

Supporting information

Resonance Raman spectra of β -carotene in solution and in photosystems revisited: An experimental and theoretical study

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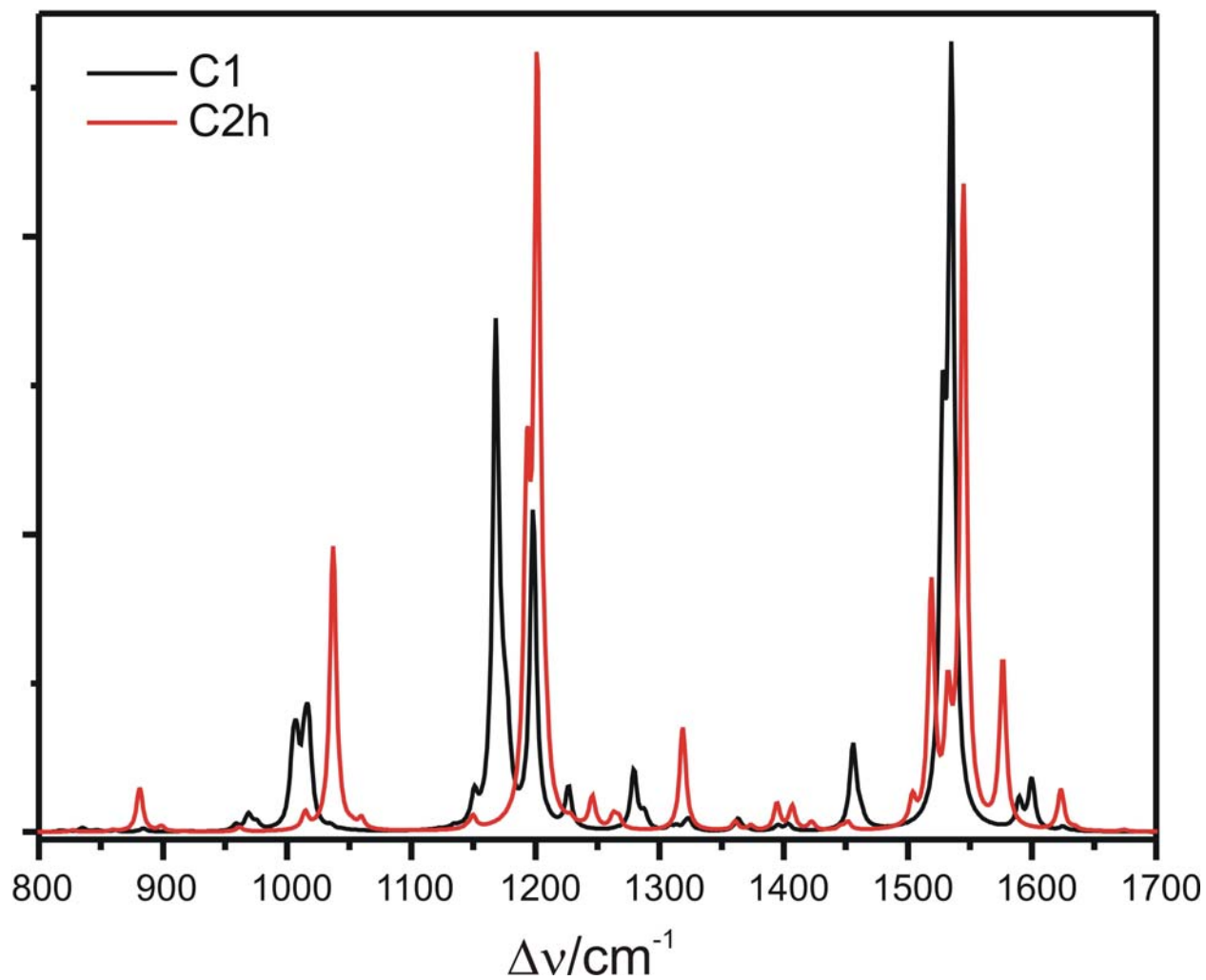


Fig. S1. Raman spectra of β -carotene calculated for the unconstrained and the C_{2h} -constrained structure.

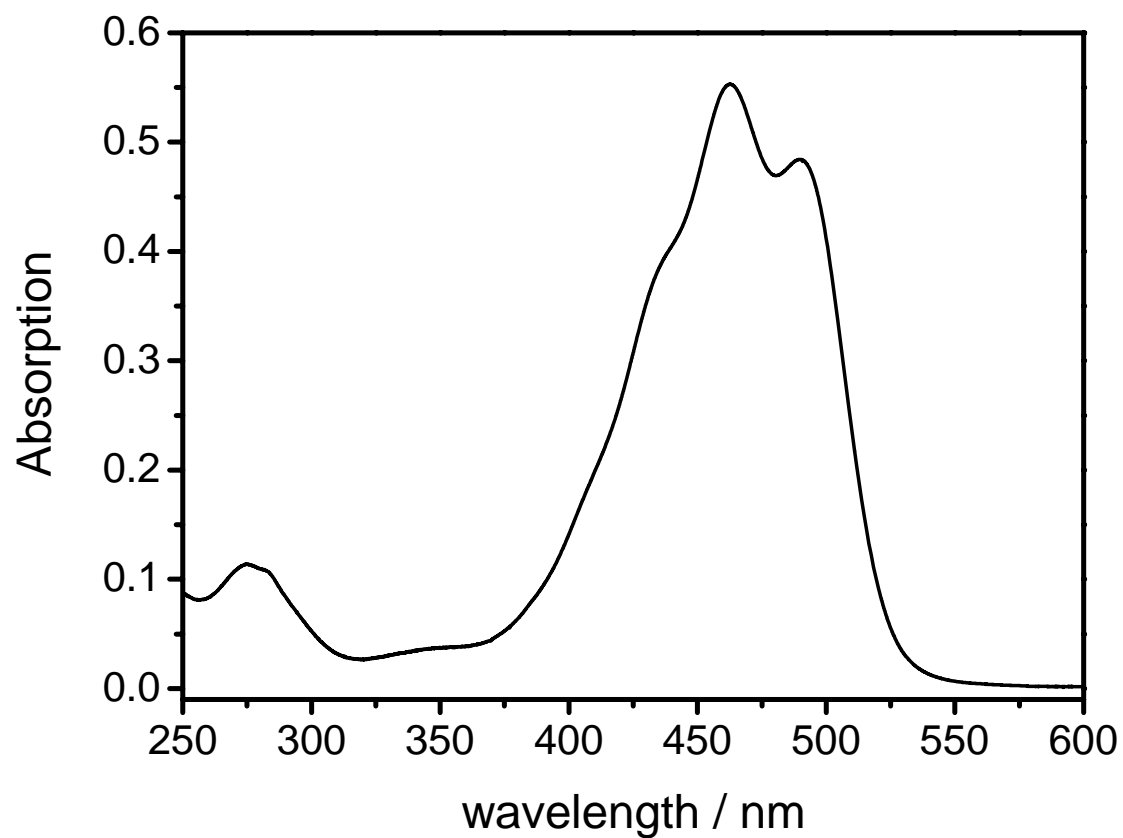


Fig. S2. Absorption spectrum of β -carotene in dichloromethane solution.

Table S1. Calculated normal modes, Raman (I_{Ra}) and IR intensities (I_{IR}) of β -carotene in its fully relaxed geometry. For numbering of the atoms, see Fig. 1.

mode No.	ν [cm^{-1}]	I_{IR} [km/mol]	I_{Ra} (rel.)	potential energy distribution			
1	3058.46	35.20	0.00	(95.74%)	(52)	C - H	STRE (24,76)
2	3057.51	33.78	0.00	(95.74%)	(20)	C - H	STRE (11,57)
3	3041.71	33.65	0.00	(6.28%)	(57)	C - H	STRE (27,78)
				(91.88%)	(59)	C - H	STRE (28,79)
4	3039.74	103.47	0.00	(41.79%)	(43)	C - H	STRE (19,72)
				(43.69%)	(45)	C - H	STRE (20,73)
				(5.03%)	(75)	C - H	STRE (35,83)
				(5.70%)	(80)	C - H	STRE (36,87)
5	3032.69	0.02	0.00	(40.50%)	(43)	C - H	STRE (19,72)
				(37.71%)	(45)	C - H	STRE (20,73)
				(9.81%)	(75)	C - H	STRE (35,83)
				(10.13%)	(80)	C - H	STRE (36,87)
6	3031.28	37.80	0.00	(12.77%)	(13)	C - H	STRE (7,54)
				(80.55%)	(15)	C - H	STRE (8,55)
7	3026.29	19.74	0.00	(86.88%)	(57)	C - H	STRE (27,78)
				(5.98%)	(59)	C - H	STRE (28,79)
8	3021.09	15.60	0.00	(63.05%)	(13)	C - H	STRE (7,54)
				(22.80%)	(23)	C - H	STRE (12,59)
				(5.43%)	(34)	C - H	STRE (15,67)
9	3017.82	30.27	0.00	(9.12%)	(13)	C - H	STRE (7,54)
				(10.83%)	(15)	C - H	STRE (8,55)
				(61.77%)	(23)	C - H	STRE (12,59)
				(9.93%)	(34)	C - H	STRE (15,67)
10	3017.64	3.41	0.00	(6.06%)	(45)	C - H	STRE (20,73)
				(22.70%)	(75)	C - H	STRE (35,83)
				(42.56%)	(80)	C - H	STRE (36,87)
				(13.47%)	(84)	C - H	STRE (37,90)
11	3017.41	6.01	0.00	(26.86%)	(84)	C - H	STRE (37,90)
				(52.21%)	(86)	C - H	STRE (38,42)
12	3017.30	28.81	0.00	(47.37%)	(84)	C - H	STRE (37,90)
				(35.27%)	(86)	C - H	STRE (38,42)
13	3016.65	5.55	0.00	(7.29%)	(13)	C - H	STRE (7,54)
				(39.64%)	(34)	C - H	STRE (15,67)
				(17.35%)	(75)	C - H	STRE (35,83)
				(14.36%)	(80)	C - H	STRE (36,87)
14	3016.48	2.64	0.00	(5.10%)	(13)	C - H	STRE (7,54)
				(33.33%)	(34)	C - H	STRE (15,67)
				(7.00%)	(43)	C - H	STRE (19,72)
				(27.83%)	(75)	C - H	STRE (35,83)
				(11.89%)	(80)	C - H	STRE (36,87)
15	3010.33	0.74	0.00	(26.78%)	(38)	C - H	STRE (16,70)

