Combined experimental and theoretical approach to study SmC→N_{CybC} phase transition studies of a four-ring bent-core liquid crystal†

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Synthesis:

[3-(4-pentyloxy-2-hydroxybenzylideneamino)-2-methyl benzoic acid], 3:

An ethanolic solution of 2-methyl-3-aminobenzoic acid **2** (0.45g, 3 mmol) was added to an ethanolic solution (20 ml) of 4-n-pentyloxy-2-hydroxybenzaldehyde **1** (0.63 g, 3mmol). The mixture was refluxed with a few drops of glacial acetic acid as catalyst for 4 hours to yield the yellow colored Schiff's base. The precipitate was collected by filtration from the hot solution and recrystallized several times from absolute ethanol to give a pure compound **3**. Yield = 0.81g, (80%).

IR ν_{max} in cm^{-1}: 1618 ($\nu_{CH=N}$, imine); 1719 ($\nu_{C=O}$, acid), 3425(ν_{O-H}, H-bonded); ^1H NMR ($CDCl_3$, 400 MHz): δ = 13.49 (s, 1H, -OH), 9.99 (s, 1H, -COOH), 8.35 (s, 1H, -CH=N-), 7.88 (d, 1H, J = 8.4Hz, ArH), 7.46 (d, 1H, J = 8.4Hz, ArH), 7.33 (t, 1H, J = 8.0 Hz, ArH), 7.29 (d, 1H, J = 7.8 Hz, ArH), 6.98 (d, 1H, J = 8.4 Hz, ArH), 6.43 (s, 1H, ArH), 4.03 (t, 2H, J = 7.8Hz, - O-CH_2-), 2.46 (s, 3H, Ar-CH_3), 1.57 (q, 2H, -O-CH_2-CH_2-), 1.29-1.21 (m, 4H, -O-$(CH_2)_2$-$(CH_2)_2$-), 0.88 (t, 3H, J = 7.8Hz, -O-$(CH_2)_4$-CH_3). Elemental analysis calculated for $C_{20}H_{23}NO_4$: C = 70.36%; H = 6.79%; N = 4.10% Found C = 70.33%; H = 6.76%; N = 4.07%.

[4-(4-heptyloxy-2-hydroxybenzylideneamino) phenol], 6 :

An ethanolic solution of 4-aminophenol **5** (0.32g, 3 mmol) was added to an ethanolic solution (20 ml) of 4-n-heptyloxysalicyldehyde **4** (0.70g, 3 mmol). The mixture was refluxed with a few drops of glacial acetic acid as catalyst for 4 hours to yield the yellow colored Schiff's base. The

precipitate was collected by filtration from the hot solution and recrystallized several times from absolute ethanol to give a pure compound **6**. Yield = 0.34g, (77%).

IR ν_{max} in cm^{-1}: 1627 ($\nu_{CH=N}$, imine); 3412(ν_{O-H}, H-bonded); ^1H NMR ($CDCl_3$, 400 MHz): δ = 13.42 and 13.39 (s, 2H, -OH), 8.39 (s, 1H, -CH=N), 7.43 (d, 1H, J = 8.4Hz, ArH), 7.22 (d, 2H, J = 8.0 Hz, ArH), 6.91 (d, 2H, J = 8.4Hz, ArH), 6.65 (d, 1H, J = 7.8 Hz, ArH), 6.34 (s, 1H, Ar-H), 4.01 (t, 2H, J = 7.8Hz, - O-CH_2-), 1.63 (q, 2H, -O-CH_2-CH_2-), 1.31-1.22 (m, 8H, -O-$(CH_2)_2$-$(CH_2)_4$-), 0.98 (t, 3H, J = 7.8Hz, -O-$(CH_2)_6$-CH_3). Elemental analysis calculated for $C_{20}H_{25}NO_3$: C = 73.37%; H = 7.70%; N = 4.28% Found C = 73.33%; H = 7.67%; N = 4.25%.

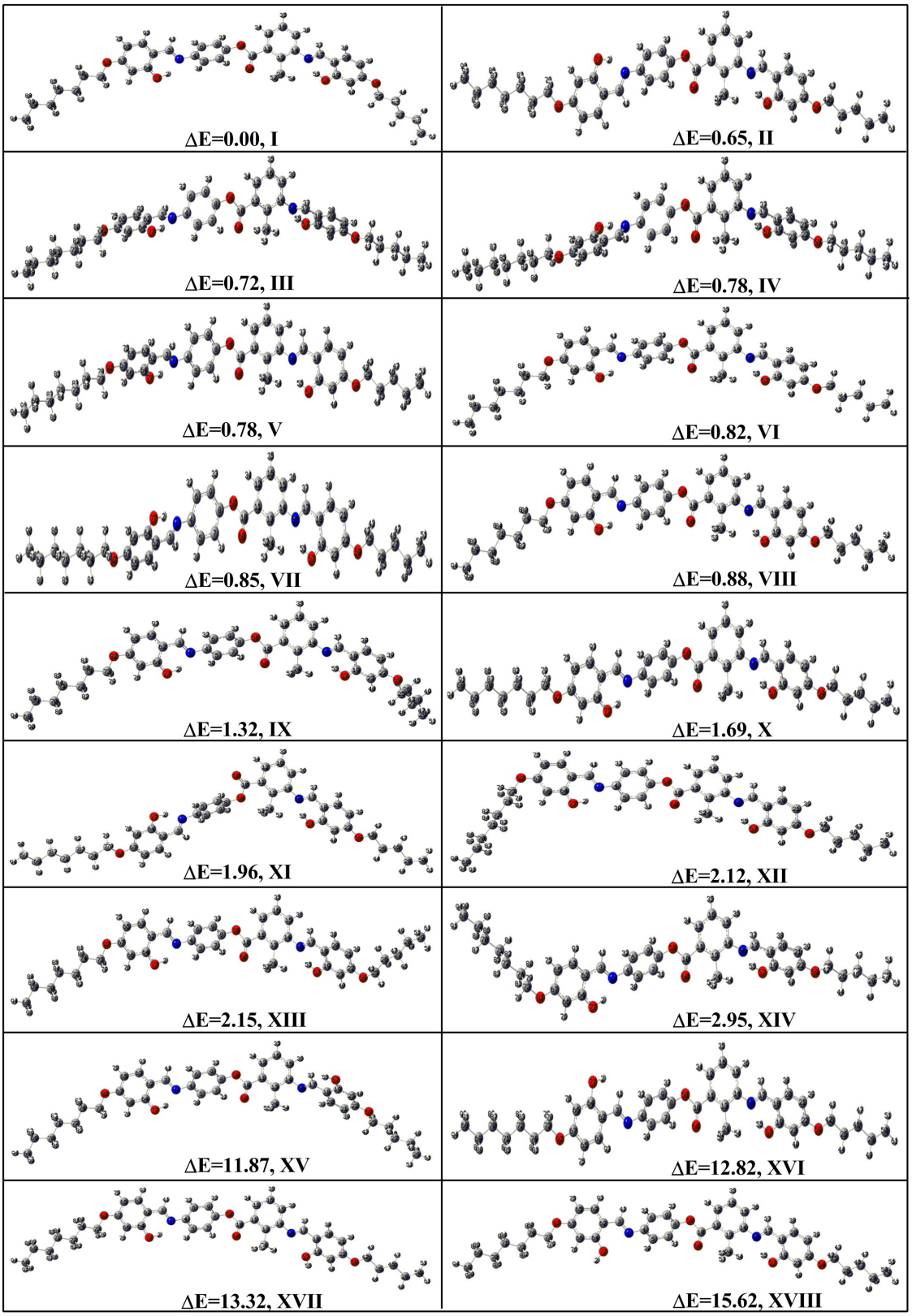

Fig. S1 All possible 18 conformers with their relative energy (kcal/mol) .

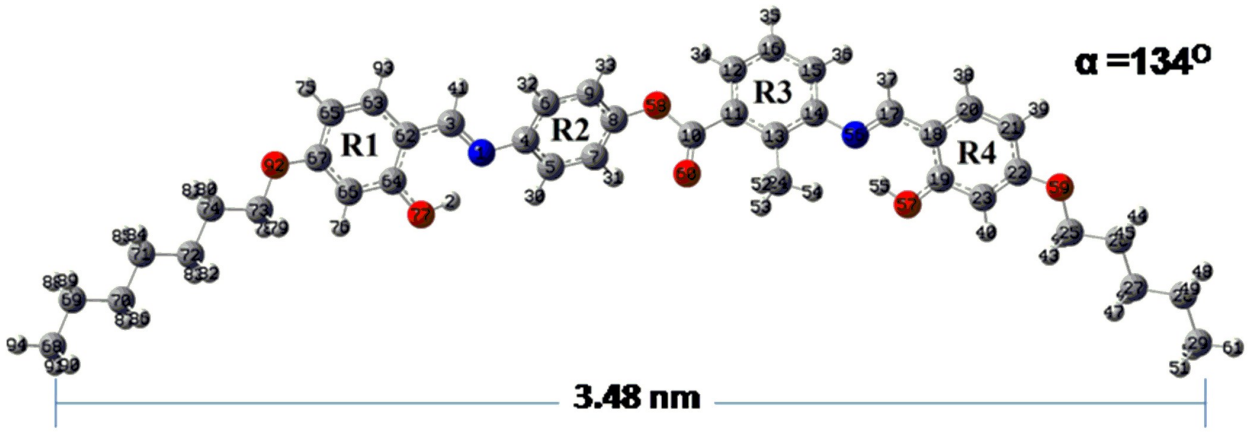

Fig. S2 Optimized structure of the most stable conformer I, with molecular length ~3.48 nm and bent angle ~134°.

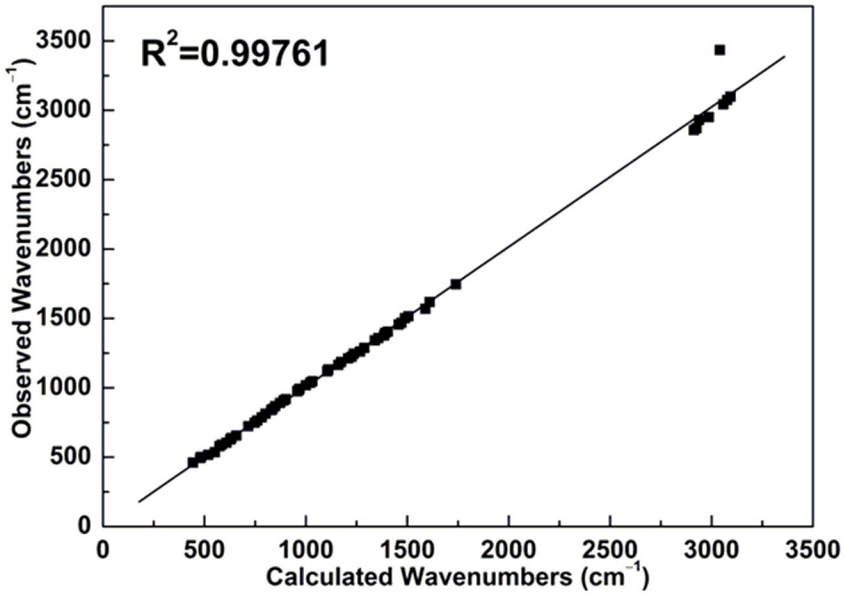

Fig. S3 The correlation graph between the calculated wavenumbers and observed wavenumbers of HAMPB.

