Electronic Supplementary Material (ESI) for Nanoscale.

Vibrational Anatomy of C_{90}, C_{96}, and C_{100} Fullertubes: Probing Frankenstein's Skeletal Structures of Fullerene Head Endcaps and Nanotube Belt Midsection

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Supporting Information

Table S1. Computed vibrational frequencies, relative IR and Raman intensities, and experimental IR and Raman features of C_{90}-D_{5h}(1)

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
E2'	1	155.0		100.0		165 m, br	173 vw	168 w, sh	173 s	**70**
E1"	1	224.9		64.4		234 m			229 w	11
E1'	1	244.1	0.9			249 w, sh	253 w, sh		246 w	45
E2'	2	245.1		0.0						**73**
A1'	1	247.8		32.5		257/265 m	259 m	259 vs	259 s	17
A1"	1	249.1								10
E2"	1	257.5								16
A2"	1	298.0	0.7			306 w, br				20
E1'	2	328.4	0.8						334 w, br, sh	22
E2"	2	329.2								25
A1'	2	332.6		12.6		338 w+, br		341 w	341 m	**67**
E2'	3	342.6		6.2		348 w			348 w	23
E1"	2	351.4		1.4		357 w			357 vw	25
E1'	3	372.9	0.2			373 vw		377 vw	377 w	**74**
E2"	3	386.7							389 vw	23
A1'	3	392.9		75.8		397 vs	398 w	397 s	397 vs	18
A2"	2	401.5	2.4							39
E2'	4	414.9		0.2		416 w+, br			417 w, sh	22
E1'	4	415.2	1.5							40
E1"	3	419.5		0.7				421 vw	422 w+, br	33
E1"	4	446.7		0.2		453 w+, br			451 vw	29
E2"	4	448.9								21
A2'	1	449.5								43
A1'	4	460.7		2.6			463 w	464 w+	464 w+	19
A2'	2	462.4								**71**
E2'	5	480.9		0.0						10
E1'	5	486.3	79.1		488 vs	485 w			488 vw	29
A1"	2	486.8								24
E1"	5	499.1		0.4		501 w			500 w	18
E2"	5	503.1								41
E1'	6	503.8	1.3		507 w					26
A2"	3	525.9	12.8							46
E2'	6	529.5		0.0		528 w			534 w	33
A2"	4	536.6	75.9		539 vs					18
E1'	7	537.1	49.5							11
A2'	3	539.5								23
E2"	6	540.1								14
E1"	6	553.6		0.0					555 vw	23
A1"	3	557.9								20
E1'	8	566.1	8.4		570 w				569 vw	27
E2"	7	569.3								41
A1'	5	607.8		1.5				608 vw	608 w+	**83**
E1"	7	620.0		0.8						**50**
E2'	7	621.0		0.0						14
A1'	6	621.6		32.9		618 m, v br	622 vw	622 w	622 m	11
A1"	4	634.1								**50**
A2'	4	639.2								14
E2'	8	649.2		0.2						42
E1"	8	654.9		0.2					658 w	29
E1"	9	663.1		13.1				668 vw	668 w	15
E1'	9	667.9	1.0							**81**