				(11.88%)	(41)	C	-	H	STRE	(18,71)
				(15.21%)	(47)	C	-	H	STRE	(21,74)
				(37.02%)	(50)	C	-	H	STRE	(23,75)
16	3009.32	126.38	0.00	(41.52%)	(38)	C	-	H	STRE	(16,70)
				(9.15%)	(41)	C	-	H	STRE	(18,71)
				(5.95%)	(47)	C	-	H	STRE	(21,74)
				(30.85%)	(50)	C	-	H	STRE	(23,75)
17	3003.49	0.18	0.00	(12.56%)	(18)	C	-	H	STRE	(10,56)
				(15.04%)	(41)	C	-	H	STRE	(18,71)
				(30.23%)	(47)	C	-	H	STRE	(21,74)
				(36.04%)	(54)	C	-	H	STRE	(25,77)
18	3002.72	5.57	0.00	(42.54%)	(18)	C	-	H	STRE	(10,56)
				(23.06%)	(41)	C	-	H	STRE	(18,71)
				(5.61%)	(47)	C	-	H	STRE	(21,74)
				(24.53%)	(54)	C	-	H	STRE	(25,77)
19	3001.30	0.36	0.00	(18.48%)	(18)	C	-	H	STRE	(10,56)
				(9.87%)	(38)	C	-	H	STRE	(16,70)
				(5.25%)	(41)	C	-	H	STRE	(18,71)
				(21.33%)	(47)	C	-	H	STRE	(21,74)
				(20.52%)	(50)	C	-	H	STRE	(23,75)
				(23.42%)	(54)	C	-	H	STRE	(25,77)
20	3000.60	16.64	0.00	(16.04%)	(18)	C	-	H	STRE	(10,56)
				(18.25%)	(38)	C	-	H	STRE	(16,70)
				(32.08%)	(41)	C	-	H	STRE	(18,71)
				(18.10%)	(47)	C	-	H	STRE	(21,74)
				(7.89%)	(50)	C	-	H	STRE	(23,75)
				(5.03%)	(54)	C	-	H	STRE	(25,77)
21	2988.44	43.91	0.00	(7.44%)	(26)	C	-	H	STRE	(13,61)
				(63.99%)	(31)	C	-	H	STRE	(14,65)
				(19.58%)	(32)	C	-	H	STRE	(14,66)
22	2987.33	56.45	0.00	(47.75%)	(90)	C	-	H	STRE	(39,91)
				(40.52%)	(91)	C	-	H	STRE	(39,92)
				(8.39%)	(96)	C	-	H	STRE	(40,96)
23	2987.15	34.01	0.00	(58.72%)	(26)	C	-	H	STRE	(13,61)
				(28.34%)	(27)	C	-	H	STRE	(13,62)
				(9.07%)	(31)	C	-	H	STRE	(14,65)
24	2983.39	34.40	0.00	(7.25%)	(91)	C	-	H	STRE	(39,92)
				(30.07%)	(95)	C	-	H	STRE	(40,95)
				(56.89%)	(96)	C	-	H	STRE	(40,96)
25	2975.64	107.61	0.01	(17.98%)	(90)	C	-	H	STRE	(39,91)
				(23.73%)	(91)	C	-	H	STRE	(39,92)
				(36.32%)	(92)	C	-	H	STRE	(39,93)
				(12.38%)	(94)	C	-	H	STRE	(40,94)
				(8.21%)	(95)	C	-	H	STRE	(40,95)
26	2974.66	151.67	0.01	(6.08%)	(26)	C	-	H	STRE	(13,61)
				(26.51%)	(27)	C	-	H	STRE	(13,62)
				(32.75%)	(28)	C	-	H	STRE	(13,63)
				(14.98%)	(30)	C	-	H	STRE	(14,64)
				(17.37%)	(32)	C	-	H	STRE	(14,66)
27	2971.17	17.19	0.00	(7.83%)	(90)	C	-	H	STRE	(39,91)
				(8.99%)	(92)	C	-	H	STRE	(39,93)

				(47.46%) (94) C - H STRE (40,94)
				(22.18%) (95) C - H STRE (40,95)
				(8.89%) (96) C - H STRE (40,96)
28	2970.46	9.68	0.00	(6.02%) (26) C - H STRE (13,61)
				(11.38%) (27) C - H STRE (13,62)
				(17.37%) (28) C - H STRE (13,63)
				(26.36%) (30) C - H STRE (14,64)
				(35.45%) (32) C - H STRE (14,66)
29	2955.89	30.44	0.00	(44.71%) (78) C - H STRE (36,85)
				(45.82%) (79) C - H STRE (36,86)
30	2955.80	7.85	0.01	(45.33%) (74) C - H STRE (35,82)
				(45.21%) (76) C - H STRE (35,84)
31	2953.50	17.03	0.01	(44.49%) (82) C - H STRE (37,88)
				(55.55%) (83) C - H STRE (37,89)
32	2953.10	17.98	0.01	(55.60%) (35) C - H STRE (15,68)
				(44.45%) (36) C - H STRE (15,69)
33	2948.69	72.94	0.01	(43.79%) (66) C - H STRE (32,46)
				(47.69%) (67) C - H STRE (32,47)
34	2948.34	53.67	0.01	(5.56%) (1) C - H STRE (2,48)
				(47.71%) (4) C - H STRE (3,50)
				(41.49%) (5) C - H STRE (3,51)
35	2933.01	95.15	0.01	(62.36%) (22) C - H STRE (12,58)
				(25.98%) (24) C - H STRE (12,60)
36	2932.73	105.35	0.01	(15.66%) (67) C - H STRE (32,47)
				(63.39%) (69) C - H STRE (33,80)
				(16.32%) (70) C - H STRE (33,81)
37	2931.78	91.72	0.01	(15.75%) (1) C - H STRE (2,48)
				(56.72%) (2) C - H STRE (2,49)
				(17.22%) (5) C - H STRE (3,51)
38	2929.44	44.56	0.01	(44.19%) (87) C - H STRE (38,43)
				(55.59%) (88) C - H STRE (38,44)
39	2917.26	67.14	0.01	(5.60%) (1) C - H STRE (2,48)
				(9.34%) (2) C - H STRE (2,49)
				(20.85%) (4) C - H STRE (3,50)
				(20.92%) (5) C - H STRE (3,51)
				(32.85%) (7) C - H STRE (4,52)
40	2915.01	35.03	0.01	(6.35%) (63) C - H STRE (31,41)
				(24.86%) (66) C - H STRE (32,46)
				(17.18%) (67) C - H STRE (32,47)
				(7.42%) (69) C - H STRE (33,80)
				(5.80%) (70) C - H STRE (33,81)
				(12.13%) (92) C - H STRE (39,93)
				(7.45%) (94) C - H STRE (40,94)
				(6.62%) (95) C - H STRE (40,95)
41	2914.67	49.21	0.01	(10.33%) (26) C - H STRE (13,61)
				(14.78%) (27) C - H STRE (13,62)
				(23.13%) (28) C - H STRE (13,63)
				(21.59%) (30) C - H STRE (14,64)
				(9.60%) (31) C - H STRE (14,65)

				(10.64%)	(32)	C	-	H	STRE	(14,66)
42	2913.93	59.16	0.01	(15.20%)	(66)	C	-	H	STRE	(32,46)
				(14.11%)	(67)	C	-	H	STRE	(32,47)
				(5.82%)	(92)	C	-	H	STRE	(39,93)
				(18.59%)	(94)	C	-	H	STRE	(40,94)
				(18.72%)	(95)	C	-	H	STRE	(40,95)
				(11.89%)	(96)	C	-	H	STRE	(40,96)
43	2912.65	1.61	0.01	(17.18%)	(74)	C	-	H	STRE	(35,82)
				(17.27%)	(76)	C	-	H	STRE	(35,84)
				(28.89%)	(78)	C	-	H	STRE	(36,85)
				(28.04%)	(79)	C	-	H	STRE	(36,86)
				(5.20%)	(80)	C	-	H	STRE	(36,87)
44	2912.35	94.17	0.00	(28.35%)	(74)	C	-	H	STRE	(35,82)
				(5.25%)	(75)	C	-	H	STRE	(35,83)
				(28.50%)	(76)	C	-	H	STRE	(35,84)
				(17.54%)	(78)	C	-	H	STRE	(36,85)
				(17.02%)	(79)	C	-	H	STRE	(36,86)
45	2910.54	73.48	0.03	(50.51%)	(82)	C	-	H	STRE	(37,88)
				(38.63%)	(83)	C	-	H	STRE	(37,89)
				(8.02%)	(84)	C	-	H	STRE	(37,90)
46	2910.06	149.62	0.01	(7.64%)	(34)	C	-	H	STRE	(15,67)
				(36.78%)	(35)	C	-	H	STRE	(15,68)
				(48.18%)	(36)	C	-	H	STRE	(15,69)
47	2909.83	8.65	0.00	(9.64%)	(26)	C	-	H	STRE	(13,61)
				(13.29%)	(27)	C	-	H	STRE	(13,62)
				(22.90%)	(28)	C	-	H	STRE	(13,63)
				(25.01%)	(30)	C	-	H	STRE	(14,64)
				(9.47%)	(31)	C	-	H	STRE	(14,65)
				(11.49%)	(32)	C	-	H	STRE	(14,66)
48	2908.95	16.27	0.00	(14.82%)	(90)	C	-	H	STRE	(39,91)
				(15.80%)	(91)	C	-	H	STRE	(39,92)
				(35.39%)	(92)	C	-	H	STRE	(39,93)
				(12.70%)	(94)	C	-	H	STRE	(40,94)
				(10.76%)	(95)	C	-	H	STRE	(40,95)
				(7.43%)	(96)	C	-	H	STRE	(40,96)
49	2905.73	11.77	0.00	(26.33%)	(4)	C	-	H	STRE	(3,50)
				(13.26%)	(5)	C	-	H	STRE	(3,51)
				(50.62%)	(7)	C	-	H	STRE	(4,52)
50	2897.60	33.95	0.01	(70.98%)	(63)	C	-	H	STRE	(31,41)
				(8.75%)	(66)	C	-	H	STRE	(32,46)
				(6.24%)	(87)	C	-	H	STRE	(38,43)
				(5.57%)	(88)	C	-	H	STRE	(38,44)
51	2892.13	36.28	0.01	(23.61%)	(22)	C	-	H	STRE	(12,58)
				(5.27%)	(23)	C	-	H	STRE	(12,59)
				(57.23%)	(24)	C	-	H	STRE	(12,60)
52	2892.06	56.30	0.01	(8.83%)	(63)	C	-	H	STRE	(31,41)
				(5.45%)	(86)	C	-	H	STRE	(38,42)
				(42.79%)	(87)	C	-	H	STRE	(38,43)
				(31.22%)	(88)	C	-	H	STRE	(38,44)
53	2891.58	30.41	0.00	(66.57%)	(1)	C	-	H	STRE	(2,48)

				(24.52%)	(2)	C - H	STRE	(2,49)
54	2890.94	38.73	0.00	(22.61%)	(69)	C - H	STRE	(33,80)
				(72.13%)	(70)	C - H	STRE	(33,81)
55	2862.33	57.79	0.02	(7.45%)	(63)	C - H	STRE	(31,41)
				(90.86%)	(64)	C - H	STRE	(31,45)
56	2859.04	34.40	0.02	(94.62%)	(8)	C - H	STRE	(4,53)
57	1633.51	6.25	0.07	(7.59%)	(12)	C = C	STRE	(6, 5)
				(6.77%)	(16)	C = C	STRE	(8, 7)
				(14.66%)	(60)	C = C	STRE	(28,27)
				(25.90%)	(62)	C = C	STRE	(30,29)
				(5.53%)	(202)	secd XY, C84-	H39	ROCK
58	1632.59	41.86	0.01	(25.29%)	(12)	C = C	STRE	(6, 5)
				(16.69%)	(16)	C = C	STRE	(8, 7)
				(5.23%)	(60)	C = C	STRE	(28,27)
				(13.72%)	(62)	C = C	STRE	(30,29)
				(6.04%)	(131)	secd XY, C63-	H14	ROCK
59	1624.85	0.68	0.52	(11.20%)	(12)	C = C	STRE	(6, 5)
				(6.39%)	(39)	C = C	STRE	(16,11)
				(8.77%)	(46)	C = C	STRE	(20,19)
				(8.03%)	(53)	C = C	STRE	(24,23)
				(9.30%)	(62)	C = C	STRE	(30,29)
60	1618.85	1.54	0.01	(7.23%)	(19)	C = C	STRE	(10, 9)
				(7.95%)	(42)	C = C	STRE	(18,17)
				(7.50%)	(49)	C = C	STRE	(22,21)
				(6.21%)	(56)	C = C	STRE	(26,25)
61	1607.97	19.70	0.02	(9.21%)	(12)	C = C	STRE	(6, 5)
				(5.73%)	(16)	C = C	STRE	(8, 7)
				(9.59%)	(42)	C = C	STRE	(18,17)
				(9.79%)	(49)	C = C	STRE	(22,21)
				(6.79%)	(60)	C = C	STRE	(28,27)
				(7.84%)	(62)	C = C	STRE	(30,29)
62	1599.70	2.92	6.89	(9.02%)	(12)	C = C	STRE	(6, 5)
				(13.79%)	(16)	C = C	STRE	(8, 7)
				(5.01%)	(46)	C = C	STRE	(20,19)
				(14.22%)	(60)	C = C	STRE	(28,27)
				(7.37%)	(62)	C = C	STRE	(30,29)
63	1589.63	0.04	3.90	(18.84%)	(19)	C = C	STRE	(10, 9)
				(8.68%)	(46)	C = C	STRE	(20,19)
				(18.37%)	(56)	C = C	STRE	(26,25)
64	1576.53	71.55	0.03	(7.48%)	(19)	C = C	STRE	(10, 9)
				(6.56%)	(42)	C = C	STRE	(18,17)
				(6.38%)	(49)	C = C	STRE	(22,21)
				(7.44%)	(56)	C = C	STRE	(26,25)
65	1571.54	57.97	0.00	(11.76%)	(19)	C = C	STRE	(10, 9)
				(13.09%)	(39)	C = C	STRE	(16,11)
				(13.11%)	(53)	C = C	STRE	(24,23)
				(12.59%)	(56)	C = C	STRE	(26,25)
66	1535.07	0.76	100.00	(11.62%)	(39)	C = C	STRE	(16,11)
				(20.28%)	(46)	C = C	STRE	(20,19)
				(11.73%)	(53)	C = C	STRE	(24,23)