Table S1 The optimized structural parameters: Bond length, bond angle and dihedral angle conformer I.

Parameters		Parameters		Parameters		Parameters	
Bond length		A(10,11,12)	118.7987	A(74,72,82)	109.4257	D(42,25,26,27)	−60.2293
R(1,3)	1.2957	A(10,11,13)	120.3002	A(74,72,83)	109.5453	D(42,25,26,44)	61.9923
R(1,4)	1.4057	A(12,11,13)	120.8983	A(82,72,83)	106.0692	D(42,25,26,45)	177.5997
R(2,77)	1.0005	A(11,12,16)	120.5105	A(74,73,78)	110.8859	D(43,25,26,27)	59.849
R(3,41)	1.0983	A(11,12,34)	119.1731	A(74,73,79)	110.8648	D(43,25,26,44)	−177.929
R(3,62)	1.4427	A(16,12,34)	120.3116	A(74,73,92)	107.908	D(43,25,26,45)	−62.322
R(4,5)	1.4049	A(11,13,14)	117.5815	A(78,73,79)	107.8948	D(59,25,26,27)	179.7917
R(4,6)	1.4056	A(11,13,24)	122.9885	A(78,73,92)	109.6791	D(59,25,26,44)	−57.9867
R(5,7)	1.3907	A(14,13,24)	119.418	A(79,73,92)	109.603	D(59,25,26,45)	57.6207
R(5,30)	1.0857	A(13,14,15)	120.5962	A(72,74,73)	112.2265	D(26,25,59,22)	−179.497
R(6,9)	1.3924	A(13,14,56)	119.0718	A(72,74,80)	110.1163	D(42,25,59,22)	59.6868

R(6,32)	1.0859	A(15,14,56)	120.2719	A(72,74,81)	110.1869	D(43,25,59,22)	−58.6801
R(7,8)	1.396	A(14,15,16)	120.8329	A(73,74,80)	108.6813	D(25,26,27,28)	179.998
R(7,31)	1.0829	A(14,15,36)	118.9844	A(73,74,81)	108.7651	D(25,26,27,46)	58.027
R(8,9)	1.3933	A(16,15,36)	120.1498	A(80,74,81)	106.6931	D(25,26,27,47)	−58.0323
R(8,58)	1.3936	A(12,16,15)	119.5579	A(2,77,64)	107.1477	D(44,26,27,28)	58.5996
R(9,33)	1.0856	A(12,16,35)	120.2741	A(67,92,73)	119.0884	D(44,26,27,46)	−63.3713
R(10,11)	1.4922	A(15,16,35)	120.164	Dihedral angle		D(44,26,27,47)	−179.431
R(10,58)	1.3775	A(18,17,37)	116.5214	D(4,1,3,41)	3.8941	D(45,26,27,28)	−58.6779
R(10,60)	1.2105	A(18,17,56)	122.7559	D(4,1,3,62)	−176.91	D(45,26,27,46)	179.3511
R(11,12)	1.4063	A(37,17,56)	120.7169	D(3,1,4,5)	−148.241	D(45,26,27,47)	63.2918
R(11,13)	1.4163	A(17,18,19)	121.5674	D(3,1,4,6)	33.9494	D(26,27,28,29)	179.9027
R(12,16)	1.3883	A(17,18,20)	120.3587	D(1,3,62,63)	−179.34	D(26,27,28,48)	−57.8575
R(12,34)	1.0824	A(19,18,20)	118.0727	D(1,3,62,64)	0.736	D(26,27,28,49)	57.6718
R(13,14)	1.4176	A(18,19,23)	120.3339	D(41,3,62,63)	−0.1095	D(46,27,28,29)	−57.8624
R(13,24)	1.5108	A(18,19,57)	121.765	D(41,3,62,64)	179.9662	D(46,27,28,48)	64.3774
R(14,15)	1.4037	A(23,19,57)	117.901	D(1,4,5,7)	−179.83	D(46,27,28,49)	179.9066
R(14,56)	1.4094	A(18,20,21)	121.9182	D(1,4,5,30)	1.0835	D(47,27,28,29)	57.7156
R(15,16)	1.391	A(18,20,38)	118.5005	D(6,4,5,7)	−1.9112	D(47,27,28,48)	179.9554
R(15,36)	1.0863	A(21,20,38)	119.5814	D(6,4,5,30)	179.0022	D(47,27,28,49)	−64.5153
R(16,35)	1.0862	A(20,21,22)	119.2234	D(1,4,6,9)	179.0727	D(27,28,29,50)	60.0343
R(17,18)	1.4425	A(20,21,39)	122.0424	D(1,4,6,32)	1.3172	D(27,28,29,51)	−59.8096
R(17,37)	1.0988	A(22,21,39)	118.7341	D(5,4,6,9)	1.2788	D(27,28,29,61)	−179.888
R(17,56)	1.2951	A(21,22,23)	120.6009	D(5,4,6,32)	−176.477	D(48,28,29,50)	−62.0065
R(18,19)	1.4234	A(21,22,59)	115.18	D(4,5,7,8)	1.3395	D(48,28,29,51)	178.1496
R(18,20)	1.4127	A(23,22,59)	124.2192	D(4,5,7,31)	−179.588	D(48,28,29,61)	58.0712
R(19,23)	1.4016	A(19,23,22)	119.8508	D(30,5,7,8)	−179.589	D(49,28,29,50)	−177.952
R(19,57)	1.3413	A(19,23,40)	117.7039	D(30,5,7,31)	−0.516	D(49,28,29,51)	62.2037
R(20,21)	1.3781	A(22,23,40)	122.4453	D(4,6,9,8)	−0.1032	D(49,28,29,61)	−57.8747
R(20,38)	1.0878	A(13,24,52)	111.3208	D(4,6,9,33)	−179.409	D(3,62,63,65)	−179.631
R(21,22)	1.4131	A(13,24,53)	111.1658	D(32,6,9,8)	177.6646	D(3,62,63,93)	0.1917
R(21,39)	1.0843	A(13,24,54)	110.5128	D(32,6,9,33)	−1.6411	D(64,62,63,65)	0.296
R(22,23)	1.3954	A(52,24,53)	105.7955	D(5,7,8,9)	−0.1178	D(64,62,63,93)	−179.881
R(22,59)	1.3555	A(52,24,54)	108.8513	D(5,7,8,58)	−176.474	D(3,62,64,66)	179.6232
R(23,40)	1.0826	A(53,24,54)	109.0502	D(31,7,8,9)	−179.193	D(3,62,64,77)	−0.4383
R(24,52)	1.0939	A(26,25,42)	110.9949	D(31,7,8,58)	4.451	D(63,62,64,66)	−0.3029
R(24,53)	1.094	A(26,25,43)	111.0133	D(7,8,9,6)	−0.4931	D(63,62,64,77)	179.6357
R(24,54)	1.0901	A(26,25,59)	107.5711	D(7,8,9,33)	178.8254	D(62,63,65,67)	−0.0755
R(25,26)	1.5221	A(42,25,43)	107.9579	D(58,8,9,6)	176.0821	D(62,63,65,75)	179.8363
R(25,42)	1.0991	A(42,25,59)	109.6688	D(58,8,9,33)	−4.5995	D(93,63,65,67)	−179.896
R(25,43)	1.0991	A(43,25,59)	109.6302	D(7,8,58,10)	−52.2171	D(93,63,65,75)	0.0156
R(25,59)	1.4312	A(25,26,27)	112.6463	D(9,8,58,10)	131.2827	D(62,64,66,67)	0.0942
R(26,27)	1.5341	A(25,26,44)	108.6262	D(58,10,11,12)	−9.1651	D(62,64,66,76)	−179.956
R(26,44)	1.0976	A(25,26,45)	108.5745	D(58,10,11,13)	171.4328	D(77,64,66,67)	−179.847
R(26,45)	1.0976	A(27,26,44)	110.08	D(60,10,11,12)	170.994	D(77,64,66,76)	0.1029
R(27,28)	1.5343	A(27,26,45)	110.0689	D(60,10,11,13)	−8.4081	D(62,64,77,2)	−0.2258
R(27,46)	1.1001	A(44,26,45)	106.6481	D(11,10,58,8)	178.8477	D(66,64,77,2)	179.7142
R(27,47)	1.1	A(26,27,28)	112.9603	D(60,10,58,8)	−1.3041	D(63,65,67,66)	−0.1453
R(28,29)	1.5318	A(26,27,46)	109.6282	D(10,11,12,16)	−178.935	D(63,65,67,92)	179.872
R(28,48)	1.099	A(26,27,47)	109.5744	D(10,11,12,34)	0.2638	D(75,65,67,66)	179.94
R(28,49)	1.099	A(28,27,46)	109.1579	D(13,11,12,16)	0.4633	D(75,65,67,92)	−0.0427
R(29,50)	1.097	A(28,27,47)	109.1871	D(13,11,12,34)	179.6622	D(64,66,67,65)	0.1343
R(29,51)	1.0969	A(46,27,47)	106.1003	D(10,11,13,14)	−179.851	D(64,66,67,92)	−179.885
R(29,61)	1.0958	A(27,28,29)	113.1535	D(10,11,13,24)	−1.1234	D(76,66,67,65)	−179.813
R(55,57)	0.9993	A(27,28,48)	109.1679	D(12,11,13,14)	0.7592	D(76,66,67,92)	0.1683
R(62,63)	1.4126	A(27,28,49)	109.1422	D(12,11,13,24)	179.4872	D(65,67,92,73)	−179.169
R(62,64)	1.4237	A(29,28,48)	109.524	D(11,12,16,15)	−0.7536	D(66,67,92,73)	0.8487

