
102	212 w	176	2.0	0.8	174	S_{62} (30), S_{58} (24)
103		152	1.4	0.4	148	S_{10} (20), S_{57} (17)
104		139	0.8	0.4	127	S_{103} (34), S_{58} (11)
105		133	1.6	0.5	122	S_{10} (14), S_{117} (13), S_{103} (13)
106		124	0.2	0.2	118	S_{105} (43)
107		112	3.3	0.2	108	S_{7} (18), S_{59} (13), S_{55} (8)#
108		107	2.7	0.3	99	S_{105} (16)
109		94	0.1	0.3	92	S_{60} (19), S_{56} (14)
110		80	2.7	0.1	72	S_{118} (15)
111		64	1.0	0.8	57	S_{110} (63)
112		59	0.7	1.3	53	S_{104} (18), S_{118} (15), S_{103} (11), S_{100} (10)
113		51	1.3	0.4	46	S_{108} (62)
114		42	1.2	0.7	38	S_{102} (33), S_{101} (16)
115		36	2.2	0.6	32	S_{106} (43), S_{105} (17)
116		32	1.0	0.7	30	S_{102} (17), S_{101} (10)
117		29	1.1	0.9	26	S_{101} (33), S_{102} (23), S_{103} (13)
118		28	0.5	0.3	25	S_{109} (29), S_{106} (19)
119		12	0.8	0.4	11	S_{119} (43)
120		9	0.3	0.3	8	S_{104} (45)

[a]This work, [b]B3LYP/6-31G*; [c]Units are km.mol^{-1}; [d]Raman activities in Å^4 (amu)$^{-1}$

[e] From scaled quantum mechanics force field, #PED value < 10%