				(5.19%) (143)secd XY, C67- H17 ROCK
				(9.44%) (175)secd XY, C75- H32 ROCK
				(9.51%) (178)secd XY, C76- H33 ROCK
				(5.27%) (190)secd XY, C80- H36 ROCK
67	1527.99	0.11	47.28	(22.36%) (42) C = C STRE (18,17) (22.66%) (49) C = C STRE (22,21)
68	1492.27	1.28	0.03	(9.84%) (114)ring sXY2, X= C58 SCIS (72.36%) (118)ring sXY2, X= C59 SCIS (8.87%) (122)ring sXY2, X= C60 SCIS
69	1491.80	2.46	0.03	(7.42%) (208)ring sXY2, X= C87 SCIS (76.12%) (212)ring sXY2, X= C88 SCIS (8.71%) (216)ring sXY2, X= C89 SCIS
70	1485.33	6.05	0.01	(64.14%) (114)ring sXY2, X= C58 SCIS (5.09%) (118)ring sXY2, X= C59 SCIS (16.89%) (157)prim XY3 , X= C70 ADEFb
71	1483.09	4.47	0.01	(5.28%) (212)ring sXY2, X= C88 SCIS (64.89%) (216)ring sXY2, X= C89 SCIS (14.60%) (246)prim XY3 , X= C95 ADEFb (5.33%) (251)prim XY3 , X= C96 ADEFb
72	1475.63	7.79	0.07	(7.20%) (212)ring sXY2, X= C88 SCIS (12.60%) (246)prim XY3 , X= C95 ADEFb (53.50%) (250)prim XY3 , X= C96 ADEFa (10.56%) (251)prim XY3 , X= C96 ADEFb
73	1473.35	4.98	0.02	(8.07%) (114)ring sXY2, X= C58 SCIS (6.72%) (118)ring sXY2, X= C59 SCIS (33.68%) (152)prim XY3 , X= C69 ADEFb (37.20%) (156)prim XY3 , X= C70 ADEFa
74	1472.33	2.30	0.03	(6.83%) (216)ring sXY2, X= C89 SCIS (36.23%) (245)prim XY3 , X= C95 ADEFa (24.15%) (250)prim XY3 , X= C96 ADEFa (19.64%) (251)prim XY3 , X= C96 ADEFb
75	1469.28	5.60	0.03	(6.63%) (114)ring sXY2, X= C58 SCIS (11.26%) (122)ring sXY2, X= C60 SCIS (42.30%) (151)prim XY3 , X= C69 ADEFa (5.39%) (156)prim XY3 , X= C70 ADEFa (21.95%) (157)prim XY3 , X= C70 ADEFb
76	1466.90	4.71	0.13	(9.52%) (118)ring sXY2, X= C59 SCIS (65.78%) (122)ring sXY2, X= C60 SCIS (5.57%) (157)prim XY3 , X= C70 ADEFb
77	1465.08	16.21	0.02	(7.86%) (161)prim XY3 , X= C71 ADEFa (16.05%) (208)ring sXY2, X= C87 SCIS (20.38%) (225)prim XY3 , X= C91 ADEFa (19.53%) (230)prim XY3 , X= C92 ADEFa (12.87%) (235)prim XY3 , X= C93 ADEFa
78	1464.76	11.59	0.08	(55.03%) (208)ring sXY2, X= C87 SCIS (5.88%) (216)ring sXY2, X= C89 SCIS (6.68%) (225)prim XY3 , X= C91 ADEFa (6.69%) (230)prim XY3 , X= C92 ADEFa (9.32%) (241)prim XY3 , X= C94 ADEFb
79	1462.04	0.19	1.41	(16.60%) (161)prim XY3 , X= C71 ADEFa

				(8.43%) (230)prim XY3 , X= C92 ADEFa
				(55.88%) (235)prim XY3 , X= C93 ADEFa
80	1461.51	1.13	0.19	(50.00%) (161)prim XY3 , X= C71 ADEFa
				(16.29%) (225)prim XY3 , X= C91 ADEFa
				(8.28%) (230)prim XY3 , X= C92 ADEFa
				(7.99%) (235)prim XY3 , X= C93 ADEFa
81	1459.74	25.53	0.05	(10.93%) (146)prim XY3 , X= C68 ADEFa
				(77.48%) (147)prim XY3 , X= C68 ADEFb
				(6.28%) (149)prim XY3 , X= C68 ROCKb
82	1457.60	1.25	0.00	(53.45%) (246)prim XY3 , X= C95 ADEFb
				(5.44%) (250)prim XY3 , X= C96 ADEFa
				(18.56%) (251)prim XY3 , X= C96 ADEFb
83	1456.98	14.93	0.32	(6.61%) (208)ring sXY2, X= C87 SCIS
				(8.08%) (240)prim XY3 , X= C94 ADEFa
				(63.12%) (241)prim XY3 , X= C94 ADEFb
				(5.27%) (243)prim XY3 , X= C94 ROCKb
84	1456.12	4.39	9.34	(29.65%) (225)prim XY3 , X= C91 ADEFa
				(29.23%) (230)prim XY3 , X= C92 ADEFa
				(8.50%) (241)prim XY3 , X= C94 ADEFb
85	1455.93	5.35	0.26	(37.64%) (151)prim XY3 , X= C69 ADEFa
				(5.73%) (152)prim XY3 , X= C69 ADEFb
				(36.72%) (157)prim XY3 , X= C70 ADEFb
86	1454.92	6.59	1.03	(78.65%) (240)prim XY3 , X= C94 ADEFa
87	1453.88	3.96	0.95	(74.34%) (146)prim XY3 , X= C68 ADEFa
				(9.55%) (147)prim XY3 , X= C68 ADEFb
88	1452.86	1.56	0.02	(43.75%) (152)prim XY3 , X= C69 ADEFb
				(43.62%) (156)prim XY3 , X= C70 ADEFa
89	1452.48	8.24	0.07	(34.04%) (226)prim XY3 , X= C91 ADEFb
				(54.97%) (231)prim XY3 , X= C92 ADEFb
90	1452.35	0.22	0.01	(55.09%) (226)prim XY3 , X= C91 ADEFb
				(33.57%) (231)prim XY3 , X= C92 ADEFb
91	1451.82	3.63	0.01	(49.01%) (245)prim XY3 , X= C95 ADEFa
				(5.42%) (250)prim XY3 , X= C96 ADEFa
				(31.64%) (251)prim XY3 , X= C96 ADEFb
92	1449.94	10.30	0.01	(88.11%) (236)prim XY3 , X= C93 ADEFb
				(7.14%) (238)prim XY3 , X= C93 ROCKb
93	1449.70	8.98	0.00	(88.24%) (162)prim XY3 , X= C71 ADEFb
				(7.11%) (164)prim XY3 , X= C71 ROCKb
94	1408.16	50.66	0.01	(9.07%) (140)secd XY, C66- H16 ROCK
				(8.23%) (172)secd XY, C74- H31 ROCK
				(6.22%) (181)secd XY, C77- H34 ROCK
				(5.85%) (193)secd XY, C81- H37 ROCK
95	1403.47	0.76	0.93	(9.24%) (140)secd XY, C66- H16 ROCK
				(5.46%) (181)secd XY, C77- H34 ROCK
				(11.36%) (193)secd XY, C81- H37 ROCK
				(6.63%) (229)prim XY3 , X= C92 SDEF

				(6.29%) (234)prim XY3 , X= C93 SDEF
96	1395.89	1.39	0.04	(6.04%) (140)secd XY, C66- H16 ROCK (17.66%) (160)prim XY3 , X= C71 SDEF (6.55%) (172)secd XY, C74- H31 ROCK (10.64%) (224)prim XY3 , X= C91 SDEF (10.03%) (234)prim XY3 , X= C93 SDEF
97	1395.30	0.11	0.72	(5.46%) (160)prim XY3 , X= C71 SDEF (7.25%) (181)secd XY, C77- H34 ROCK (9.72%) (224)prim XY3 , X= C91 SDEF (17.23%) (229)prim XY3 , X= C92 SDEF (15.36%) (234)prim XY3 , X= C93 SDEF
98	1389.53	4.36	0.03	(7.70%) (116)ring sXY2, X= C58 WAGG (43.86%) (150)prim XY3 , X= C69 SDEF (39.00%) (155)prim XY3 , X= C70 SDEF
99	1387.57	3.75	0.05	(10.52%) (218)ring sXY2, X= C89 WAGG (42.11%) (244)prim XY3 , X= C95 SDEF (37.00%) (249)prim XY3 , X= C96 SDEF
100	1379.49	7.81	0.00	(88.63%) (145)prim XY3 , X= C68 SDEF
101	1379.17	1.06	0.00	(86.61%) (239)prim XY3 , X= C94 SDEF
102	1376.89	76.83	0.00	(10.80%) (160)prim XY3 , X= C71 SDEF (29.68%) (224)prim XY3 , X= C91 SDEF (28.18%) (229)prim XY3 , X= C92 SDEF (9.66%) (234)prim XY3 , X= C93 SDEF
103	1372.87	6.27	0.08	(8.82%) (116)ring sXY2, X= C58 WAGG (9.19%) (120)ring sXY2, X= C59 WAGG (19.27%) (124)ring sXY2, X= C60 WAGG (13.34%) (160)prim XY3 , X= C71 SDEF (5.13%) (229)prim XY3 , X= C92 SDEF (9.62%) (234)prim XY3 , X= C93 SDEF
104	1371.31	55.51	0.06	(6.62%) (116)ring sXY2, X= C58 WAGG (7.58%) (120)ring sXY2, X= C59 WAGG (10.69%) (124)ring sXY2, X= C60 WAGG (10.66%) (210)ring sXY2, X= C87 WAGG (6.74%) (224)prim XY3 , X= C91 SDEF (13.15%) (234)prim XY3 , X= C93 SDEF
105	1369.62	22.74	0.11	(11.97%) (160)prim XY3 , X= C71 SDEF (18.47%) (210)ring sXY2, X= C87 WAGG (6.96%) (214)ring sXY2, X= C88 WAGG (12.47%) (218)ring sXY2, X= C89 WAGG (5.74%) (229)prim XY3 , X= C92 SDEF (5.92%) (249)prim XY3 , X= C96 SDEF
106	1367.04	2.45	0.00	(6.27%) (140)secd XY, C66- H16 ROCK (15.73%) (160)prim XY3 , X= C71 SDEF (5.49%) (172)secd XY, C74- H31 ROCK (7.45%) (193)secd XY, C81- H37 ROCK (6.37%) (224)prim XY3 , X= C91 SDEF (16.89%) (234)prim XY3 , X= C93 SDEF
107	1366.16	3.16	0.00	(43.42%) (150)prim XY3 , X= C69 SDEF (46.51%) (155)prim XY3 , X= C70 SDEF
108	1364.90	3.85	0.01	(11.14%) (214)ring sXY2, X= C88 WAGG