R(63,65)	1.3785	A(29,28,49)	109.5316	D(11,12,16,35)	178.5149	D(90,68,69,70)	59.8946
R(63,93)	1.0879	A(48,28,49)	106.0755	D(34,12,16,15)	−179.943	D(90,68,69,88)	−178.012
R(64,66)	1.4019	A(28,29,50)	111.2316	D(34,12,16,35)	−0.6749	D(90,68,69,89)	−62.189
R(64,77)	1.3404	A(28,29,51)	111.2087	D(11,13,14,15)	−1.7053	D(91,68,69,70)	−59.8459
R(65,67)	1.4128	A(28,29,61)	111.3283	D(11,13,14,56)	−178.895	D(91,68,69,88)	62.2472
R(65,75)	1.0843	A(50,29,51)	107.5437	D(24,13,14,15)	179.5196	D(91,68,69,89)	178.0705
R(66,67)	1.3952	A(50,29,61)	107.6648	D(24,13,14,56)	2.3297	D(94,68,69,70)	−179.971
R(66,76)	1.0825	A(51,29,61)	107.6776	D(11,13,24,52)	−54.4497	D(94,68,69,88)	−57.8774
R(67,92)	1.3566	A(14,56,17)	120.7205	D(11,13,24,53)	63.2258	D(94,68,69,89)	57.9459
R(68,69)	1.5321	A(19,57,55)	107.1757	D(11,13,24,54)	−175.538	D(68,69,70,71)	−179.856
R(68,90)	1.097	A(8,58,10)	120.3318	D(14,13,24,52)	124.256	D(68,69,70,86)	−57.6274
R(68,91)	1.097	A(22,59,25)	119.3422	D(14,13,24,53)	−118.069	D(68,69,70,87)	57.8335
R(68,94)	1.0959	A(3,62,63)	120.4144	D(14,13,24,54)	3.1675	D(88,69,70,71)	57.9202
R(69,70)	1.5342	A(3,62,64)	121.5641	D(13,14,15,16)	1.4636	D(88,69,70,86)	−179.852
R(69,88)	1.0993	A(63,62,64)	118.0215	D(13,14,15,36)	−176.451	D(88,69,70,87)	−64.3908
R(69,89)	1.0993	A(62,63,65)	121.9797	D(56,14,15,16)	178.6197	D(89,69,70,71)	−57.6056
R(70,71)	1.5338	A(62,63,93)	118.4697	D(56,14,15,36)	0.7054	D(89,69,70,86)	64.6224
R(70,86)	1.1003	A(65,63,93)	119.5504	D(13,14,56,17)	−140.034	D(89,69,70,87)	−179.917
R(70,87)	1.1002	A(62,64,66)	120.3035	D(15,14,56,17)	42.767	D(69,70,71,72)	179.8946
R(71,72)	1.5344	A(62,64,77)	121.8173	D(14,15,16,12)	−0.2035	D(69,70,71,84)	57.7852
R(71,84)	1.0999	A(66,64,77)	117.8791	D(14,15,16,35)	−179.473	D(69,70,71,85)	−57.9275
R(71,85)	1.0999	A(63,65,67)	119.2052	D(36,15,16,12)	177.6866	D(86,70,71,72)	57.7064
R(72,74)	1.5342	A(63,65,75)	122.0298	D(36,15,16,35)	−1.5826	D(86,70,71,84)	−64.4029
R(72,82)	1.1	A(67,65,75)	118.765	D(37,17,18,19)	179.6268	D(86,70,71,85)	179.8844
R(72,83)	1.0999	A(64,66,67)	119.9191	D(37,17,18,20)	0.0391	D(87,70,71,72)	−57.8639
R(73,74)	1.5222	A(64,66,76)	117.6323	D(56,17,18,19)	0.502	D(87,70,71,84)	−179.973
R(73,78)	1.0992	A(67,66,76)	122.4486	D(56,17,18,20)	−179.086	D(87,70,71,85)	64.314
R(73,79)	1.0992	A(65,67,66)	120.5702	D(18,17,56,14)	−176.485	D(70,71,72,74)	−179.58
R(73,92)	1.4307	A(65,67,92)	115.2697	D(37,17,56,14)	4.426	D(70,71,72,82)	−57.4398
R(74,80)	1.0976	A(66,67,92)	124.1601	D(17,18,19,23)	−179.703	D(70,71,72,83)	58.1079
R(74,81)	1.0976	A(69,68,90)	111.1857	D(17,18,19,57)	0.1872	D(84,71,72,74)	−57.3998
Bond angle		A(69,68,91)	111.1789	D(20,18,19,23)	−0.1062	D(84,71,72,82)	64.7399
A(3,1,4)	121.3903	A(69,68,94)	111.429	D(20,18,19,57)	179.784	D(84,71,72,83)	−179.713
A(1,3,41)	120.997	A(90,68,91)	107.502	D(17,18,20,21)	179.7418	D(85,71,72,74)	58.1935
A(1,3,62)	122.5596	A(90,68,94)	107.6808	D(17,18,20,38)	−0.2495	D(85,71,72,82)	−179.667
A(41,3,62)	116.4388	A(91,68,94)	107.6763	D(19,18,20,21)	0.14	D(85,71,72,83)	−64.1191
A(1,4,5)	117.8654	A(68,69,70)	113.1892	D(19,18,20,38)	−179.851	D(71,72,74,73)	179.786
A(1,4,6)	123.481	A(68,69,88)	109.4605	D(18,19,23,22)	0.0737	D(71,72,74,80)	58.5769
A(5,4,6)	118.6184	A(68,69,89)	109.4959	D(18,19,23,40)	−179.98	D(71,72,74,81)	−58.8485
A(4,5,7)	121.2136	A(70,69,88)	109.2255	D(57,19,23,22)	−179.821	D(82,72,74,73)	57.7919
A(4,5,30)	118.5753	A(70,69,89)	109.1981	D(57,19,23,40)	0.1259	D(82,72,74,80)	−63.4173
A(7,5,30)	120.2048	A(88,69,89)	106.0202	D(18,19,57,55)	0.7166	D(82,72,74,81)	179.1573
A(4,6,9)	120.448	A(69,70,71)	113.5667	D(23,19,57,55)	−179.391	D(83,72,74,73)	−58.0985
A(4,6,32)	120.0311	A(69,70,86)	109.2031	D(18,20,21,22)	−0.1372	D(83,72,74,80)	−179.308
A(9,6,32)	119.4832	A(69,70,87)	109.2101	D(18,20,21,39)	179.9954	D(83,72,74,81)	63.267
A(5,7,8)	119.127	A(71,70,86)	109.2752	D(38,20,21,22)	179.8541	D(78,73,74,72)	60.4484
A(5,7,31)	120.5431	A(71,70,87)	109.3356	D(38,20,21,39)	−0.0133	D(78,73,74,80)	−177.522
A(8,7,31)	120.3234	A(86,70,87)	105.9707	D(20,21,22,23)	0.1001	D(78,73,74,81)	−61.729
A(7,8,9)	120.709	A(70,71,72)	113.3283	D(20,21,22,59)	−179.894	D(79,73,74,72)	−59.3801
A(7,8,58)	122.7122	A(70,71,84)	109.3518	D(39,21,22,23)	179.972	D(79,73,74,80)	62.6498
A(9,8,58)	116.4852	A(70,71,85)	109.3615	D(39,21,22,59)	−0.0224	D(79,73,74,81)	178.4425
A(6,9,8)	119.8601	A(72,71,84)	109.2255	D(21,22,23,19)	−0.0695	D(92,73,74,72)	−179.413
A(6,9,33)	120.9805	A(72,71,85)	109.2733	D(21,22,23,40)	179.9866	D(92,73,74,80)	−57.3832
A(8,9,33)	119.1558	A(84,71,85)	106.0419	D(59,22,23,19)	179.9243	D(92,73,74,81)	58.4096
A(11,10,58)	111.0144	A(71,72,74)	113.1945	D(59,22,23,40)	−0.0195	D(74,73,92,67)	179.176
A(11,10,60)	126.4819	A(71,72,82)	109.1653	D(21,22,59,25)	179.5372	D(78,73,92,67)	−59.9287

A(58,10,60)	122.5034	A(71,72,83)	109.1921	D(23,22,59,25)	−0.457	D(79,73,92,67)	58.3513

Note: Bond length in angstrom, bond angle and dihedral angles are in degree.

Table S2 Observed and calculated vibrational wavenumbers (in cm^{-1}) of conformers I.