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
E2"	8	676.8								**52**
E1"	10	684.7		0.0					679 vw	9
E2'	9	688.5		0.0					690 w	33
E2"	9	692.3								15
E2'	10	699.5		4.2					703 w	**60**
E1'	10	705.0	2.3							17
A1"	5	706.4								**51**
A2"	5	707.6	0.3							1
A1'	7	709.0		0.7			712 vw	712 w	712 vw	1
E2'	11	719.9		0.1					722 w	11
A2'	5	726.8								13
E2"	10	730.4							734 vw	19
E1"	11	737.8		0.3					742 w	25
E1'	11	744.0	0.9							13
E2'	12	751.1		0.0					752 w	**60**
E2"	11	751.9								18
E1'	12	754.8	0.4							6
E2"	12	762.8								13
A1"	6	767.4								35
E2'	13	769.8		0.1					770 vw	14
E2"	13	774.7								**60**
A1"	7	778.5								30
E2'	14	780.8		0.1						19
E1"	12	781.0		1.0		780 vw			781 vw	35
A2"	6	786.3	0.7							32
E2'	15	799.2		0.8					798 w	**78**
E1'	13	801.0	11.3							25
A2'	6	813.4								**87**
E1'	14	815.6	24.7		815 s					**72**
E1'	15	821.8	0.0							**49**
E2"	14	842.1								45
E1"	13	847.2		0.4						**57**
A2'	7	870.4								12
A2'	8	878.4								38
E2'	16	912.9		0.1			926 vw		917 vw, br	**64**
E1"	14	946.6		0.8		943 vw, br	947 w	948 m	947 w	**79**
A1'	8	947.9		0.8		943 vw, br	947 w	948 m	947 w	33
A1"	8	954.4								34
E2'	17	981.7		0.4		981 vw			981 vw	20
E2"	15	1002.1				1002 vw			1004 vw	41
A2"	7	1053.6	1.9							23
E1'	16	1076.0	3.1						1077 vw	35
E1'	17	1080.5	13.3		1085 m	1085 vw, br		1087 vw	1086 w	**75**
E2"	16	1086.9								35
E1"	15	1101.6		6.7					1102 vw	**58**
E2'	18	1111.0		3.2			1124 vw	1124 vw	1114/ 1124 w/ vw	18
A1'	9	1121.6		1.1			1129 vw	1129 vw	1129 vw	32
A2"	8	1160.6	11.3		1159 vw					**52**
E1"	16	1160.8		0.0					1160 w	42
E2'	19	1172.8		0.0					1167/ 1173 vw/ w	21
E2"	17	1193.0								37
E1'	18	1195.6	18.6		1196 s					16
A2"	9	1207.2	32.0		1216 w+			1216 vw	1215 sh	19
A1"	9	1207.6								31

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
E1'	19	1209.9	11.7		1216 w+					25
A1'	10	1210.0		11.0		1216 m, br	1222 vw	1220 vw	1220 m	**83**
A2'	9	1223.4								**77**
A1'	11	1232.7		0.1		1233 w, sh	1235 w, br	1233 w, br	1233 vw	12
E2"	18	1245.1								37
E1"	17	1247.5		2.9			1240 vw	1242 vw		20
E1"	18	1253.9		0.0						**81**
E2'	20	1254.3		5.1					1264 w	20
A2'	10	1270.8								24
E2'	21	1285.2		0.4						40
E1'	20	1287.5	2.9		1300 w					17
E1"	19	1287.6		2.9		1297 w, br			1300 vw	49
E2"	19	1297.1								**81**
E1'	21	1304.1	0.0							44
E2'	22	1314.0		0.1					1323 w, sh	21
A2"	10	1317.4	0.0							**74**
A1"	10	1322.1								2
E2"	20	1325.1								47
A1'	12	1327.8		90.7		1329 vs, br	1330 w+	1332 w+	1330 vs	**63**
A2'	11	1333.3								10
E1'	22	1334.7	2.3				1335 w, sh	1337 w, sh	1335 s, sh	**62**
E2"	21	1346.7								32
E1"	20	1347.7		0.2		1346 w, sh			1347 w	33
E1'	23	1354.8	0.9						1366 w	**53**
E2'	23	1374.4		1.5				1386 vw	1386 w+	**63**
E1"	21	1388.6		0.0						7
E2'	24	1390.4		0.6						**59**
E2"	22	1395.7								17
A2"	11	1412.2	0.0							29
A1"	11	1419.1								45
E1'	24	1431.0	39.2		1437 s					6
E1"	22	1435.9		3.6						28
E2"	23	1436.8								30
E1"	23	1438.5		1.4						5
E2'	25	1439.0		2.6				1441 vw	1440 w+	44
A1'	13	1445.0		16.9		1446 m, br	1450 w	1450 s	1449 vs, br	20
E1'	25	1449.0	11.0							40
E2"	24	1460.5								24
A2"	12	1463.6	100.0		1462 w+				1463 w, br	11
A1'	14	1480.3		34.5		1484 m, br	1488 vs	1489 vs	1487 vs	33
E2'	26	1505.7		0.2				1503 vw	1504 vw	12
E1"	24	1509.0		11.8					1516 w	27
E2"	25	1513.8								11
E2'	27	1540.3		0.3					1526 w	48
E1'	26	1547.4	0.6							37
A1"	12	1552.5								**66**
A2"	13	1553.8	11.6		1564 vw					3
E2'	28	1556.0		5.4						5
E2"	26	1556.2								3
A2'	12	1557.9								45
E1'	27	1561.8	5.0						1573 sh	19
E1"	25	1563.0		20.5			1577 w+	1578 m	1576 s, sh	8
A1'	15	1565.2		13.8		1578 m, br	1581 m	1582 vs	1581 s	8