				(37.69%) (244)prim XY3 , X= C95 SDEF
				(35.82%) (249)prim XY3 , X= C96 SDEF
109	1363.54	0.14	1.45	(9.38%) (172)secd XY, C74- H31 ROCK (10.64%) (181)secd XY, C77- H34 ROCK (15.11%) (224)prim XY3 , X= C91 SDEF (16.53%) (229)prim XY3 , X= C92 SDEF
110	1362.04	2.37	0.24	(18.84%) (210)ring sXY2, X= C87 WAGG (14.23%) (214)ring sXY2, X= C88 WAGG (10.08%) (215)ring sXY2, X= C88 TWIST (10.41%) (219)ring sXY2, X= C89 TWIST (7.13%) (244)prim XY3 , X= C95 SDEF (8.92%) (249)prim XY3 , X= C96 SDEF
111	1359.78	7.83	0.13	(6.50%) (9) C - C STRE (4, 3) (13.62%) (117)ring sXY2, X= C58 TWIST (23.48%) (120)ring sXY2, X= C59 WAGG (10.77%) (121)ring sXY2, X= C59 TWIST (24.30%) (124)ring sXY2, X= C60 WAGG
112	1352.26	0.63	0.02	(46.84%) (116)ring sXY2, X= C58 WAGG (20.82%) (120)ring sXY2, X= C59 WAGG (8.90%) (121)ring sXY2, X= C59 TWIST
113	1350.78	0.26	0.01	(5.23%) (210)ring sXY2, X= C87 WAGG (31.93%) (214)ring sXY2, X= C88 WAGG (6.38%) (215)ring sXY2, X= C88 TWIST (36.72%) (218)ring sXY2, X= C89 WAGG (6.58%) (244)prim XY3 , X= C95 SDEF
114	1331.49	0.69	0.08	(5.58%) (39) C = C STRE (16,11) (11.66%) (166)secd XY, C72- H30 ROCK (9.75%) (187)secd XY, C79- H35 ROCK
115	1329.72	54.38	0.01	(6.14%) (60) C = C STRE (28,27) (7.23%) (166)secd XY, C72- H30 ROCK (7.49%) (187)secd XY, C79- H35 ROCK (5.91%) (199)secd XY, C83- H38 ROCK (5.30%) (202)secd XY, C84- H39 ROCK
116	1323.76	1.55	1.22	(12.84%) (60) C = C STRE (28,27) (41.40%) (202)secd XY, C84- H39 ROCK
117	1321.06	0.56	0.75	(15.80%) (16) C = C STRE (8, 7) (40.12%) (131)secd XY, C63- H14 ROCK (7.46%) (134)secd XY, C64- H15 ROCK
118	1313.60	0.01	0.52	(11.56%) (46) C = C STRE (20,19) (5.51%) (131)secd XY, C63- H14 ROCK (8.88%) (175)secd XY, C75- H32 ROCK (8.98%) (178)secd XY, C76- H33 ROCK
119	1310.55	8.37	0.00	(9.61%) (39) C = C STRE (16,11) (5.05%) (53) C = C STRE (24,23) (10.61%) (134)secd XY, C64- H15 ROCK (10.21%) (143)secd XY, C67- H17 ROCK (8.47%) (166)secd XY, C72- H30 ROCK (6.66%) (190)secd XY, C80- H36 ROCK (6.47%) (199)secd XY, C83- H38 ROCK
120	1308.42	0.43	0.53	(8.91%) (53) C = C STRE (24,23)

				(6.38%) (175)secd XY, C75- H32 ROCK
				(6.64%) (178)secd XY, C76- H33 ROCK
				(8.05%) (187)secd XY, C79- H35 ROCK
				(8.68%) (190)secd XY, C80- H36 ROCK
				(9.69%) (199)secd XY, C83- H38 ROCK
121	1298.99	19.49	0.00	(6.58%) (40) C - C STRE (17,16)
				(6.78%) (51) C - C STRE (23,22)
				(13.99%) (175)secd XY, C75- H32 ROCK
				(12.78%) (178)secd XY, C76- H33 ROCK
122	1288.11	2.60	1.72	(17.68%) (211)ring sXY2, X= C87 TWIST
				(32.50%) (219)ring sXY2, X= C89 TWIST
123	1286.39	1.97	0.53	(31.25%) (117)ring sXY2, X= C58 TWIST
				(19.42%) (125)ring sXY2, X= C60 TWIST
124	1279.32	0.61	8.12	(5.00%) (134)secd XY, C64- H15 ROCK
				(17.62%) (143)secd XY, C67- H17 ROCK
				(18.05%) (190)secd XY, C80- H36 ROCK
				(5.80%) (199)secd XY, C83- H38 ROCK
125	1277.72	6.85	0.00	(15.74%) (143)secd XY, C67- H17 ROCK
				(6.27%) (166)secd XY, C72- H30 ROCK
				(6.32%) (175)secd XY, C75- H32 ROCK
				(5.84%) (178)secd XY, C76- H33 ROCK
				(6.61%) (187)secd XY, C79- H35 ROCK
				(14.46%) (190)secd XY, C80- H36 ROCK
126	1266.16	8.80	0.05	(5.21%) (73) C - C STRE (34,33)
				(12.35%) (199)secd XY, C83- H38 ROCK
				(11.29%) (202)secd XY, C84- H39 ROCK
				(10.91%) (211)ring sXY2, X= C87 TWIST
				(7.78%) (215)ring sXY2, X= C88 TWIST
				(5.13%) (218)ring sXY2, X= C89 WAGG
				(7.41%) (222)ring tXY2, X= C90 WAGG
				(6.25%) (253)prim XY3 , X= C96 ROCKb
127	1265.25	9.43	0.09	(5.20%) (3) C - C STRE (2, 1)
				(7.29%) (112)ring tXY2, X= C57 WAGG
				(5.57%) (116)ring sXY2, X= C58 WAGG
				(9.35%) (121)ring sXY2, X= C59 TWIST
				(9.81%) (125)ring sXY2, X= C60 TWIST
				(13.47%) (131)secd XY, C63- H14 ROCK
				(11.21%) (134)secd XY, C64- H15 ROCK
				(6.49%) (154)prim XY3 , X= C69 ROCKb
128	1226.59	0.25	5.56	(5.98%) (21) C - C STRE (11,10)
				(6.52%) (40) C - C STRE (17,16)
				(8.67%) (46) C = C STRE (20,19)
				(5.93%) (51) C - C STRE (23,22)
				(5.38%) (55) C - C STRE (25,24)
				(8.03%) (140)secd XY, C66- H16 ROCK
				(5.18%) (172)secd XY, C74- H31 ROCK
				(7.03%) (193)secd XY, C81- H37 ROCK
129	1217.41	47.44	0.06	(5.26%) (3) C - C STRE (2, 1)
				(7.77%) (33) C - C STRE (14, 1)
				(5.57%) (100) 6-membered ring BEND
				(9.54%) (115)ring sXY2, X= C58 ROCK
				(21.06%) (125)ring sXY2, X= C60 TWIST
				(13.97%) (153)prim XY3 , X= C69 ROCKa

130	1216.42	5.42	0.01	(5.78%) (73) C - C STRE (34,33) (9.34%) (93) C - C STRE (39,34) (22.69%) (211)ring sXY2, X= C87 TWIST (10.25%) (217)ring sXY2, X= C89 ROCK (13.86%) (252)prim XY3 , X= C96 ROCKa
131	1210.68	6.87	0.18	(16.94%) (121)ring sXY2, X= C59 TWIST (6.04%) (140)secd XY, C66- H16 ROCK (5.93%) (193)secd XY, C81- H37 ROCK
132	1209.40	11.41	0.01	(15.42%) (121)ring sXY2, X= C59 TWIST (5.79%) (140)secd XY, C66- H16 ROCK (5.98%) (193)secd XY, C81- H37 ROCK
133	1207.86	2.02	0.03	(8.40%) (97) C - C STRE (40,34) (6.06%) (210)ring sXY2, X= C87 WAGG (32.23%) (215)ring sXY2, X= C88 TWIST (6.30%) (221)ring tXY2, X= C90 ROCK (6.26%) (247)prim XY3 , X= C95 ROCKa (6.07%) (248)prim XY3 , X= C95 ROCKb
134	1205.19	7.03	0.17	(6.72%) (40) C - C STRE (17,16) (5.97%) (51) C - C STRE (23,22) (5.53%) (166)secd XY, C72- H30 ROCK (13.84%) (172)secd XY, C74- H31 ROCK (10.70%) (175)secd XY, C75- H32 ROCK (11.04%) (178)secd XY, C76- H33 ROCK (12.59%) (181)secd XY, C77- H34 ROCK
135	1198.16	0.23	42.76	(6.65%) (17) C - C STRE (9, 8) (8.41%) (58) C - C STRE (27,26) (5.42%) (140)secd XY, C66- H16 ROCK (6.48%) (166)secd XY, C72- H30 ROCK (8.22%) (187)secd XY, C79- H35 ROCK (7.20%) (193)secd XY, C81- H37 ROCK
136	1187.63	1.26	0.12	(5.35%) (21) C - C STRE (11,10) (19.40%) (44) C - C STRE (19,18) (21.19%) (48) C - C STRE (21,20) (6.25%) (55) C - C STRE (25,24) (5.29%) (143)secd XY, C67- H17 ROCK (5.29%) (190)secd XY, C80- H36 ROCK
137	1180.84	2.46	0.25	(14.03%) (65) C - C STRE (31,30) (18.44%) (89) C - C STRE (38,30) (5.62%) (106) 6-membered ring BEND (6.93%) (210)ring sXY2, X= C87 WAGG (11.59%) (242)prim XY3 , X= C94 ROCKa
138	1179.79	2.28	0.04	(16.60%) (10) C - C STRE (5, 4) (16.40%) (25) C - C STRE (12, 5) (9.18%) (124)ring sXY2, X= C60 WAGG (5.38%) (126)ring tXY C68- C61 ROCK (15.48%) (148)prim XY3 , X= C68 ROCKa
139	1177.36	34.50	9.27	(5.12%) (72) C - C STRE (34,29) (5.57%) (97) C - C STRE (40,34) (6.41%) (106) 6-membered ring BEND (6.90%) (215)ring sXY2, X= C88 TWIST (7.97%) (219)ring sXY2, X= C89 TWIST (10.98%) (248)prim XY3 , X= C95 ROCKb
140	1173.75	10.32	7.72	(5.42%) (11) C - C STRE (6, 1)

				(7.06%) (29) C - C STRE (13, 1)
				(9.95%) (100) 6-membered ring BEND
				(9.73%) (117)ring sXY2, X= C58 TWIST
				(12.59%) (159)prim XY3 , X= C70 ROCKb
141	1168.13	0.44	66.66	(12.19%) (21) C - C STRE (11,10)
				(13.87%) (44) C - C STRE (19,18)
				(13.89%) (48) C - C STRE (21,20)
				(11.32%) (55) C - C STRE (25,24)
142	1154.75	0.94	0.02	(12.44%) (21) C - C STRE (11,10)
				(10.03%) (44) C - C STRE (19,18)
				(7.49%) (48) C - C STRE (21,20)
				(11.82%) (55) C - C STRE (25,24)
143	1150.81	1.21	3.70	(5.08%) (21) C - C STRE (11,10)
				(6.82%) (44) C - C STRE (19,18)
				(8.50%) (48) C - C STRE (21,20)
				(7.27%) (55) C - C STRE (25,24)
144	1134.73	16.08	0.23	(5.31%) (21) C - C STRE (11,10)
				(8.04%) (117)ring sXY2, X= C58 TWIST
				(5.64%) (119)ring sXY2, X= C59 ROCK
				(8.67%) (123)ring sXY2, X= C60 ROCK
				(13.68%) (125)ring sXY2, X= C60 TWIST
				(9.29%) (153)prim XY3 , X= C69 ROCKa
145	1133.81	1.16	0.11	(5.05%) (61) C - C STRE (29,28)
				(7.33%) (209)ring sXY2, X= C87 ROCK
				(14.81%) (211)ring sXY2, X= C87 TWIST
				(9.66%) (219)ring sXY2, X= C89 TWIST
				(5.47%) (243)prim XY3 , X= C94 ROCKb
				(9.55%) (252)prim XY3 , X= C96 ROCKa
146	1123.15	7.28	0.04	(5.47%) (55) C - C STRE (25,24)
				(15.61%) (61) C - C STRE (29,28)
				(8.13%) (209)ring sXY2, X= C87 ROCK
				(6.46%) (217)ring sXY2, X= C89 ROCK
				(5.42%) (242)prim XY3 , X= C94 ROCKa
147	1122.12	1.04	0.05	(17.31%) (14) C - C STRE (7, 6)
				(5.92%) (21) C - C STRE (11,10)
				(5.69%) (100) 6-membered ring BEND
				(5.62%) (123)ring sXY2, X= C60 ROCK
148	1060.71	5.24	0.02	(11.72%) (6) C - C STRE (3, 2)
				(7.66%) (9) C - C STRE (4, 3)
				(5.55%) (117)ring sXY2, X= C58 TWIST
				(7.30%) (120)ring sXY2, X= C59 WAGG
				(22.21%) (149)prim XY3 , X= C68 ROCKb
				(8.56%) (154)prim XY3 , X= C69 ROCKb
149	1054.44	5.23	0.04	(5.19%) (68) C - C STRE (32,31)
				(10.00%) (71) C - C STRE (33,32)
				(6.65%) (214)ring sXY2, X= C88 WAGG
				(6.68%) (219)ring sXY2, X= C89 TWIST
				(20.38%) (243)prim XY3 , X= C94 ROCKb
				(5.69%) (252)prim XY3 , X= C96 ROCKa
				(6.63%) (253)prim XY3 , X= C96 ROCKb
150	1048.66	3.52	0.03	(5.14%) (68) C - C STRE (32,31)