Wavenumber (unscaled)	Scaled	FTIR	CONTRIBUTIONS
3250.64	3125.16		R3[ν(C12H)](97)
3246.30	3120.99		R4[ν(C23H40)](92) R1[ν(C66H)](7)
3246.29	3120.98		R1[ν(C66H)](92) R4[ν(C23H40)](7)
3245.51	3120.24		R2[ν(CH)](99)
3228.18	3103.57		R4[ν(C21H)](96)
3227.19	3102.62		R1[ν(C65H)](96)
3217.73	3093.52	3098	R2[ν(CH)](99)
3209.37	3085.49		R2[ν(CH)](95)
3209.19	3085.32		R3[ν(CH)](93) R2[ν(C5H)](4)
3200.53	3076.99	3074	R2[ν(CH)](98)
3193.23	3069.97		R3[ν(CH)](99)
3183.01	3060.15		R4[ν(CH)](98)
3181.08	3058.29	3042	R1[ν(CH)](99)
3173.69	3051.18		$\nu_a[(C24H_3)]$(99)
3163.24	3041.14	3435	ν(O57H)(98)
3140.20	3018.99		ν(O77H)(98)
3129.66	3008.85		$\nu_a[(C24H_3)]$(100)
3114.10	2993.90		$\nu_a[(C29H_3)]$(100)
3111.99	2991.87		$\nu_a[(C68H_3)]$(99)
3108.36	2988.38		$\nu_a[(C29H_3)]$(96)
3106.87	2986.95	2951	$\nu_a[(C68H_3)]$(98)
3096.49	2976.97		$\nu_a[(C74H_2)]$(76) $\nu_a[(C73H_2)]$(10) $\nu_a[(C72H_2)]$(10)
3095.32	2975.85		$\nu_a[(C26H_2)]$(75) $\nu_a[(C25H_2)]$(12) $\nu_a[(C27H_2)]$(8)
3078.07	2959.26		$\nu_s[(C24H_3)]$(100)
3072.64	2954.03		$\nu_a[(C71H_2)]$(32) $\nu_a[(C70H_2)]$(29) $\nu_a[(C69H_2)]$(18) $\nu_a[(C72H_2)]$(8)
3065.35	2947.03		$\nu_a[(C28H_2)]$(61) $\nu_a[(C27H_2)]$(20) $\nu_a[(C25H_2)]$(8) $\nu_a[(C29H_2)]$(8)
3058.16	2940.11		ν[(C3H)](98)
3057.22	2939.21		$\nu_a[(C73H_2)]$(33) $\nu_a[(C69H_2)]$(32) $\nu_a[(C72H_2)]$(16) $\nu_a[(C71H_2)]$(11)
3056.90	2938.91	2930	$\nu_a[(C25H_2)]$(79) $\nu_a[(C26H_2)]$(17)
3055.30	2937.36		$\nu_a[(C73H_2)]$(54) $\nu_a[(C74H_2)]$(17) $\nu_a[(C69H_2)]$(14) $\nu_a[(C72H_2)]$(8)
3054.95	2937.03		ν[(C17H)](98)
3049.22	2931.52		$\nu_s[(C74H_2)]$(93)
3048.78	2931.10		$\nu_s[(C26H_2)]$(92)
3043.31	2925.84	2870	$\nu_s[(C29H_3)]$(97)
3042.17	2924.74		$\nu_s[(C68H_3)]$(97)
3041.67	2924.26		$\nu_a[(C27H_2)]$(69) $\nu_a[(C28H_2)]$(27)
3041.39	2923.99		$\nu_a[(C72H_2)]$(48) $\nu_a[(C69H_2)]$(18) $\nu_a[(C70H_2)]$(17) $\nu_a[(C71H_2)]$(13)
3034.76	2917.62		$\nu_a[(C70H_2)]$(48) $\nu_a[(C71H_2)]$(33) νa[$(C69H_2)$](9) $\nu_a[(C72H_2)]$(9)
3030.07	2913.11	2857	$\nu_s[(C28H_2)]$(87) $\nu_a[(C27H_2)]$(6)
3029.51	2912.57		$\nu_s[(C69H_2)]$(57) $\nu_s[(C71H_2)]$(20) $\nu_a[(C70H_2)]$(13)
3022.44	2905.78		$\nu_s[(C72H_2)]$(40) $\nu_s[(C69H_2)]$(28) $\nu_s[(C73H_2)]$(14) $\nu_s[(C71H_2)]$(10)
3020.93	2904.32		$\nu_s[(C25H_2)]$(67) $\nu_s[(C27H_2)]$(25)
3018.21	2901.71		$\nu_s[(C73H_2)]$(58) $\nu_s[(C71H_2)]$(29) $\nu_s[(C69H_2)]$(9)
3015.39	2899.00		$\nu_s[(C27H_2)]$(65) $\nu_s[(C25H_2)]$(30)
3013.98	2897.64		$\nu_s[(C71H_2)]$(39) $\nu_s[(C72H_2)]$(26) $\nu_s[(C73H_2)]$(19) $\nu_s[(C70H_2)]$(14)
3012.23	2895.96		$\nu_s[(C70H_2)]$(66) $\nu_s[(C72H_2)]$(23)
1809.44	1739.60	1746	ν(C=O)(77) ρ(C10O58)(7) (C10C)(6)
1691.33	1626.04		R1[ν(CC)(19)+δ_{in}(O77H)(8)+δ_a(5)] R4[ν(CC)(17)+δ_{in}(O57H)(6)+δ_a(4)]
1691.04	1625.76		R4[ν(CC)(20)+δ_{in}(O57H)(7)+δ_a(4)] R1[ν(CC)(17)+δ_{in}(O77H)(7)+δa(4)] ν(C17N)(4)
1679.97	1615.12		ν(C3N)(32) R2[ν(CC)](19) ρ(C3H)(11) R1[ν(C3C)(7)+δ_{in}(C62C3)(4)]
1674.97	1610.32	1618	ν(C17N)(40) δ(C17H)(13) R4[ν(C17C)(9)+δ_{in}(C18C17)(6)+ν(C18C20)(5)]
1653.06	1589.25	1570	R2[ν(CC)(37)+δ_{in}(CH)(7)] ν(C3N)(10) R1[ν(CC)](8) ρ(C3H)(4) R2[δ'a](3)
1638.18	1574.95		R3[ν(CC)(66)+δ_{in}(CH)(15)+δ'_a(10)]
1630.34	1567.41		R3[ν(CC)(18)+δ_a(4)+δ_{in}(C15H)(3)] R4[ν(CC)(12)+δ_{in}(O57H)(7)] R2[ν(CC)](12)
1630.08	1567.16		R2[ν(CC)(50)+δ_{in}(CH)(7)+δ'_a(4)+δ_a(3)] R3[ν(C15C16)](4)
1622.80	1560.16		R1[ν(CC)(33)+δ_{in}(O77H)(24)+δ'_a(4)+δ_{in}(C64O)(4)+δ_{in}(C67O)(3)] ν(C3N)(10)
1618.26	1555.80		R3[ν(CC)(23)+ν(C17N)(8)+δ_a(4)+δ_{in}(C16H)(4)] R4[δ_{in}(O57H)(14)+ν(CC)(13)]
1567.16	1506.67		R1[ν(CC)(27)+δ_{in}(CH)(22)+ν(C67O)(6)+δ_{in}(O77H)(5)] δ_{sci}(C73H2)(14)
1566.03	1505.58	1516	R4[ν(CC)(27)+δ_{in}(CH)(25)+ν(C22O)(6)+δ_{in}(O57H)(6)] $\delta_{sci}(C25H_2)$(18)
1549.89	1490.06		$\delta_{sci}(C73H_2)$(29) R2[δ_{in}(CH)(21)+ν(CC)(14)+ν(C4N)(3)] $\delta_{sci}(C74H_2)$(9) $\delta_{sci}(C72H_2)$(6)
1548.43	1488.66	1501	$\delta_{sci}(C25H_2)$(37) $\delta_{sci}(C26H_2)$(16) $\delta_{sci}(C27H_2)$(12) $\delta_{sci}(C28H_2)$(6) R4[ν(C21C22)(4)+δin(C21H)(3)]