				(13.26%) (164)prim XY3 , X= C71 ROCKb
				(7.01%) (228)prim XY3 , X= C91 ROCKb
				(8.84%) (233)prim XY3 , X= C92 ROCKb
				(26.94%) (238)prim XY3 , X= C93 ROCKb
151	1048.26	2.33	0.06	(5.38%) (68) C - C STRE (32,31)
				(39.16%) (164)prim XY3 , X= C71 ROCKb
				(9.58%) (228)prim XY3 , X= C91 ROCKb
				(6.50%) (238)prim XY3 , X= C93 ROCKb
152	1047.58	1.73	0.05	(9.42%) (68) C - C STRE (32,31)
				(5.37%) (71) C - C STRE (33,32)
				(5.91%) (164)prim XY3 , X= C71 ROCKb
				(9.42%) (233)prim XY3 , X= C92 ROCKb
				(22.80%) (238)prim XY3 , X= C93 ROCKb
				(7.14%) (243)prim XY3 , X= C94 ROCKb
153	1046.51	3.27	0.00	(9.79%) (6) C - C STRE (3, 2)
				(19.56%) (9) C - C STRE (4, 3)
				(5.57%) (120)ring sXY2, X= C59 WAGG
				(8.18%) (148)prim XY3 , X= C68 ROCKa
				(6.16%) (153)prim XY3 , X= C69 ROCKa
154	1046.00	0.31	0.02	(13.06%) (164)prim XY3 , X= C71 ROCKb
				(27.43%) (228)prim XY3 , X= C91 ROCKb
				(20.72%) (233)prim XY3 , X= C92 ROCKb
				(14.20%) (238)prim XY3 , X= C93 ROCKb
155	1044.65	0.01	0.00	(32.15%) (228)prim XY3 , X= C91 ROCKb
				(37.33%) (233)prim XY3 , X= C92 ROCKb
				(5.68%) (238)prim XY3 , X= C93 ROCKb
156	1035.03	0.38	0.38	(25.84%) (163)prim XY3 , X= C71 ROCKa
				(16.30%) (227)prim XY3 , X= C91 ROCKa
				(6.55%) (232)prim XY3 , X= C92 ROCKa
				(10.40%) (237)prim XY3 , X= C93 ROCKa
157	1034.80	1.06	0.02	(9.67%) (163)prim XY3 , X= C71 ROCKa
				(5.75%) (227)prim XY3 , X= C91 ROCKa
				(15.86%) (232)prim XY3 , X= C92 ROCKa
				(26.46%) (237)prim XY3 , X= C93 ROCKa
158	1018.06	11.98	3.90	(15.32%) (149)prim XY3 , X= C68 ROCKb
				(10.03%) (154)prim XY3 , X= C69 ROCKb
				(8.71%) (158)prim XY3 , X= C70 ROCKa
				(7.78%) (159)prim XY3 , X= C70 ROCKb
				(16.13%) (227)prim XY3 , X= C91 ROCKa
159	1017.48	11.01	3.55	(7.58%) (72) C - C STRE (34,29)
				(10.88%) (89) C - C STRE (38,30)
				(7.53%) (232)prim XY3 , X= C92 ROCKa
				(5.85%) (242)prim XY3 , X= C94 ROCKa
				(5.05%) (247)prim XY3 , X= C95 ROCKa
				(11.90%) (248)prim XY3 , X= C95 ROCKb
160	1016.63	14.23	5.44	(17.21%) (232)prim XY3 , X= C92 ROCKa
				(13.55%) (243)prim XY3 , X= C94 ROCKb
				(11.14%) (247)prim XY3 , X= C95 ROCKa
				(18.68%) (253)prim XY3 , X= C96 ROCKb
161	1014.44	16.50	6.95	(14.01%) (149)prim XY3 , X= C68 ROCKb
				(13.30%) (154)prim XY3 , X= C69 ROCKb
				(8.15%) (163)prim XY3 , X= C71 ROCKa

				(14.14%) (227)prim XY3 , X= C91 ROCKa
162	1007.97	31.24	7.22	(15.06%) (232)prim XY3 , X= C92 ROCKa (14.92%) (237)prim XY3 , X= C93 ROCKa (7.41%) (253)prim XY3 , X= C96 ROCKb
163	1006.53	33.49	6.70	(5.85%) (25) C - C STRE (12, 5) (6.27%) (132)secd XY, C63- H14 OUT (5.83%) (135)secd XY, C64- H15 OUT (5.81%) (148)prim XY3 , X= C68 ROCKa (5.62%) (159)prim XY3 , X= C70 ROCKb (11.80%) (163)prim XY3 , X= C71 ROCKa (9.69%) (227)prim XY3 , X= C91 ROCKa (5.09%) (255)torsion C64- C63 TORS
164	1000.52	55.73	3.70	(16.45%) (135)secd XY, C64- H15 OUT (10.80%) (255)torsion C64- C63 TORS
165	998.81	57.29	0.26	(8.66%) (188)secd XY, C79- H35 OUT (10.68%) (200)secd XY, C83- H38 OUT (8.16%) (267)torsion C76- C75 TORS (5.91%) (271)torsion C80- C79 TORS (6.00%) (275)torsion C84- C83 TORS
166	995.64	0.43	0.93	(19.97%) (200)secd XY, C83- H38 OUT (7.40%) (267)torsion C76- C75 TORS (13.35%) (275)torsion C84- C83 TORS
167	992.07	4.81	1.01	(7.17%) (135)secd XY, C64- H15 OUT (9.59%) (149)prim XY3 , X= C68 ROCKb (5.31%) (153)prim XY3 , X= C69 ROCKa (11.85%) (158)prim XY3 , X= C70 ROCKa
168	988.05	0.52	0.11	(7.25%) (209)ring sXY2, X= C87 ROCK (12.42%) (213)ring sXY2, X= C88 ROCK (5.77%) (217)ring sXY2, X= C89 ROCK (14.33%) (243)prim XY3 , X= C94 ROCKb (14.34%) (247)prim XY3 , X= C95 ROCKa (7.64%) (252)prim XY3 , X= C96 ROCKa (10.79%) (253)prim XY3 , X= C96 ROCKb
169	985.66	1.22	0.03	(5.60%) (135)secd XY, C64- H15 OUT (5.68%) (144)secd XY, C67- H17 OUT (12.35%) (167)secd XY, C72- H30 OUT (9.33%) (188)secd XY, C79- H35 OUT (6.66%) (255)torsion C64- C63 TORS (10.73%) (263)torsion C72- C67 TORS (7.79%) (271)torsion C80- C79 TORS (5.56%) (275)torsion C84- C83 TORS
170	982.22	1.38	0.59	(6.64%) (167)secd XY, C72- H30 OUT (10.49%) (188)secd XY, C79- H35 OUT (6.95%) (191)secd XY, C80- H36 OUT (8.15%) (263)torsion C72- C67 TORS (6.55%) (267)torsion C76- C75 TORS (12.03%) (271)torsion C80- C79 TORS
171	973.99	10.63	0.36	(6.60%) (65) C - C STRE (31,30) (10.37%) (71) C - C STRE (33,32) (6.51%) (73) C - C STRE (34,33) (12.69%) (213)ring sXY2, X= C88 ROCK (14.71%) (242)prim XY3 , X= C94 ROCKa

				(7.78%) (253)prim XY3 , X= C96 ROCKb
172	968.24	11.00	0.33	(7.94%) (3) C - C STRE (2, 1) (6.37%) (6) C - C STRE (3, 2) (18.25%) (119)ring sXY2, X= C59 ROCK (14.99%) (148)prim XY3 , X= C68 ROCKa (9.74%) (154)prim XY3 , X= C69 ROCKb (6.11%) (159)prim XY3 , X= C70 ROCKb
173	928.50	0.46	0.01	(26.44%) (173)secd XY, C74- H31 OUT (26.02%) (182)secd XY, C77- H34 OUT
174	924.39	0.45	0.01	(21.05%) (68) C - C STRE (32,31) (11.54%) (73) C - C STRE (34,33) (7.28%) (89) C - C STRE (38,30) (8.10%) (93) C - C STRE (39,34) (6.75%) (97) C - C STRE (40,34) (5.61%) (242)prim XY3 , X= C94 ROCKa (6.31%) (247)prim XY3 , X= C95 ROCKa
175	923.64	0.05	0.01	(9.71%) (3) C - C STRE (2, 1) (15.41%) (9) C - C STRE (4, 3) (5.93%) (25) C - C STRE (12, 5) (19.49%) (29) C - C STRE (13, 1) (5.15%) (148)prim XY3 , X= C68 ROCKa (13.06%) (158)prim XY3 , X= C70 ROCKa (15.69%) (159)prim XY3 , X= C70 ROCKb
176	918.99	0.33	0.54	(7.52%) (132)secd XY, C63- H14 OUT (34.00%) (141)secd XY, C66- H16 OUT (8.09%) (144)secd XY, C67- H17 OUT (11.13%) (194)secd XY, C81- H37 OUT (5.63%) (257)torsion C66- C65 TORS
177	918.48	0.32	0.01	(13.97%) (93) C - C STRE (39,34) (21.82%) (97) C - C STRE (40,34) (5.63%) (247)prim XY3 , X= C95 ROCKa (23.71%) (248)prim XY3 , X= C95 ROCKb (22.47%) (252)prim XY3 , X= C96 ROCKa
178	917.08	3.26	0.09	(7.62%) (141)secd XY, C66- H16 OUT (5.44%) (144)secd XY, C67- H17 OUT (12.40%) (191)secd XY, C80- H36 OUT (32.03%) (194)secd XY, C81- H37 OUT (6.23%) (203)secd XY, C84- H39 OUT
179	916.46	0.70	0.06	(7.03%) (9) C - C STRE (4, 3) (7.53%) (29) C - C STRE (13, 1) (23.48%) (33) C - C STRE (14, 1) (25.33%) (153)prim XY3 , X= C69 ROCKa (9.84%) (159)prim XY3 , X= C70 ROCKb
180	908.14	0.05	0.00	(9.68%) (144)secd XY, C67- H17 OUT (19.90%) (173)secd XY, C74- H31 OUT (8.77%) (176)secd XY, C75- H32 OUT (8.89%) (179)secd XY, C76- H33 OUT (20.14%) (182)secd XY, C77- H34 OUT (9.79%) (191)secd XY, C80- H36 OUT
181	895.52	15.16	0.00	(5.26%) (72) C - C STRE (34,29) (8.06%) (89) C - C STRE (38,30)