1546.52	1486.83		R2[δ_{in}(CH)(23)+ν(CC)(15)] δ_{sci}(C74H_2)(8) δ_{sci}(C72H_2)(8) δ_{sci}(C73H_2)(8) δ_{sci}(C71H_2)(6) δ_{sci}(C70H_2)(4) R1[ν(C65C67)](3)
1542.99	1483.43		δ_{sci}(C69H_2)(23) δ_{sci}(C70H_2)(17) δ_a(C68H_3)(17) δ_{sci}(C73H_2)(17) δ_{sci}(C71H_2)(9)
1540.92	1481.44		δ_a(C29H_3)(28) δ_{sci}(C28H_2)(27) δ_{sci}(C25H_2)(24) δ_{sci}(C27H_2)(10)
1536.15	1476.86		δ_a(C68H_3)(25) δ_{sci}(C73H_2)(18) δ_{sci}(C72H_2)(17) δ_{sci}(C71H_2)(15) δ_{sci}(C74H_2)(8) δ_{sci}(C69H_2)(7)
1531.09	1471.99		δ_a(C29H_3)(33) δ_{sci}(C26H_2)(33) δ_{sci}(C25H_2)(13) δ_{sci}(C27H_2)(12)
1530.30	1471.23	1468	δ'_a(C29H_3)(91) ρ(C29H_3)(5)
1529.42	1470.39		δ'_a(C68H_3)(91) ρ(C68H_3)(6)
1528.09	1469.10		δ_{sci}(C74H_2)(35) δ_a(C68H_3)(21) δ_{sci}(C70H_2)(19) δ_{sci}(C73H_2)(8) δ_{sci}(C71H_2)(6)
1521.28	1462.56		δ_{sci}(C74H_2)(27) δ_{sci}(C72H_2)(27) δ_{sci}(C69H_2)(26) δ_a(C68H_3)(13)
1521.05	1462.34		δ_{sci}(C26H_2)(39) δ_{sci}(C27H_2)(20) δ_{sci}(C28H2)(15) δ_a(C29H_3)(15)
1519.56	1460.90		δ'_a(C24H_3)(82) ρ(C24H_3)(5)
1517.42	1458.85		δ_{sci}(C28H_2)(47) δ_{sci}(C27H_2)(42) δ_a(C29H_3)(5)
1515.98	1457.46	1456	δ_{sci}(C71H_2)(45) δ_{sci}(C72H_2)(32) δ_{sci}(C69H_2)(13) δ_a(C68H_3)(4)
1515.37	1456.88		δ_a(C24H_3)(19) R4[ν(CC)(13)+δ_{in}(CH)(9)+ν(C19O)(4)] R3[δ_{in}(C16H)](11) ν(C14N)(3)
1515.31	1456.82		δ_{sci}(C70H_2)(49) δ_{sci}(C69H_2)(21) δ_{sci}(C71H_2)(11) δ_{sci}(C74H_2)(4)
1513.69	1455.27		R1[ν(CC)(40)+δ_{in}(CH)(17)+δ_{in}(O77H)(10)+ν(C64O)(7)+ ν(C3C)(5) +δ_{in}(C62C3)(4)] ν(C3N)(4)
1512.16	1453.79		R4[ν(CC)(21)+δ_{in}(CH)(10)+δ_{in}(O57H)(7)+ν(C19O)(4)] δ_a(C24H_3)(19) R3[δ_{in}(C16H)](5) ρ'(C24H_3)(4)
1493.35	1435.71		R3[δ_{in}(CH)(32)+ν(CC)(26)] δ_a(C24H_3)(14) ν(C13C24)(5) R3[δ_{in}(C14N)](4) ν(C10C)(4)
1481.43	1424.24		R3[ν(CC)(29)+δ_{in}(C15H)(15)+δ_{in}(C11C10)(6)+δ_{in}(C14N)(4)] δ_a(C24H_3)(17) δ(C24H_3)(4)
1464.34	1407.81		R2[ν(CC)(20)+δ_{in}(CH)(12)] R1[δ_{in}(O77H)(15)+ν(C66C67)(8)+ν(C64O)(8)+ν(C67O)(3)]
1462.29	1405.84		R2[ν(CC)(24)+δ_{in}(CH)(19)] R1[ν(CC)(11)+ν(C64O)(9)+δ_{in}(O77H)(9)+ν(C67O)(4)]
1460.40	1404.02	1404	R4[δ_{in}(O57H)(23)+ν(CC)(23)+ν(C19O)(16)+ν(C22O)(7)+δ_{tri}(5)+δ_{in}(C22O)(4)] ω(C25H_2)(4)
1447.46	1391.58		ω(C25H_2)(36) δ(C29H_3)(16) ω(C26H_2)(15) ν(C25C)(8) ν(C26C27)(4) ω(C27H_2)(3)
1446.82	1390.97	1396	ω(C73H_2)(49) ω(C74H_2)(17) ν(C73C74)(10) ν(C72C74)(4) ω(C72H_2)(3)
1441.79	1386.14	1377	δ(C68H_3)(87) ν(C68C69)(7)
1440.67	1385.06		δ(C29H_3)(59) δ(C24H_3)(17) ω(C25H_2)(8) ν(C28C29)(5)
1440.23	1384.64		δ(C24H_3)(67) δ(C29H_3)(13) δ_a(C24H_3)(5) ν(C13C24)(5) ω(C25H_2)(3)
1428.11	1372.98		ω(C71H_2)(26) ω(C70H_2)(22) ω(C72H_2)(14) ν(C70C71)(9) ω(C69H_2)(8) ν(C71C72)(7) ν(C69C70)(5)
1423.71	1368.76		ω(C27H_2)(38) ω(C28H_2)(28) ν(C27C28)(10) ω(C25H_2)(8) ν(C26C27)(5) ν(C28C29)(3)
1416.98	1362.29		ω(C72H_2)(25) ω(C69H_2)(22) ω(C70H_2)(16) ω(C73H_2)(6) ν(C69C70)(6) ω(C74H_2)(4) ν(C72C74)(3)
1412.00	1357.49	1358	ρ(C17H)(45) ν(C17N)(8) R4[ν(C17C)(5)+δ_{in}(C20H)(3)+ν(C19O)(3)] R3[δ_{in}(C15H)](3)
1411.82	1357.32		ρ(C3H)(41) ν(C3N)(7) R1[ν(C3C)(5)+δ_{in}(C63H)(3)] R2[ν(C6C9)](4) ω(C73H_2)(3)
1394.02	1340.21	1341	R4[ν(CC)(62)+δ_{in}(CH)(8)+ν(C17C)(7)+ν(C19O)(3)] δ(C17H)(3)
1393.27	1339.49		R1[ν(CC)(64)+δ_{in}(CH)(9)+ν(C3C)(6)]
1376.26	1323.13		ω(C69H_2)(29) ω(C71H_2)(22) ω(C74H_2)(16) ω(C73H_2)(8) ω(C72H_2)(8)
1371.81	1318.86		ω(C28H_2)(39) ω(C26H_2)(25) ω(C25H_2)(12) ω(C27H_2)(7)
1353.22	1300.98		ϒ(C72H_2)(38) ϒ(C69H_2)(25) ϒ(C70H_2)(14) ϒ(C71H_2)(12)
1351.08	1298.93		ϒ(C28H_2)(44) ϒ(C27H_2)(43) ϒ(C25H_2)(6)
1349.14	1297.06		ϒ(C71H_2)(41) ϒ(C70H_2)(35) ϒ(C74H_2)(10) ϒ(C73H_2)(5)
1344.18	1292.29		R2[ν(CC)](75)
1340.01	1288.29	1288	ϒ(C26H_2)(46) ϒ(C25H_2)(13) ϒ(C27H_2)(12) R3[ν(C13C14)](3)
1339.87	1288.15		R3[ν(CC)](54) ϒ(C26H_2)(5)
1339.46	1287.76		R2[δ_{in}(CH)](31) R1[ν(CC)(11)+δ_{tri}(7)+ν(C64O)(7)+ν(C67O)(6)+δ_{in}(C65H)(4)]
1337.04	1285.43		ϒ(C74H_2)(40) ϒ(C72H_2)(21) ϒ(C69H_2)(19) ϒ(C73H_2)(9) ϒ(C70H_2)(5)
1335.11	1283.57		R3[ν(CC)](18) R4[ν(CC)(14)+δ_{in}(CH)(9)+δ_{tri}(8)+ν(C22O)(8)+ν(C19O)(6)+δ_{in}(C22O)(4)] ω(C25H_2)(3)
1331.20	1279.81		R2[δ_{in}(CH)(37)+ν(CC)(16)+δ_{in}(C4N)(3)] R1[ν(C65C67)(4)+ν(C67O)(3)+δ_{tri}(3)]
1327.42	1276.18		ϒ(C73H_2)(35) ϒ(C69H_2)(21) ϒ(C72H_2)(10) ϒ(C71H_2)(8) ρ(C74H_2)(5) ϒ(C74H_2)(5) ϒ(C70H_2)(4) ρ(C70H_2)(3)
1318.27	1267.38	1261	ω(C70H_2)(25) ω(C74H_2)(25) ω(C69H_2)(13) ω(C73H_2)(9) ω(C71H_2)(5) ω(C72H_2)(5)
1315.63	1264.85		ϒ(C25H_2)(38) ϒ(C28H_2)(30) ϒ(C27H_2)(11) ρ(C26H_2)(8) ρ(C29H_3)(4) ρ(C27H_2)(4)
1295.44	1245.44		ν(C14N)(23)δ(C17H)(9) R3[δ_{in}(C15H)(9)+δ_{tri}(7)+ν(CC)(7)] R4[ν(C17C)](7) ν(C10C)(4)
1286.74	1237.07		ω(C26H_2)(38) ω(C27H_2)(34) ω(C28H_2)(9) ω(C25H_2)(7) ρ'(C29H_3)(3)
			R2[ν(C4N)](10) ρ(C3H)(9) R1[ν(C3C)(9)+ν(C62C63)(5)] ϒ(C73H_2)(8) ϒ(C70H_2)(6) ϒ(C74H_2)(4) ϒ(C69H_2)(4) ρ(C72H_2)(4)
1285.77	1236.14	1246	ϒ(C71H_2)(3)
			ϒ(C73H_2)(11) ϒ(C70H_2)(8) R2[ν(C4N)](8) ρ(C3H)(7) R1[ν(C3C)(7)+ν(C62C63)(4)] ϒ(C74H_2)(6) ϒ(C69H_2)(6) ρ(C72H_2)(5)
1285.71	1236.08		ϒ(C71H_2)(4)
1274.84	1225.64	1223	R4[δ_{in}(CH)(25)+ν(CC)(16)+ν(C19O)(7)+δ_{in}(C19O)(5)+δ_{in}(C18C17)(3)] ν(C10C)(7) R3[δ_{in}(C12H)(6)+ν(C11C12)(6)]
1272.59	1223.47		R1[δ_{in}(CH)(38)+ν(CC)(24)+ν(C64O)(9)+δ_{in}(C64O)(6)+(C62C3)(5)]
1269.44	1220.44		R3[ν(CC)(20)+δ_{in}(CH)(19)+δ_{in}(C13C24)(3)] R4[δ_{in}(C20H)(11)+ν(C18C20)(8)] ν(C10C)(8)
1262.48	1213.74		ω(C72H_2)(26) ω(C71H_2)(25) ω(C74H_2)(19) ω(C70H_2)(14)
1256.93	1208.42	1213	R4[ν(C17C)(14)+ν(CC)(12)+ν(C22O)(5)+δ_{in}(C21H)(3)] ν(C10C)(11) R2[ν(C8O)](6) R3[ν(C13C14)(4)+δ_{tri}(4)]δ(C17H)(4)
1252.72	1204.36		ϒ(C25H_2)(22) ϒ(C26H_2)(17) ρ(C28H_2)(16) ρ(C29H_3)(12) ϒ(C27H_2)(8) ρ(C27H_2)(7) ρ(C25H_2)(5) ρ'(C29H_3)(4) ϒ(C28H_2)(3)
1244.49	1196.45		R2[ν(C8O)(27)+ν(CC)(11)+ν(C4N)(4)] ν(C10O58)(7) R1[ν(C67O)](5)
1241.82	1193.88		R4[δ_{in}(C23H)(33)+ν(C22O)(24)+ν(C19O)(16)] ν(C25O)(4)
1239.28	1191.44		R1[δ_{in}(C66H)(27)+ν(C67O)(18)+ν(C64O)(11)] ν(C73O)(3)
			ρ(C69H_2)(13) ρ(C70H_2)(10) ρ(C68H_3)(9) ϒ(C73H_2)(9) R1[δ_{in}(C66H)(7)+ν(C67O)(5)] ϒ(C74H_2)(7) ϒ(C72H_2)(6) ρ(C71H_2)(5)
1238.44	1190.63		ρ(C73H_2)(4) ϒ(C71H_2)(4)
1225.12	1177.83		ν(C13C24)(27) R3[δ_{in}(CH)(18)+ν(CC)(17)+δ_{tri}(7)]
1221.42	1174.27	1186	R2[ν(C4N)(18)+δ_{tri}(13)+ν(C8O)(11)+δ_{in}(CH)(6)+ν(C4C5)(3)] R1[ν(C3C)(6)+ν(C62C63)(5)+δ_{tri}(3)] ν(C10O58)(3)
1207.27	1160.67	1165	R3[δ_{in}(CH)(52)+ν(C15C16)(10)+δ_{tri}(7)] ν(C14N)(7) ν(C13C24)(6)
1204.16	1157.68		ρ(C73H_2)(31) ρ(C74H_2)(16) ρ(C72H_2)(11) ϒ(C73H_2)(11) ρ(C71H_2)(8) ρ(C70H_2)(6) ρ(C69H_2)(4)