				(5.27%) (106) 6-membered ring BEND
				(5.30%) (203)secd XY, C84- H39 OUT
				(13.68%) (217)ring sXY2, X= C89 ROCK
				(6.39%) (242)prim XY3 , X= C94 ROCKa
182	895.21	20.94	0.01	(6.24%) (11) C - C STRE (6, 1)
				(7.93%) (25) C - C STRE (12, 5)
				(5.51%) (100) 6-membered ring BEND
				(17.47%) (115)ring sXY2, X= C58 ROCK
				(5.54%) (130)skel, C62 C64 C63 BEND
				(8.01%) (148)prim XY3 , X= C68 ROCKa
183	881.34	0.11	0.01	(7.12%) (144)secd XY, C67- H17 OUT
				(6.27%) (167)secd XY, C72- H30 OUT
				(32.14%) (176)secd XY, C75- H32 OUT
				(31.31%) (179)secd XY, C76- H33 OUT
				(5.74%) (188)secd XY, C79- H35 OUT
				(6.04%) (191)secd XY, C80- H36 OUT
184	872.65	10.00	0.11	(21.13%) (6) C - C STRE (3, 2)
				(9.21%) (9) C - C STRE (4, 3)
				(7.63%) (29) C - C STRE (13, 1)
				(5.25%) (33) C - C STRE (14, 1)
				(16.85%) (123)ring sXY2, X= C60 ROCK
				(6.41%) (132)secd XY, C63- H14 OUT
185	870.19	1.19	0.12	(8.93%) (68) C - C STRE (32,31)
				(14.36%) (71) C - C STRE (33,32)
				(8.25%) (85) C - C STRE (37,26)
				(6.77%) (209)ring sXY2, X= C87 ROCK
186	868.55	4.77	0.11	(7.07%) (37) C - C STRE (15, 9)
				(14.06%) (132)secd XY, C63- H14 OUT
				(9.13%) (135)secd XY, C64- H15 OUT
				(5.76%) (144)secd XY, C67- H17 OUT
187	863.65	2.92	0.02	(5.39%) (93) C - C STRE (39,34)
				(5.69%) (176)secd XY, C75- H32 OUT
				(5.68%) (182)secd XY, C77- H34 OUT
				(9.44%) (188)secd XY, C79- H35 OUT
				(11.27%) (191)secd XY, C80- H36 OUT
				(7.34%) (200)secd XY, C83- H38 OUT
				(13.53%) (203)secd XY, C84- H39 OUT
188	860.60	1.50	0.31	(5.03%) (37) C - C STRE (15, 9)
				(16.27%) (77) C - C STRE (35,17)
				(15.37%) (81) C - C STRE (36,22)
				(5.60%) (167)secd XY, C72- H30 OUT
189	854.35	2.07	0.42	(5.46%) (81) C - C STRE (36,22)
				(12.24%) (144)secd XY, C67- H17 OUT
				(18.83%) (167)secd XY, C72- H30 OUT
				(7.35%) (173)secd XY, C74- H31 OUT
				(5.17%) (179)secd XY, C76- H33 OUT
190	852.42	6.22	0.46	(6.95%) (77) C - C STRE (35,17)
				(5.17%) (182)secd XY, C77- H34 OUT
				(14.20%) (188)secd XY, C79- H35 OUT
				(8.13%) (191)secd XY, C80- H36 OUT
				(6.03%) (200)secd XY, C83- H38 OUT
				(10.13%) (203)secd XY, C84- H39 OUT

191	846.09	1.10	0.02	(5.91%) (115)ring sXY2, X= C58 ROCK (6.19%) (123)ring sXY2, X= C60 ROCK (13.54%) (209)ring sXY2, X= C87 ROCK (12.15%) (217)ring sXY2, X= C89 ROCK
192	845.38	1.09	0.00	(11.34%) (115)ring sXY2, X= C58 ROCK (14.35%) (123)ring sXY2, X= C60 ROCK (16.71%) (209)ring sXY2, X= C87 ROCK (10.22%) (217)ring sXY2, X= C89 ROCK
193	842.76	4.46	0.02	(8.93%) (77) C - C STRE (35,17) (9.57%) (81) C - C STRE (36,22) (7.06%) (123)ring sXY2, X= C60 ROCK
194	820.15	0.07	0.03	(16.08%) (37) C - C STRE (15, 9) (5.64%) (77) C - C STRE (35,17) (7.02%) (81) C - C STRE (36,22) (16.94%) (85) C - C STRE (37,26)
195	809.64	1.78	0.00	(10.54%) (37) C - C STRE (15, 9) (17.99%) (77) C - C STRE (35,17) (17.11%) (81) C - C STRE (36,22) (9.01%) (85) C - C STRE (37,26)
196	780.01	4.22	0.13	(9.74%) (65) C - C STRE (31,30) (15.57%) (73) C - C STRE (34,33) (6.96%) (89) C - C STRE (38,30) (16.57%) (93) C - C STRE (39,34) (8.41%) (97) C - C STRE (40,34)
197	777.25	3.97	0.14	(15.43%) (3) C - C STRE (2, 1) (10.81%) (10) C - C STRE (5, 4) (7.40%) (25) C - C STRE (12, 5) (8.92%) (29) C - C STRE (13, 1) (16.02%) (33) C - C STRE (14, 1)
198	729.21	7.72	0.01	(5.75%) (3) C - C STRE (2, 1) (10.59%) (10) C - C STRE (5, 4) (7.49%) (33) C - C STRE (14, 1) (10.44%) (119)ring sXY2, X= C59 ROCK (6.60%) (129)ring tXY C63- C62 WAGG (7.75%) (130)skel, C62 C64 C63 BEND (5.31%) (133)skel, C63 C65 C64 BEND
199	723.32	5.20	0.01	(11.91%) (65) C - C STRE (31,30) (7.65%) (73) C - C STRE (34,33) (7.45%) (198)skel, C82 C84 C83 BEND (8.56%) (201)skel, C83 C85 C84 BEND (10.98%) (213)ring sXY2, X= C88 ROCK
200	663.76	0.85	0.01	(7.35%) (171)skel, C73 C75 C74 BEND (7.79%) (180)skel, C76 C78 C77 BEND (5.31%) (186)skel, C78 C80 C79 BEND (14.09%) (205)ring tXY C84- C85 WAGG
201	659.04	6.56	0.03	(5.50%) (171)skel, C73 C75 C74 BEND (14.57%) (205)ring tXY C84- C85 WAGG (5.17%) (221)ring tXY2, X= C90 ROCK
202	641.89	8.46	0.01	(16.31%) (129)ring tXY C63- C62 WAGG (5.50%) (184)tert XY3 , X= C78 ADEFa (7.22%) (186)skel, C78 C80 C79 BEND

203	630.39	2.42	0.00	(12.78%) (129)ring tXY C63- C62 WAGG (5.59%) (139)skel, C65 C67 C66 BEND (9.56%) (165)skel, C67 C73 C72 BEND (7.45%) (169)tert XY3 , X= C73 ADEFa (5.85%) (186)skel, C78 C80 C79 BEND
204	604.62	0.99	0.00	(7.78%) (138)tert XY3 , X= C65 ADEFb (14.36%) (139)skel, C65 C67 C66 BEND (5.94%) (186)skel, C78 C80 C79 BEND (6.31%) (192)skel, C80 C82 C81 BEND
205	595.43	0.28	0.03	(6.01%) (185)tert XY3 , X= C78 ADEFb (10.45%) (192)skel, C80 C82 C81 BEND (6.93%) (196)tert XY3 , X= C82 ADEFa
206	567.50	7.90	0.04	(10.53%) (11) C - C STRE (6, 1) (11.15%) (25) C - C STRE (12, 5) (9.66%) (29) C - C STRE (13, 1) (24.76%) (100) 6-membered ring BEND (5.83%) (115)ring sXY2, X= C58 ROCK (5.47%) (119)ring sXY2, X= C59 ROCK
207	566.73	2.85	0.01	(9.98%) (72) C - C STRE (34,29) (11.33%) (89) C - C STRE (38,30) (8.50%) (97) C - C STRE (40,34) (24.74%) (106) 6-membered ring BEND (5.08%) (213)ring sXY2, X= C88 ROCK (6.14%) (217)ring sXY2, X= C89 ROCK
208	538.01	3.18	0.00	(6.52%) (136)t-planXY3umbr C65 SOUT (5.24%) (168)t-planXY3umbr C73 SOUT (7.58%) (183)t-planXY3umbr C78 SOUT (11.96%) (195)t-planXY3umbr C82 SOUT (6.32%) (204)ring tXY C84- C85 ROCK
209	534.58	0.04	0.00	(11.89%) (136)t-planXY3umbr C65 SOUT (6.63%) (168)t-planXY3umbr C73 SOUT (5.87%) (183)t-planXY3umbr C78 SOUT (10.96%) (195)t-planXY3umbr C82 SOUT
210	530.65	3.34	0.00	(19.76%) (168)t-planXY3umbr C73 SOUT (14.61%) (183)t-planXY3umbr C78 SOUT
211	525.91	0.56	0.21	(9.52%) (168)t-planXY3umbr C73 SOUT (9.25%) (170)tert XY3 , X= C73 ADEFb (6.30%) (174)skel, C74 C76 C75 BEND (5.88%) (177)skel, C75 C77 C76 BEND (9.15%) (183)t-planXY3umbr C78 SOUT (8.23%) (185)tert XY3 , X= C78 ADEFb
212	522.53	1.19	0.25	(7.23%) (168)t-planXY3umbr C73 SOUT (6.93%) (170)tert XY3 , X= C73 ADEFb (15.11%) (183)t-planXY3umbr C78 SOUT
213	519.50	1.36	0.09	(6.54%) (136)t-planXY3umbr C65 SOUT (5.05%) (168)t-planXY3umbr C73 SOUT
214	492.47	3.10	0.23	(5.65%) (98) 6-membered ring BEND (6.77%) (111)ring tXY2, X= C57 ROCK (29.25%) (136)t-planXY3umbr C65 SOUT (5.03%) (137)tert XY3 , X= C65 ADEFa

215	489.15	0.33	0.06	(7.76%) (99) 6-membered ring BEND (8.69%) (105) 6-membered ring BEND (14.84%) (195)t-planXY3umbr C82 SOUT (5.94%) (197)tert XY3 , X= C82 ADEFb
216	479.44	0.40	0.11	(13.73%) (99) 6-membered ring BEND (8.08%) (104) 6-membered ring BEND (5.49%) (105) 6-membered ring BEND (9.78%) (195)t-planXY3umbr C82 SOUT (7.03%) (222)ring tXY2, X= C90 WAGG
217	474.09	6.45	0.01	(10.94%) (98) 6-membered ring BEND (12.29%) (99) 6-membered ring BEND (8.63%) (104) 6-membered ring BEND (5.09%) (110)ring tXY2, X= C57 SCIS (5.09%) (137)tert XY3 , X= C65 ADEFa
218	470.94	1.84	0.07	(5.47%) (97) C - C STRE (40,34) (5.12%) (98) 6-membered ring BEND (21.59%) (105) 6-membered ring BEND (5.31%) (196)tert XY3 , X= C82 ADEFa (5.49%) (220)ring tXY2, X= C90 SCIS (8.11%) (221)ring tXY2, X= C90 ROCK
219	446.99	1.97	0.01	(5.52%) (98) 6-membered ring BEND (14.17%) (138)tert XY3 , X= C65 ADEFb (13.66%) (169)tert XY3 , X= C73 ADEFa (10.01%) (184)tert XY3 , X= C78 ADEFa (9.95%) (197)tert XY3 , X= C82 ADEFb
220	432.89	0.27	0.06	(11.19%) (98) 6-membered ring BEND (6.87%) (112)ring tXY2, X= C57 WAGG (15.70%) (126)ring tXY C68- C61 ROCK (6.81%) (127)ring tXY C68- C61 WAGG (6.10%) (265)torsion C74- C73 TORS (8.64%) (267)torsion C76- C75 TORS (5.49%) (269)torsion C78- C77 TORS
221	430.41	0.67	0.08	(13.84%) (126)ring tXY C68- C61 ROCK (9.56%) (265)torsion C74- C73 TORS (14.78%) (267)torsion C76- C75 TORS (10.09%) (269)torsion C78- C77 TORS
222	421.78	0.57	0.05	(5.05%) (73) C - C STRE (34,33) (12.91%) (104) 6-membered ring BEND (10.25%) (206)ring tXY C94- C86 ROCK (10.43%) (207)ring tXY C94- C86 WAGG (23.10%) (222)ring tXY2, X= C90 WAGG
223	412.13	3.89	0.18	(5.09%) (110)ring tXY2, X= C57 SCIS (15.32%) (111)ring tXY2, X= C57 ROCK (12.68%) (112)ring tXY2, X= C57 WAGG (42.99%) (127)ring tXY C68- C61 WAGG
224	402.98	5.41	0.24	(15.42%) (105) 6-membered ring BEND (45.44%) (207)ring tXY C94- C86 WAGG (14.49%) (221)ring tXY2, X= C90 ROCK
225	394.79	1.06	0.00	(15.28%) (170)tert XY3 , X= C73 ADEFb (6.50%) (171)skel, C73 C75 C74 BEND