1202.56	1156.14		$\rho(C25H_2)(33)$ $\rho(C26H_2)(18)$ $\rho(C27H_2)(13)$ $\Upsilon(C25H_2)(12)$ $\rho(C28H_2)(10)$ $\rho(C29H_3)(5)$
1195.07	1148.94		R2[δ_{in}(CH)(69)+(CC)(13)+ν(C8O)(6)]
1160.87	1116.06		ν(C10O58)(16) R3[δ_{in}(CH)(12)+ν(C12C16)(8)+δ_{in}(C11C10)(7)] ν(C14N)(9) δ(C10O58)(9) ρ'(C24H_3)(5)
1155.68	1111.07	1132	R4[δ_{in}(C21H)(26)+ν(C20C21)(6)] ρ'(C29H_3)(7) ν(C25C)(6) ν(C27C28)(6) δ_{sci}(C27H_2)(4) δ_{sci}(C28H_2)(3) δ_{sci}(C26H_2)(3)
			R1[δ_{in}(CH)(22)+ν(C63C65)(5)] ρ'(C68H_3)(7) ν(C69C70)(6) ν(C73C74)(4) δ_{sci}(C70C)(4) δ_{sci}(C71C)(4) δ_{sci}(C69C)(3) δ_{sci}(C72C)(3)
1155.11	1110.52	1130	ν(C70C71)(3)
1150.01	1105.62	1119	R1[δ_{in}(CH)(25)+ν(C63C65)(6)] ρ'(C68H3)(6) ν(C69C70)(4)
			R4[δ_{in}(CH)(20)+ν(C20C21)(6)] ρ'(C29H_3)(7) ν(C27C28)(6) δ_{in}(C65H)(4) δ_{sci}(C27H_2)(3) ν(C25O)(3) δ_{sci}(C28H_2)(3) δ_{sci}(C26H_2)(3)
1149.24	1104.88		ν(C25C)(3)
1139.88	1095.88		R2[δ_{in}(CH)(65)+ν(CC)(25)]
1117.98	1074.82		R3[ν(CC)(39)+δ_{in}(CH)(18)+δ_{tri}(13)+δ_{in}(C14N)(3)] ν(C13C24)(7) ν(C10O58)(4)
1091.31	1049.18		ν(C73C74)(38) ν(C69C70)(13) ρ'(C68H_3)(8) δ_{sci}(C73C)(6) δ_{sci}(C74C)(5) ω(C69H_2)(5)
1075.52	1034.01		ν(C70C71)(34) ν(C71C72)(24) ν(C69C70)(12) ν(C72C74)(10) ν(C68C69)(7) ν(C73O)(4)
1073.75	1032.31	1047	ν(C27C28)(30) ν(C25C)(26) ν(C28C29)(17) ν(C25O)(7) ω(C28H_2)(5) ν(C26C27)(4)
1072.88	1031.46		ν(C25C)(36) ν(C26C27)(35) ν(C28C29)(8) ν(C27C28)(6) ω(C27H_2)(4)
1070.49	1029.17		ρ(C24H_3)(50) ρ'(C24H_3)(24) R3[δ_{oop}(C13C24)(10) δ'$_a$(C24H_3)(5) R3[δ_{puc}](5)
1064.98	1023.88		ν(C73O)(31) ν(C68C69)(18) ν(C73C74)(14) ν(C69C70)(11) ν(C71C72)(10) R1[ν(C65C67)](4)
1062.77	1021.75	1036	ν(C72C74)(30) ν(C73O)(25) ν(C68C69)(13) δ_{sci}(C73C)(4) δ_{sci}(C74C)(3) ρ'(C68H_3)(3)
1053.79	1013.12		ν(C25O)(58) R4[ν(C21C22)](8) δ_{sci}(C25C)(4) ρ'(C29H_3)(4)
1040.59	1000.43	1018	ρ'(C24H_3)(26) ν(C10O58)(19) ρ(C24H_3)(13) R3[ν(C11C13)](6) δ_a(C24H_3)(4)
1036.48	996.47		Υ(C71H_2)(20) Υ(C70H_2)(17) Υ(C72H_2)(15) Υ(C74H_2)(8) Υ(C69H_2)(8) ρ(C73H_2)(8)ρ(C68H_3)(6) ρ(C74H_2)(5) ρ(C69H_2)(4)
1036.05	996.06		ν(C72C74)(26) ν(C71C72)(14) ν(C70C71)(13) ν(C68C69)(10) ν(C73O)(10) R1[ν(C65C67)](6)
1032.75	992.88		R2[δ_{tri}(46)+ν(CC)(30)+δ_{in}(CH)(9)]
1031.19	991.39		ν(C28C29)(39) ν(C26C27)(31) ρ'(C29H3)(6) δ_{sci}(C25C)(4) δ_{sci}(C26H2)(3)
1008.05	969.13	993	ν(C70C71)(25) ν(C68C69)(20) ν(C71C72)(19) ν(C73C74)(9) δ_{sci}(C71C)(4) ρ'(C68H3)(3)
1007.94	969.04		δ_{oop}(C17H)(65) τ(C17N)(14) R4[τ(C17C)(8)+δ_{oop}(C18C17)(4)+δ_{oop}(C20H)(3)]
1003.98	965.23	984	δ_{oop}(C3H)(64) τ(C3N)(14) R1[τ(C3C)(7)+δ_{oop}(C63H)(4)+δ_{oop}(C62C3)(4)]
1001.71	963.05	982	Υ(C27H_2)(21) Υ(C26H_2)(17) ρ(C25H_2)(16) Υ(C28H_2)(16) ρ(C29H_3)(12) ρ(C26H_2)(5) ρ(C28H_2)(4) ρ'(C29H_3)(4)
996.34	957.88	974	R4[δ_{tri}(24)+ν(CC)(24)+δ_{in}(CH)(8)+ν(C22O)(6)+ν(C19O)(5)+δ_{in}(C19O)(3)+δ_{in}(C22O)(3)] ν(C25O)(8) ν(C26C27)(5)
994.98	956.57		R1[δ_{tri}(22)+ν(CC)(20)+δ_{in}(CH)(6)+ν(C67O)(5)+ν(C64O)(4)+δ_{in}(C67O)(3)] ν(C73O)(10) ν(C71C72)(4) ν(C72C74)(3)
977.31	939.59		R3[δ_{oop}(CH)(86)+δ_{puc}(11)]
959.91	922.86		R2[δ_{oop}(CH)(79)+δ_{puc}(12)]
949.06	912.43		R2[δ_{oop}(CH)(82)+δ_{puc}(8)+τ_a(3)]
			ρ(C73H_2)(15) ρ(C71H_2)(14) Υ(C74H_2)(13) Υ(C69H_2)(12) ρ(C68H_3)(11) Υ(C72H_2)(7) Υ(C70H_2)(7) ρ(C70H_2)(6) ρ(C72H_2)(5)
946.34	909.81		ρ'(C68H_3)(3)
943.28	906.87		R4[δ_{oop}(CH)(83)+δ_{puc}(5)+τ'$_a$(5)]
941.16	904.83		R1[δ_{oop}(CH)(84)+δ_{puc}(5)+τ'$_a$(5)]
936.75	900.59	918	R3[δ_{oop}(CH)(40)+ δ_{oop}(C14N)(4)+τ_a(3)] δ(C17H)(7) ν(C14N)(6) δ_{in}(N56C)(5)
926.31	890.56	908	R3[δ_{oop}(CH)(49)+ ν(C13C14)(3)] ν(C10O58)(4) ν(C14N)(4) ρ'(C24H_3)(4) δ(C17H)(3)
			δ(C3H)(11) ν(C27C28)(8) δ_{in}(N1C)(7) ρ'(C29H_3)(7) R1[ν(C62C64)(4)+δ_{tri}(3)] R2[ν(C4C6)(4)+ν(C4N)(4)] ν(C28C29)(4)
908.89	873.80		ν(C69C70)(4) ρ'(C68H_3)(3)
907.88	872.84	891	ν(C27C28)(20) ρ'(C29H_3)(17) ν(C28C29)(10) ρ(C29H_3)(5) δ(C3H)(4) δ_{sci}(C27H_2)(4) ν(C69C70)(3) ω(C28H_2)(3)
905.12	870.18		ν(C69C70)(21) ρ'(C68H_3)(18) ν(C68C69)(11) ρ(C68H_3)(6) δ(C3H)(5) δ_{sci}(C70C)(4) ω(C69H_2)(3) δ_{in}(N1C)(3)
883.05	848.97	868	R2[δ_{oop}(CH)(17)+δ_{oop}(C8O)(6)] δ_{in}(O58C)(8) δ(C17H)(7) ρ(C10O58)(6) ν(C10O58)(6) R4[ν(C18C19)(5)+δ_{tri}(5)] δ_{in}(N56C)(5)
879.89	845.93		ρ(C25H_2)(20) ρ(C27H_2)(19) ρ(C29H_3)(13) Υ(C26H_2)(9) Υ(C28H_2)(9) R4[δ_{oop}(C23H)](7) ρ(C26H_2)(5) Υ(C25H_2)(4) ρ'(C29H_3)(4)
869.70	836.13	846	R2[δ_{oop}(CH)(22)+δ_{oop}(C8O)(5)+ν(C8O)(5)+τ'$_a$(4)+ν(C7C8)(4)+δ_{oop}(C4N)(3)] R4[δ_{tri}(5)+ν(C18C19)(4)] δ_{in}(O58C)(3) δ(C17H)(3)
			R1[δ_{oop}(C66H)(24)+δ_{puc}(6)] ρ(C70H_2)(10) ρ(C73H_2)(10) ρ(C72H_2)(8) ρ(C74H_2)(6) ρ(C68H_3)(6) Υ(C71H_2)(4) Υ(C69H_2)(4)
862.26	828.98	839	Υ(C74H_2)(3)
851.91	819.03		R4[δ_{oop}(C23H)(45)+τ(C19O)(17)+δ_{puc}(13)+δ_{oop}(C22O)(4)+δ_{oop}(C19O)(5)]
851.09	818.24		R3[δ_{tri}(12)+δ_a(4)] R1[δ_{tri}(5)+ν(C62C64)(4)] R4[δ_{oop}(C23H)](5) ν(C13C24)(4) R2[δ'$_a$](3)
846.90	814.21		R1[δ_{oop}(C66H)(39)+τ(C64O)(13)+δ_{puc}(11)+δ_{oop}(C64O)(5)+δ_{oop}(C67O)(3)] ρ(C72H_2)(4) ρ(C73H_2)(4) ρ(C70H_2)(4)
833.84	801.65	814	R2[δ_{oop}(CH)(29)+δ_{oop}(C4N)(3)] R3[δ_{tri}(10)+δ'$_a$(4)] R1[τ(C64O)(8)+δ_{oop}(C66H)(5)] ν(C13C24)(4)
833.52	801.35		R4[τ(C19O)(41)+δ_{oop}(CH)(25)+δ_{puc}(11)+δ_{oop}(C22O)(6)+δ_{oop}(C19O)(5)]
828.57	796.59		R1[τ(C64O)(41)+δ_{oop}(CH)(16)+δ_{puc}(8)+C67O)(4)+δ_{oop}(C64O)(4)] R2[δ_{oop}(CH)](12)
824.76	792.93		R2[δ_{oop}(CH)](71) R1[τ(C64O)](3)
821.97	790.24		R3[δ_{oop}(CH)(30)+δ_{puc}(19)+δ_{oop}(C11C10)(9)+δ_{oop}(C14N)(5)+δ_{oop}(C13C24)(3)] δ_{oop}(C=O)((8)
814.18	782.76	787	R4[δ_{oop}(CH)(21)+τ_a(3)] R1[δ_{oop}(CH)](9) ρ(C10O58)(6) δ_{in}(O58C)(4) R2[δ_{tri}](3)
812.83	781.45		R4[δ_{oop}(CH)(45)+τa(7)+δ_{oop}(C22O)(4)+δ_{oop}(C18C17)(3)+δ_{oop}(C19O)(3)] R1[δ_{oop}(C65H)(7)+δ_{oop}(C63H)(3)]
810.77	779.47		R1[δ_{oop}(CH)(49)+τa(7)+δ_{oop}(C67O)(4)+δ_{oop}(C64O)(3)+δ_{oop}(C62C3)(3)] ρ(C10O58)(3)
791.13	760.60	764	ρ(C74H_2)(27) ρ(C71H_2)(16) ρ(C69H_2)(14) ρ(C73H_2)(9) ρ(C68H_3)(7) Υ(C72H_2)(4) Υ(C70H_2)(3) Υ(C73H_2)(3)
786.12	755.78		ρ(C26H_2)(35) ρ(C28H_2)(20) ρ(C25H_2)(10) ρ(C29H_3)(9) Υ(C27H_2)(5) Υ(C25H_2)(4)
777.87	747.84	748	R3[ν(CC)(11)+δ'a(7)] ν(C13C24)(10) R2[δ_{tri}(7)+ν(C8O)(6)] δ(C10O58)
764.77	735.25		R4[ν(CC)(22)+ δ'$_a$(15)+δ_{tri}(11)+ν(C19O)(7)+ν(C22O)(6)+δa(4)] δ(O59C)(3) δ_{sci}(C25C)(3)
764.02	734.53		R1[ν(CC)(20)+δ'$_a$(14)+δ_{tri}(13)+ν(C67O)(6)+ν(C64O)(6)] δ_{in}(O92C)(4) δ_{sci}(C73C)(3)
754.51	725.38		δ_{oop}(C10O58)(39) R3[δ_{oop}(CH)(29)+δ_{oop}(C11C10)(14)]
752.59	723.54		ρ(C72H_2)(29) ρ(C69H_2)(21) ρ(C74H_2)(14) ρ(C71H_2)(7) ρ(C70H_2)(6) ρ(C68H_3)(4)
745.19	716.42	723	ρ(C27H_2)(35) ρ(C28H_2)(33) ρ(C26H_2)(9) τ(C27C28)(6) ρ(C29H_3)(5) τ(C26C27)(4)
740.28	711.70		ρ(C70H_2)(29) ρ(C71H_2)(24) ρ(C69H_2)(16) ρ(C72H_2)(10) τ(C70C71)(5) τ(C69C70)(5) τ(C71C72)(4)
730.58	702.38		R2[δ_{puc}(40)+δ_{oop}(C4N)(10)+δ_{oop}(C8O)(9)] R1[δ_{puc}(9)+δ_{oop}(C64O)(4)+δ_{oop}(C62C3)(3)] R3[δ_{puc}](5)
728.29	700.18		R3[δ_{puc}(24)+δ_{oop}(C14N)(10)+δ_{oop}(C16H)(6)+δ_{oop}(C13C24)(5)] R4[δ_{puc}(14)+δ_{oop}(C19O)(6)+δ_{oop}(C18C17)(5)] R2[δ_{puc}](8) R1[δ_{puc}](3)