				(6.09%) (174)skel, C74 C76 C75 BEND
				(6.06%) (177)skel, C75 C77 C76 BEND
				(6.81%) (180)skel, C76 C78 C77 BEND
				(15.25%) (185)tert XY3 , X= C78 ADEFb
226	384.78	1.09	0.12	(5.56%) (11) C - C STRE (6, 1)
				(19.66%) (98) 6-membered ring BEND
				(6.87%) (101) 6-membered ring TORS
				(12.42%) (111)ring tXY2, X= C57 ROCK
				(6.13%) (112)ring tXY2, X= C57 WAGG
				(17.41%) (126)ring tXY C68- C61 ROCK
227	374.81	0.95	0.01	(9.76%) (109) 6-membered ring TORS
				(5.09%) (204)ring tXY C84- C85 ROCK
				(23.90%) (206)ring tXY C94- C86 ROCK
				(7.65%) (223)ring tXY2, X= C90 TWIST
				(5.37%) (273)torsion C82- C81 TORS
228	371.34	0.54	0.09	(7.54%) (138)tert XY3 , X= C65 ADEFb
				(5.87%) (142)skel, C66 C72 C67 BEND
				(5.83%) (174)skel, C74 C76 C75 BEND
229	367.02	0.60	0.01	(5.33%) (103) 6-membered ring TORS
				(5.87%) (126)ring tXY C68- C61 ROCK
				(10.78%) (128)ring tXY C63- C62 ROCK
				(12.87%) (206)ring tXY C94- C86 ROCK
				(7.01%) (257)torsion C66- C65 TORS
230	366.10	1.31	0.00	(9.12%) (184)tert XY3 , X= C78 ADEFa
				(5.86%) (189)skel, C79 C81 C80 BEND
				(6.64%) (197)tert XY3 , X= C82 ADEFb
				(6.75%) (206)ring tXY C94- C86 ROCK
				(5.25%) (207)ring tXY C94- C86 WAGG
				(5.96%) (221)ring tXY2, X= C90 ROCK
				(9.44%) (223)ring tXY2, X= C90 TWIST
231	355.81	0.19	0.03	(11.30%) (196)tert XY3 , X= C82 ADEFa
				(8.56%) (204)ring tXY C84- C85 ROCK
				(11.15%) (220)ring tXY2, X= C90 SCIS
				(14.13%) (222)ring tXY2, X= C90 WAGG
232	347.90	5.52	0.03	(5.82%) (128)ring tXY C63- C62 ROCK
				(5.86%) (169)tert XY3 , X= C73 ADEFa
				(5.55%) (256)torsion C65- C64 TORS
				(5.82%) (273)torsion C82- C81 TORS
233	340.91	0.39	0.23	(5.52%) (99) 6-membered ring BEND
				(9.87%) (110)ring tXY2, X= C57 SCIS
				(8.94%) (113)ring tXY2, X= C57 TWIST
				(9.27%) (273)torsion C82- C81 TORS
234	332.04	0.74	0.42	(12.59%) (110)ring tXY2, X= C57 SCIS
				(5.75%) (113)ring tXY2, X= C57 TWIST
				(5.75%) (256)torsion C65- C64 TORS
				(10.86%) (257)torsion C66- C65 TORS
235	315.73	0.08	0.15	(18.63%) (110)ring tXY2, X= C57 SCIS
				(13.84%) (113)ring tXY2, X= C57 TWIST
				(20.11%) (220)ring tXY2, X= C90 SCIS
236	314.73	0.20	0.07	(10.30%) (110)ring tXY2, X= C57 SCIS
				(16.50%) (113)ring tXY2, X= C57 TWIST

				(22.59%) (220)ring tXY2, X= C90 SCIS
237	308.18	0.47	0.67	(6.13%) (110)ring tXY2, X= C57 SCIS (5.01%) (112)ring tXY2, X= C57 WAGG (5.50%) (129)ring tXY C63- C62 WAGG (7.67%) (130)skel, C62 C64 C63 BEND (5.32%) (165)skel, C67 C73 C72 BEND (9.34%) (169)tert XY3 , X= C73 ADEFa
238	292.17	0.57	0.95	(5.38%) (204)ring tXY C84- C85 ROCK (5.57%) (205)ring tXY C84- C85 WAGG (5.37%) (220)ring tXY2, X= C90 SCIS (7.95%) (223)ring tXY2, X= C90 TWIST (6.84%) (264)torsion C73- C72 TORS (5.27%) (265)torsion C74- C73 TORS (5.34%) (274)torsion C83- C82 TORS (5.17%) (281)torsion C95- C90 TORS
239	287.49	0.10	0.30	(11.95%) (264)torsion C73- C72 TORS (8.52%) (265)torsion C74- C73 TORS (8.70%) (269)torsion C78- C77 TORS (15.96%) (270)torsion C79- C78 TORS (7.44%) (273)torsion C82- C81 TORS (5.24%) (274)torsion C83- C82 TORS
240	272.97	0.55	0.01	(66.02%) (282)torsion C96- C90 TORS
241	271.34	0.80	0.00	(7.71%) (137)tert XY3 , X= C65 ADEFa (9.21%) (139)skel, C65 C67 C66 BEND (6.21%) (170)tert XY3 , X= C73 ADEFb (10.23%) (192)skel, C80 C82 C81 BEND (5.60%) (196)tert XY3 , X= C82 ADEFa (5.58%) (197)tert XY3 , X= C82 ADEFb (10.36%) (282)torsion C96- C90 TORS
242	268.21	0.16	0.04	(61.98%) (260)torsion C69- C57 TORS (19.37%) (261)torsion C70- C57 TORS
243	259.45	0.39	0.02	(6.10%) (101) 6-membered ring TORS (30.03%) (103) 6-membered ring TORS (7.23%) (111)ring tXY2, X= C57 ROCK (12.85%) (260)torsion C69- C57 TORS
244	257.87	0.46	0.07	(5.32%) (103) 6-membered ring TORS (19.98%) (107) 6-membered ring TORS (21.28%) (109) 6-membered ring TORS (11.60%) (223)ring tXY2, X= C90 TWIST (7.47%) (280)torsion C94- C86 TORS (7.56%) (281)torsion C95- C90 TORS
245	249.05	0.20	0.01	(14.56%) (109) 6-membered ring TORS (7.03%) (221)ring tXY2, X= C90 ROCK (15.04%) (280)torsion C94- C86 TORS (16.69%) (281)torsion C95- C90 TORS
246	238.64	0.56	0.93	(7.88%) (171)skel, C73 C75 C74 BEND (7.16%) (180)skel, C76 C78 C77 BEND (16.13%) (280)torsion C94- C86 TORS (6.85%) (281)torsion C95- C90 TORS
247	236.75	2.17	0.37	(5.44%) (101) 6-membered ring TORS

				(6.26%)	(254)torsion	C63- C62	TORS
				(8.83%)	(259)torsion	C68- C61	TORS
				(7.31%)	(264)torsion	C73- C72	TORS
248	228.68	2.21	0.01	(18.87%)	(261)torsion	C70- C57	TORS
				(5.57%)	(266)torsion	C75- C74	TORS
				(5.66%)	(268)torsion	C77- C76	TORS
				(17.47%)	(281)torsion	C95- C90	TORS
249	224.86	0.82	0.05	(6.20%)	(265)torsion	C74- C73	TORS
				(19.35%)	(266)torsion	C75- C74	TORS
				(19.41%)	(268)torsion	C77- C76	TORS
				(8.40%)	(269)torsion	C78- C77	TORS
				(10.14%)	(270)torsion	C79- C78	TORS
				(6.37%)	(272)torsion	C81- C80	TORS
				(7.51%)	(280)torsion	C94- C86	TORS
250	220.90	2.12	0.01	(6.50%)	(258)torsion	C67- C66	TORS
				(5.67%)	(259)torsion	C68- C61	TORS
				(8.21%)	(264)torsion	C73- C72	TORS
				(7.49%)	(270)torsion	C79- C78	TORS
				(6.49%)	(272)torsion	C81- C80	TORS
251	219.76	0.07	0.20	(5.87%)	(171)skel, C73 C75 C74	BEND	
				(6.46%)	(180)skel, C76 C78 C77	BEND	
				(7.40%)	(260)torsion C69- C57	TORS	
				(32.46%)	(261)torsion C70- C57	TORS	
				(17.21%)	(281)torsion C95- C90	TORS	
252	207.91	0.23	0.00	(5.20%)	(196)tert XY3 , X= C82	ADEFa	
				(8.38%)	(198)skel, C82 C84 C83	BEND	
				(5.61%)	(259)torsion C68- C61	TORS	
				(16.79%)	(280)torsion C94- C86	TORS	
253	196.62	0.30	0.00	(5.61%)	(205)ring tXY C84- C85	WAGG	
				(5.92%)	(261)torsion C70- C57	TORS	
254	183.41	0.04	0.28	(12.52%)	(259)torsion C68- C61	TORS	
				(10.66%)	(274)torsion C83- C82	TORS	
				(11.09%)	(280)torsion C94- C86	TORS	
255	173.86	0.81	0.57	(11.23%)	(129)ring tXY C63- C62	WAGG	
				(5.36%)	(138)tert XY3 , X= C65	ADEFb	
				(5.40%)	(171)skel, C73 C75 C74	BEND	
				(5.35%)	(180)skel, C76 C78 C77	BEND	
256	172.76	4.23	0.14	(5.61%)	(133)skel, C63 C65 C64	BEND	
				(6.00%)	(205)ring tXY C84- C85	WAGG	
257	162.16	0.39	1.23	(8.92%)	(256)torsion C65- C64	TORS	
				(22.66%)	(259)torsion C68- C61	TORS	
				(5.59%)	(274)torsion C83- C82	TORS	
				(11.39%)	(279)torsion C93- C82	TORS	
258	152.32	0.05	0.10	(5.08%)	(256)torsion C65- C64	TORS	
				(5.55%)	(259)torsion C68- C61	TORS	
				(31.63%)	(262)torsion C71- C65	TORS	
				(5.19%)	(277)torsion C91- C73	TORS	
				(5.43%)	(278)torsion C92- C78	TORS	
				(30.62%)	(279)torsion C93- C82	TORS	
259	145.15	0.31	0.21	(36.29%)	(262)torsion C71- C65	TORS	