717.45	689.75	669	R4[δ_{puc}(32)+δ_{oop}(C19O)(14)+δ_{oop}(C18C17)(8)+δ_{oop}(C22O)(3)] R1[δ_{puc}(13)+δ_{oop}(C64O)(6)+δ_{oop}(C62C3)(3)] R3[δ_{puc}](5)
715.43	687.81		R1[δ_{puc}(30)+δ_{oop}(C64O)(13)+δ_{oop}(C62C3)(7)+(C67O)(3)] R2[δ_{puc}](10) R4[δ_{puc}(10)+δ_{oop}(C19O)(4)] R3[δ_{puc}](3)
684.41	657.99	656	R3[δ_a(12)+δ_{puc}(8)+δ'_a(7)] R2[δ_{puc}](8) δ(C17H)(6) R4[δ_a](5) δ(C10O58)(4)
658.79	633.37		R4[δ_{oop}(C22O)(35)+τ_a(19)+δ_{oop}(C19O)(19)+δ_{puc}(10)+τ'_a(7)+δ_{oop}(C20H)(5)]
658.16	632.76	638	R1[δ_{oop}(C67O)(35)+δ_{oop}(C64O)(19)+τ_a(19)+δ_{puc}(10)+τ'_a(7)+δ_{oop}(C63H)(5)]
652.90	627.70	627	R2[δ_a(40)+δ'_a(26)+δ_{in}(C4N)(5)+δ_{in}(C8O)(4)]
633.47	609.02	604	R1[δ_a](15) δ_s(C=O)(8) R2[δ_a(8)+δ'_a(6)] δ(C3H)(7) R3[δ_a](5) δ_{sci}(C73C)(4) δ_{in}(O92C)(4)
609.05	585.54	590	R4[δ_a(7)+δ_{in}(C18C17)(6)+δ'_a(5)+δ_{in}(C22O)(4)] R3[δ_{in}(C11C10)(8)+δ_{puc}(7)+τ_a(5)+ δ_{oop}(C14N)(4)] δ_{in}(N56C)(6) δ(O59C)(4)
608.15	584.67		R4[δ_{in}(CC)(21)+δ_a(8)+δ_{in}(C19O)(5)+δ_{in}(C22O)(3)] R3[δ'_a(8)+δ_{in}(C14N)(7)+ν(C14C15)(4)] δ(C17H)(7) ν(C13C24)(5)
597.51	574.44	579	R1[δ_{in}(C62C3)(21)+δ'_a(16)+δ_{in}(C67O)(12)+δ_{in}(C64O)(9)+ν(C62C63)(6)+ν(C64O)(3)] δ_{in}(N1C)(5) R2[δ_a](4) δ_{in}(O92C)(4)
573.86	551.71	536	R4[δ'_a](13) R3[τ_a(12)+δ_{oop}(C14N)(9)+δ_{oop}(C11C10)(6)+δ_{puc}(5)] R1[δ_a](3)
564.45	542.66		R3[τ_a(13)+δ_{oop}(C14N)(10)+δ_{puc}(9)+δ_{in}(C14N)(5)+δ_{in}(C13C24)(4)+δ_{oop}(C11C10)(4)+δ_a(4)] R2[δ'_a](4) R1[δ_a](4)
551.50	530.21		R2[δ_{oop}(C8O)(25)+τ'_a(21)+δ_{oop}(C4N)(20)+τ_a(6)]
539.71	518.87	517	R3[δ_a(20)+δ'_a(5)+τ_a(3)] R4[δ_{in}(C19O)(9)+δ_a(6)] δ_{sci}(C25C)(6)
536.88	516.16		R1[δ'_a(28)+δ_{in}(C67O)(11)+δ_{in}(C64O)(10)] δ_{in}(O92C)(9) δ_{sci}(C74C)(6)
532.25	511.70		R4[δ'_a(22)+δ_{in}(C22O)(7)+δ_{in}(C19O)(5)] δ(O59C)(6) δ_{in}(O92C)(5) R2[δ'_a](4) R3[δ_{in}(C14N)(4)
			δ(O59C)(10) R4[δ_{in}(C22O)(9)+δ'_a(8)+δ_{in}(C19O)(5)] R3[δ_{in}(C14N)(7)+δ_{in}(C11C10)(4)+δ_{in}(C13C24)(3)] R2[δ'_a](6) δ_{in}(O92C)(4)
527.52	507.16		δ_{sci}(C26H_2)(3)
503.60	484.16	501	R3[τ'_a(35)+δ_{oop}(C13C24)(16)+δ_{oop}(C11C10)(7)+δ_{puc}(4)+δ_{oop}(C16H)(4)]
498.93	479.67	494	R2[δ_{in}(C4N)(14)+δ_a(7)] R3[τ'_a(14)+δ_{oop}(C13C24)(7)] δ(C3H)(7) R1[δ_{in}(C62C3)(4)+δ_{oop}(C62C3)(3)+τ'_a(3)] δ_{in}(N1C)(4)
482.04	463.43		R1[δ_{in}(C64O)(14)+δ_a(10)] δ_{sci}(C72C)(13) δ_{sci}(C70C)(8) δ_{sci}(C69C)(8)
469.93	451.79		R1[τ'_a(27)+τ_a(11)+δ_{oop}(C62C3)(11)+δ_{oop}(C64O)(8)+δ_{oop}(C67O)(6)+δ_{oop}(C65H)(6)+δ_{puc}(3)] R4[τ'_a](5)
469.68	451.55		R4[τ'a(27)+τa(12)+δoop(C18C17)(11)+δoop(C19O)(8)+δoop(C22O)(6)+δoop(C21H)(6)+δpuc(4)] R1[τ'a](5)
461.15	443.35	461	R4[δ_{in}(C19O)(18)+δ_a(9)+τ'_a(6)] δ(C17H)(8) δ_{sci}(C27H_2)(7) R3[δ_a(5)+δ_{in}(C13C24)(4)] δ(O59C)(4)
			R4[δ_{in}(C18C17)(7)+δ_a(3)] R3[δ'_a(6)+δ_{in}(C13C24)(4)+δ_{in}(C11C10)(3)] δ_{sci}(C71C)(6) δ_{sci}(C26H2)(6) δ_{in}(N56C)(5) δ(O59C)(4)
446.05	428.83		δ_{sci}(C74C)(4) δ(C10O58)(3)
443.04	425.93		R1[δ_{in}(C64O)](15) δ_{sci}(C71C)(15) δ_{sci}(C69C)(12) δ_{sci}(C74C)(7) δ_{in}(O92C)(6) δ_{sci}(C72C)(4)
434.49	417.72		δ_{sci}(C28H_2)(23) R4[δ_{in}(C19O)](18) δ_{sci}(C26H_2)(8) δ_{sci}(C27H_2)(7) δ(O59C)(4) δ_{sci}(C25C)(4)
432.72	416.01		R2[τ_a(28)+δ_{oop}(CH)(10)+δ_{puc}(9)+δ_{oop}(C8O)(7)+δ_{in}(C8O)(4)] R1[τ'_a(5)+δ_{puc}(4)+δ_{in}(C64O)(3)] τ(C3N)(3)
427.83	411.32		R2[τ_a(43)+τ'_a(23)+δ_{oop}(CH)(12)+δ_{puc}(3)]
411.58	395.69		R3[δ_{in}(C13C24)(24)+δ'_a(6)] δ_s(C=O)(8) R2[δ_{in}(C8O)](7) ν(C10C)(4) R4[δ_a](3)
			δ_{sci}(C70C)(11) δ_{in}(O92C)(6) R3[δ'_a](5) R1[δ_{in}(C67O)(5)+δ_a(4)+δ_{in}(C64O)(3)] ν(C10C)(4) δ_{sci}(C71C)(4) R2[δ_{in}(C8O)](3) ν(C69C70)(3)
406.86	391.15		δ_{in}(N1C)(3) ν(C70C71)(3)
399.28	383.86		R4[δ_{oop}(C18C17)(21)+δ_{puc}(9)+τ(C17C)(7)+τ'_a(5)+δ_{oop}(C21H)(3)] τ(C17N)(9) R3[τ_a](7) R3[δ_{in}(C13C24)(3)
382.92	368.14		R2[δ_{in}(C8O)](19) R1[δ_{oop}(C62C3)(10)+τ(C3C)(3)] δ_s(C=O)(7) R4[δ_{oop}(C18C17)](5) R3[δ_{in}(C13C24)](3)
366.87	352.71		R1[δ_{oop}(C62C3)(23)+τ(C3C)(15)+τ_a(4)] R2[δ_{oop}(C4N)(8)+δ_{puc}(5)] δ_{in}(O58C)(5) τ(N1C4)(4)
			R4[τ(C17C)(14)+δ_{oop}(C18C17)(6)+δ_{in}(C18C17)(5)+δ_{in}(C22O)(3)] R3[δ_{in}(C14N)(8)+δ_{in}(C13C24)(6)+τ_a(6)] τ(C14N)(6) δ_{sci}(C26H_2)(3)
344.67	331.36		R2[δ_{in}(C8O)](3)
334.11	321.21		δ_{sci}(C69C)(26) δ_{sci}(C73C)(16) δ_{sci}(C72C)(12) R1[δ_{in}(C67O)(10)+δ_{in}(C64O)(5)] δ_{sci}(C71C)(7)
			δ_{sci}(C28H_2)(10) R4[δ_{in}(C22O)(10)+δ_{oop}(C18C17)(4)] δ_{sci}(C27H_2)(7) R3[τ_a(7)+δ_{oop}(C11C10)(4)+δ_{oop}(C13C24)(5)+τ'_a(4)] δ_{sci}(C26H_2)(7)
322.76	310.30		R4[τ(C17C)](6) δ_{sci}(C25C)(4) δ_{in}(N56C)(4)
307.69	295.81		R1[δ_{in}(C62C3)(7)+τ(C3C)(6)+δ_a(5)] R2[δ_{in}(C4N)](5) R3[δ_{in}(C13C24)](5) δ_{sci}(C28H_2)(4)
291.27	280.03		R3[δ_{in}(C11C10)](12) R1[δ_{in}(C62C3)](8) R2[δ_{oop}(C8O)](4) δ_{sci}(C28H_2)(3)
281.47	270.60		R1[τ(C3C)(13) +δ_{in}(C62C3)(4)+τ(C64O)(4)] R2[τ'_a](10) τ(N1C4)(6) R2[δ_{in}(C4N)(4)+τ_a(3)] δ_{in}(O58C)(4) R3[δ_{in}(C11C10)(4)
			R4[τ(C17C)(10)+τ_a(7)+τ(C19O)(6)+δ_{puc}(4)+δ_{in}(C18C17)(3)] δ_{sci}(C28H_2)(4) δ_{sci}(C25C)(4) R3[δ_{oop}(C13C24)(4)+δ_{in}(C11C10)(3)]
262.97	252.82		R1[δ_{in}(C62C3)(3)
253.90	244.10		R1[τ_a(13)+τ(C3C)(10)+δ_{puc}(9)+τ(C64O)(8)+δ_{oop}(C66H)(6)] R4[τ_a](5) τ(N1C4)(4) τ(C73O)(3)
250.49	240.83		τ(C28C29)(82) τ(C26C27)(3)
246.90	237.37		τ(C68C69)(90) τ(C70C71)(4)
244.22	234.79		R4[δ_{puc}(13)+τ_a(12)+δ_{oop}(C23H)(10)+τ'a(7)+τ(C19O)(7)+δ_{oop}(C19O)(3)] τC25O)(4) τ(C28C29)(3)
241.69	232.36		R3[δ_{oop}(C13C24)(8)+δ_{oop}(C11C10)(7)+τ'_a(6)+δ_{oop}(C14N)(6)] R4[δ_{in}(C18C17)](7) R1[τ_a(7)+δ_{puc}(6)+δ_{oop}(C66H)(5)+τ'_a(4)] R2[τ'_a](3)
229.59	220.73		R4[τ'_a(30)+τ(C17C)(12)+τ_a(9)+δ_{puc}(6)+δ_{oop}(C23H)(5)+δ_{oop}(C18C17)(5)] R1[τ'_a(7)+τ(C3C)(3)] τ(C14N)(3)
227.73	218.94		R1[τ'_a(29)+τ(C3C)(13)+τ_a(11)+δ_{oop}(C62C3)(5)+δ_{puc}(5)+δ_{oop}(C66H)(4)] R4[τ'_a(5)+τ_a(3)] τ(C67O)(4)
221.07	212.54		δ_{sci}(C70C)(17) δ_{sci}(C74C)(16) R1[δ_{in}(C67O)](11) δ_{sci}(C69C)(10) δ_{sci}(C72C)(3)
198.22	190.57		R3[τ_a(36)+δ_{oop}(C11C10)(9)+δ_{oop}(C12H)(4)] R4[δ_{in}(C18C17)(6)+τ(C17C)(3)] δ_{sci}(C27H2)(5) δ(O59C)(4)
193.89	186.40		R4[δ_a](5) δ_{sci}(C72C)(5) ν(C73C74)(4) δ_{sci}(C69C)(4) δ_{sci}(C73C)(4) ν(C72C74)(4) R2[δ'_a](4) δ_{sci}(C28H_2)(3)
179.21	172.29		τ(C73C74)(11) τ(C67O)(11) τ(C22O)(6) τ(C71C72)(5) R1[τ_a](5) R4[τ_a](4) τ(C25C26)(4) R2[τ'_a](4) R3[δ_{in}(C11C10)](3)
176.75	169.92		τ(C24C)(80) δ'_a(C24H3)(7)
170.80	164.21		τ(C73C74)(15) τ(C71C72)(12) τ(C22O)(11) τ(C25C26)(10) τ(C67O)(7) τ(C69C70)(5)
			δ_{sci}(C27H_2)(8) τ(C71C72)(7) τ(C73C74)(7) δ_{sci}(C28H_2)(5) R2[τ'_a](5) R4[δ_{in}(C22O)](4) δ_{sci}(C26H2)(4) ρ(C10O58)(3) δ(O59C)(3)
166.86	160.42		δ_{sci}(C73C)(3)
161.97	155.72		τ(C25C26)(19) τ(C22O)(12) τ(C27C28)(7) τ(C26C27)(5) R4[τ'_a](3)
156.68	150.64		τ(C72C74)(30) τ(C69C70)(17) τ(C71C72)(15) τ(C67O)(12) τ(C70C71)(7) τ(C73O)(5) R1[τ'_a](3)
146.69	141.03		δ_{sci}(C27H_2)(12) δ(O59C)(6) δ_{in}(N56C)(6) R4[δ_{in}(C22O)(4)+δ_a(4)] R3[τ'_a](4) δ_{sci}(C73C)(3) δ_{sci}(C26H_2)(3)
138.31	132.97		τ(C26C27)(26) τC25O)(23) τ(C27C28)(18) R4[τ(C19O)](5) τ(C28C29)(3)
			τ(C67O)(12) τ(C73O)(9) τ(C69C70)(6) τ(C70C71)(6) τ(C27C28)(5) τ(C72C74)(5) R1[τ(C64O)(6)+τ_a(4)+δ_{oop}(C62C3)(4)] R2[τ'_a](4)
132.28	127.17		R4[τ_a](3)
130.42	125.39		τ(C27C28)(12) R4[τ_a](10) R3[τ'_a](6) τ(C14N)(4) R4[τ(C19O)](4) τ(C22O)(4) τ(C17N)(4)
114.83	110.39		τ(C70C71)(16) τ(C67O)(8) δ_{sci}(C71C)(6) δ_{sci}(C70C)(5) R1[τ_a](4) δ_{in}(O92C)(4)
109.73	105.49		τ(C69C70)(27) τ(C70C71)(18) τ(C73C74)(11) τ(C73O)(10) τ(C71C72)(6) τ(C67O)(5)

104.64	100.60	δ_{sci}(C71C)(7) R1[τa](6) δ_{sci}(C70C)(6) δ_{in}(O92C)(4) τ(C10O)(4) R2[τ'$_a$](4) τ(C73C74)(4) δ_{sci}(C72C)(3) τ(C69C70)(3)
100.22	96.35	τ(C22O)(10) R3[τ'$_a$](9) τC25O)(8) τ(C27C28)(5) τ(C24C)(5) R1[τ$_a$](5) R4[δ_{oop}(C18C17)](4) τ(C26C27)(4)
88.65	85.22	τ(C22O)(9) R2[τ(C8O)](8) τ(C26C27)(6) τC25O)(5) δ_{in}(N56C)(5) δ_{in}(N1C)(4) τ(C27C28)(4) δ_{in}(O58C)(3) R1[τ(C3C)](3)
76.26	73.32	R2[τ(C8O)](14) δ_{sci}(C72C)(7) δ_{sci}(C71C)(6) δ(C3H)(5) R1[δ_{in}(C62C3)](5) δ_{sci}(C70C)(4)
75.19	72.29	τ(C26C27)(11) R4[τ$_a$(9)+τ(C19O)(8)+τ(C17C)(4)] τ(C22O)(5) R2[τ(C8O)](3) τ(C73O)(3)
63.00	60.57	τ(C73O)(13) τ(C67O)(12) R2[τ(C8O)](9) τ(C3N)(6) τ(C10C)(5) τ(C71C72)(4) R1[δ_{oop}(C62C3)](4) τ(C70C71)(4) τ(C26C27)(3)
		δ_{sci}(C26H$_2$)(6) R2[τ(C8O)](6) τ(C25C26)(6) δ_{sci}(C25C)(5) τ(C67O)(5) τ(C10C)(4) δ_{in}(N56C)(4) τ(C73O)(4) τ(C27C28)(4) δ(O59C)(4)
58.84	56.57	R1[τ(C3C)](3) τ(N1C4)(3)
54.02	51.93	τ(C25C26)(16) τ(C26C27)(13) τC25O)(10) τ(C27C28)(9) τ(C24C)(5) τ(C10C)(5) R2[τ(C8O)](4)
51.22	49.24	τ(C73C74)(15) τ(N1C4)(14) τ(C72C74)(14) τ(C71C72)(11) τ(C67O)(8) τ(C70C71)(6) R2[τ(C8O)](5) τ(C69C70)(4)
		τ(N1C4)(18) R2[τ(C8O)](15) δ_{in}(O58C)(6) τ(C17N)(5) τC25O)(5) R4[τ(C17C)(5)+δ_{oop}(C18C17)(5)] R1[τ(C3C)](4) R2[δ_{in}(C8O)](4)
44.92	43.18	τ(C10C)(3)
44.34	42.63	R2[τ(C8O)](29) τ(C10C)(12) δ_{in}(O58C)(4) δ_{in}(N1C)(4) τ(N1C4)(4) R4[τ(C17C)](3)
		τ(C10O)(13) τ(N1C4)(9) τ(C72C74)(6) R1[δ_{oop}(C62C3)(5)+τ$_a$(4)] τ(C14N)(4) τ(C17N)(4) τ(C70C71)(4) R4[δ_{oop}(C18C17)](3)
39.60	38.07	τ(C3N)(3)
36.39	34.99	R2[τ(C8O)](22) τ(C10C)(15) τ(C24C)(8) τ(N1C4)(7) R1[τ(C3C)](3) δ_{sci}(C74C)(3)
		τ(C14N)(14) τC25O)(7) τ(C3N)(7) τ(C22O)(6) τ(C17N)(6) R1[δ_{oop}(C62C3)](5) τ(C72C74)(5) τ(C73O)(4) δ_{in}(O58C)(3)
28.32	27.23	R4[δ_{oop}(C18C17)](3)
26.67	25.64	R2[τ(C8O)](26) τ(C10C)(24) τ(C24C)(11) R2[δ_{in}(C8O)](5) δ_{in}(O58C)(4) τ(C14N)(3)
21.01	20.20	R2[τ(C8O)](30) δ_{in}(O58C)(7) τC25O)(4) δ_{sci}(C74C)(4) δ_{sci}(C73C)(4) δ_{in}(N56C)(4) τ(C22O)(4) δ_{in}(O92C)(3)
17.10	16.44	τ(C10C)(34) τ(C24C)(16) τ(C10O)(6) τ(C67O)(5) τ(C73O)(4) τ(C22O)(3) τ(C14N)(3)
14.80	14.23	τ(C10C)(13) R2[τ(C8O)](10) τ(C73O)(9) τC25O)(7) τ(C22O)(7) τ(C24C)(6) τ(C67O)(6) τ(C14N)(3)
10.71	10.30	τ(C10C)(26) τ(C10O)(12) τ(C73O)(9) τ(C72C74)(7) τ(C14N)(6) τ(C17N)(3) τ(C73C74)(3)
7.07	6.80	τ(C10C)(25) R2[τ(C8O)](18) δ_{in}(O58C)(12) R2[δ_{in}(C8O)](9)
6.50	6.25	τ(C10C)(21) τ(C73O)(13) τ(C24C)(12) τ(C67O)(5) τC25O)(5) τ(C10O)(5) τ(C3N)(4) τ(C14N)(3) R1[δ_{oop}(C62C3)](3)

Proposed assignment and potential energy distribution (PED) for vibrational normal modes.

Types of vibrations: ν, stretching; δ, deformation(bending); oop, out-of-plane bending; ρ, rocking; τ, torsion; ϒ, twisting; ω, wagging.

[a] Potential energy distribution (contribution ≥ 3)