				(39.15%) (279)torsion	C93- C82	TORS
260	138.25	0.03	0.03	(19.26%) (262)torsion	C71- C65	TORS
				(15.38%) (277)torsion	C91- C73	TORS
				(33.43%) (278)torsion	C92- C78	TORS
				(8.00%) (279)torsion	C93- C82	TORS
261	136.26	0.55	0.01	(58.25%) (277)torsion	C91- C73	TORS
				(35.55%) (278)torsion	C92- C78	TORS
262	133.29	0.29	0.10	(56.29%) (108) 6-membered ring	TORS	
				(10.22%) (109) 6-membered ring	TORS	
				(9.09%) (278)torsion	C92- C78	TORS
263	121.31	0.03	0.04	(26.10%) (101) 6-membered ring	TORS	
				(9.36%) (103) 6-membered ring	TORS	
				(6.29%) (127)ring tXY	C68- C61	WAGG
				(9.34%) (259)torsion	C68- C61	TORS
264	115.07	0.02	0.02	(15.85%) (101) 6-membered ring	TORS	
				(9.33%) (108) 6-membered ring	TORS	
				(5.76%) (272)torsion	C81- C80	TORS
				(5.68%) (277)torsion	C91- C73	TORS
				(5.94%) (278)torsion	C92- C78	TORS
265	112.70	0.26	0.03	(13.37%) (101) 6-membered ring	TORS	
266	109.46	0.10	0.14	(9.60%) (101) 6-membered ring	TORS	
				(12.03%) (102) 6-membered ring	TORS	
267	90.33	0.08	0.12	(6.15%) (130)skel, C62 C64 C63	BEND	
				(7.26%) (165)skel, C67 C73 C72	BEND	
268	89.02	0.08	0.06	(8.94%) (102) 6-membered ring	TORS	
				(6.43%) (204)ring tXY	C84- C85	ROCK
				(5.49%) (255)torsion	C64- C63	TORS
				(6.71%) (275)torsion	C84- C83	TORS
269	82.24	0.03	0.30	(5.83%) (128)ring tXY	C63- C62	ROCK
				(5.43%) (204)ring tXY	C84- C85	ROCK
270	76.89	0.02	0.74	(15.67%) (258)torsion	C67- C66	TORS
				(7.18%) (264)torsion	C73- C72	TORS
				(6.26%) (266)torsion	C75- C74	TORS
				(6.58%) (268)torsion	C77- C76	TORS
				(5.64%) (270)torsion	C79- C78	TORS
				(14.82%) (272)torsion	C81- C80	TORS
				(5.04%) (276)torsion	C85- C84	TORS
271	66.69	0.04	0.00	(19.61%) (102) 6-membered ring	TORS	
				(11.50%) (107) 6-membered ring	TORS	
272	62.75	0.63	0.35	(5.15%) (265)torsion	C74- C73	TORS
				(12.19%) (266)torsion	C75- C74	TORS
				(12.29%) (268)torsion	C77- C76	TORS
				(5.78%) (269)torsion	C78- C77	TORS
				(5.44%) (275)torsion	C84- C83	TORS
273	52.41	0.11	0.04	(24.14%) (102) 6-membered ring	TORS	
				(5.04%) (103) 6-membered ring	TORS	
				(15.12%) (107) 6-membered ring	TORS	
274	46.97	0.12	0.12	(12.49%) (107) 6-membered ring	TORS	

				(11.68%) (254)torsion C63- C62 TORS
				(5.10%) (270)torsion C79- C78 TORS
				(12.12%) (276)torsion C85- C84 TORS
275	42.09	0.11	0.02	(7.99%) (102) 6-membered ring TORS
				(8.08%) (107) 6-membered ring TORS
				(10.58%) (130)skel, C62 C64 C63 BEND
				(5.59%) (133)skel, C63 C65 C64 BEND
				(5.36%) (198)skel, C82 C84 C83 BEND
				(10.63%) (201)skel, C83 C85 C84 BEND
276	37.65	0.03	0.03	(6.55%) (107) 6-membered ring TORS
				(5.26%) (257)torsion C66- C65 TORS
				(7.24%) (264)torsion C73- C72 TORS
				(9.67%) (270)torsion C79- C78 TORS
				(10.79%) (273)torsion C82- C81 TORS
				(7.24%) (275)torsion C84- C83 TORS
277	28.59	0.00	0.19	(5.95%) (254)torsion C63- C62 TORS
				(7.27%) (256)torsion C65- C64 TORS
				(8.37%) (257)torsion C66- C65 TORS
				(6.32%) (266)torsion C75- C74 TORS
				(6.07%) (268)torsion C77- C76 TORS
				(5.04%) (273)torsion C82- C81 TORS
				(6.16%) (274)torsion C83- C82 TORS
				(7.56%) (276)torsion C85- C84 TORS
278	22.82	0.00	0.51	(7.43%) (130)skel, C62 C64 C63 BEND
				(5.19%) (139)skel, C65 C67 C66 BEND
				(8.49%) (142)skel, C66 C72 C67 BEND
				(5.29%) (186)skel, C78 C80 C79 BEND
				(10.16%) (189)skel, C79 C81 C80 BEND
				(5.95%) (192)skel, C80 C82 C81 BEND
				(7.43%) (201)skel, C83 C85 C84 BEND
279	15.90	0.01	0.30	(23.43%) (254)torsion C63- C62 TORS
				(13.37%) (256)torsion C65- C64 TORS
				(13.47%) (258)torsion C67- C66 TORS
				(8.75%) (264)torsion C73- C72 TORS
				(5.48%) (266)torsion C75- C74 TORS
				(6.48%) (269)torsion C78- C77 TORS
280	15.25	0.01	0.32	(7.64%) (270)torsion C79- C78 TORS
				(11.83%) (272)torsion C81- C80 TORS
				(14.31%) (274)torsion C83- C82 TORS
				(33.71%) (276)torsion C85- C84 TORS
281	10.74	0.10	0.02	(6.84%) (142)skel, C66 C72 C67 BEND
				(6.79%) (165)skel, C67 C73 C72 BEND
				(8.36%) (171)skel, C73 C75 C74 BEND
				(12.38%) (174)skel, C74 C76 C75 BEND
				(12.20%) (177)skel, C75 C77 C76 BEND
				(7.99%) (180)skel, C76 C78 C77 BEND
				(5.92%) (186)skel, C78 C80 C79 BEND
				(5.91%) (189)skel, C79 C81 C80 BEND
282	7.92	0.02	0.03	(5.36%) (173)secd XY, C74- H31 OUT
				(5.23%) (176)secd XY, C75- H32 OUT
				(5.02%) (179)secd XY, C76- H33 OUT
				(8.16%) (265)torsion C74- C73 TORS
				(7.63%) (267)torsion C76- C75 TORS
				(7.25%) (269)torsion C78- C77 TORS

Table S2. Calculated electronic transitions and oscillator strengths of carotene

Gaussian (C _{2H}) Wavelength, nm (energy, eV)	Gaussian (C _{2H}) oscillator strength	character	Turbomole (C ₁) Wavelength, nm (energy, eV)	Turbomole (C ₁) oscillator strength	character
618.6 (2.0)	4.0193 (B _U)	H → L (68)	556.26 (2.23)	3.8342 (BU)	H → L (97.9)
523.46 (2.37)	0 (A _G)	H-1 → L (63), H → L+1 (37)	468.65 (2.65)	0.0001	H-1 → L (68.6), H → L+1 (29.7)
403.75 (3.07)	0.0984 (B _U)	H-2 → L (72), H → L+2 (24)	378.01 (3.28)	0.1388	H-2 → L (82.4), H → L+2 (13.5)
390.2 (3.18)	0 (A _G)	H → L+1 (45), H-1 → L (19) H-3 → L (6)	372.08 (3.33)	0.0033	H → L+1 (57.3), H-1 → L (25.1) H-3 → L (15.5)
364.02 (3.41)	0.1001 (B _U)	H-1 → L+1 (62), H → L+2 (34)	334.85 (3.7)	0.1696	H-1 → L+1 (66.5), H → L+2 (31.3)
333.44 (3.72)	0 (A _G)	H-3 → L (76), H → L+3 (14)	324.5 (3.82)	0.0002	H-3 → L (77.2), H → L+1 (10.4) H → L+3 (6.2)
311.69 (3.98)	0.281 (B _U)	H-4 → L (32), H → L+2 (21) H-1 → L+1 (16), H-2 → L (10)	316.14 (3.92)	0.0879	H-4 → L (54.8), H → L+2 (22.3) H-1 → L+1 (13.1)
307.68 (4.03)	0 (A _G)	H-2 → L+1 (73), H-1 → L+2 (16) H → L+3 (9)	292.33 (4.24)	0.0010	H-2 → L+1 (83.5), H → L+3 (7.2)
293.52 (4.22)	0 (A _G)	H-1 → L+2 (57), H → L+3 (37)	280.47 (4.42)	0.2698	H-4 → L (37.9), H → L+2 (28.8) H-1 → L+1 (13.9), H → L+4 (5.6) H-3 → L+1 (5.1)
289.78 (4.28)	0.1857 (B _U)	H-4 → L (54), H → L+2 (10) H-1 → L+1 (6), H → L+4 (9)	274.65 (4.53)	0.0054	H-1 → L+2 (65.2), H-5 → L (27.4)

Table S3. Bond lengths (in Å) and angles (in degree) of the calculated unconstrained geometries in the S_0 and S_2 state.

bond length	ground state (S_0)	excited state (S_2)	angle	ground state (S_0)	excited state (S_2)
C2-C1	1.553	1.553			
C3-C2	1.532	1.531	C3-C2-C1	112.787	112.912
C4-C3	1.535	1.534	C4-C3-C2	109.792	109.590
C5-C4	1.522	1.520	C5-C4-C3	114.117	114.218
C6-C5	1.363	1.372	C6-C5-C4	122.789	122.814
C7-C6	1.477	1.462	C7-C6-C5	123.329	123.996
C8-C7	1.358	1.374	C8-C7-C6	126.396	127.871
C9-C8	1.457	1.439	C9-C8-C7	126.564	126.135
C10-C9	1.373	1.394	C10-C9-C8	118.226	118.334
C11-C10	1.436	1.415	C11-C10-C9	128.379	128.510
C12-C5	1.515	1.514	C12-C5-C4	112.992	113.148
C13-C1	1.552	1.553	C13-C1-C2	107.460	107.059
C14-C1	1.555	1.555	C14-C1-C13	108.555	108.727
C15-C9	1.512	1.512	C15-C9-C8	118.485	119.099
C16-C11	1.369	1.393	C16-C11-C10	122.732	122.891
C17-C16	1.445	1.419	C17-C16-C11	126.883	126.815
C18-C17	1.379	1.407	C18-C17-C16	118.316	118.547
C19-C18	1.430	1.404	C19-C18-C17	128.317	128.370
C20-C19	1.373	1.402	C20-C19-C18	123.477	123.754
C21-C20	1.430	1.403	C21-C20-C19	123.647	123.707
C22-C21	1.379	1.408	C22-C21-C20	128.197	128.420
C23-C22	1.445	1.419	C23-C22-C21	118.401	118.506
C24-C23	1.369	1.393	C24-C23-C22	126.750	126.863
C25-C24	1.436	1.414	C25-C24-C23	122.894	122.841
C26-C25	1.373	1.395	C26-C25-C24	128.242	128.549
C27-C26	1.457	1.437	C27-C26-C25	118.327	118.307
C28-C27	1.359	1.375	C28-C27-C26	126.400	126.116
C29-C28	1.477	1.461	C29-C28-C27	125.751	127.194
C30-C29	1.363	1.373	C30-C29-C28	122.712	123.588
C31-C30	1.520	1.518	C31-C30-C29	122.917	122.973
C32-C31	1.533	1.532	C32-C31-C30	113.711	113.817
C33-C32	1.532	1.531	C33-C32-C31	109.307	108.888
C34-C33	1.553	1.554	C34-C33-C32	112.657	112.659
C35-C17	1.514	1.514	C35-C17-C16	118.556	119.287
C36-C22	1.514	1.514	C36-C22-C21	123.090	122.167
C37-C26	1.512	1.512	C37-C26-C25	123.247	122.532
C38-C30	1.515	1.513	C38-C30-C29	124.392	124.397
C39-C34	1.554	1.554	C39-C34-C33	109.911	109.750
C40-C34	1.554	1.555	C40-C34-C33	107.257	106.856