Red – IR-active modes, purple – Raman-active modes, grey – silent modes (neither IR nor Raman active), green – weak experimental features tentatively assigned to inactive modes.

Table S2. Computed vibrational frequencies, relative IR and Raman intensities, and experimental IR and Raman features of C_{96}-D_{3d}(3)

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
Eg	1	147.3		100.0		158 s, br	166 m	166 m	164 w	**43**
Eg	2	220.8		60.9		229 s	226 w	226 w+	226 w	13
A2u	1	225.4	0.0							**45**
A1u	1	230.1								37
Eu	1	232.0	1.5				242 w+	243 vw, sh		33
A1g	1	235.8		28.1		243 s	246 s, sh	247 w+	243 vw, br	09
A1u	2	248.5								08
Eu	2	253.5	0.5			261 w				03
A2u	2	293.5	0.1							06
Eu	3	305.1	0.2			301 vw				12
Eg	3	318.7		6.0		310 w				21
A1g	2	322.0		11.8		327 m	327 m	327 w	326 w	17
Eg	4	327.0		3.4		333 w+, sh	332 vw	332 vw	332 vw, sh	13
A2g	1	330.3								03
A1g	3	343.4		5.4		353 w+	353 m	354 w	353 w	**41**
Eg	5	349.1		1.2						**42**
Eu	4	382.3	1.6							20
A1g	4	386.5		58.8		392 vs	391 m	392 m	391 w	03
Eu	5	388.7	1.2							11
A2u	3	397.8	5.3							24
Eu	6	401.8	0.9				402 vw			28
A2g	2	415.0					407 vw			**40**
A1u	3	417.4								37
A2u	4	420.6	1.8							10
Eg	6	429.7		0.2			418 w	418 vw		06
Eu	7	438.3	2.1							18
Eg	7	443.8		0.4			433 vw	433 vw		15
A1g	5	448.6		9.3		451 s	451 s	451 s	451 m	14
Eu	8	454.8	30.4		457 s		457 vw			28
Eg	8	467.0		0.1						16
Eu	9	474.3	49.8		475 s	477 vw	471/ 477 vw	472 vw	470 vw	20
Eg	9	484.5		0.2		487 vw	488 w	488 w	487 w	14
A2g	3	485.1								18
Eg	10	496.2		0.3		500 vw	500 w	501 w	499 vw	13
A1g	6	513.4		0.7						26
A1u	4	517.1								4
A2u	5	518.1	69.1		522 m					12
Eu	10	519.2	15.7		522 m	520 w, br			520 vw, br	21
A2u	6	526.7	39.2		532 vs	530 vw	533 w	533 vw	531 vw	21
Eu	11	529.1	96.1		532 vs					6
A1u	5	531.4								4
A2g	4	537.6								17
A2g	5	552.2					541 w	541 vw	540 vw	31
Eg	11	555.6		0.1			557 vw		557 vw	7
Eu	12	562.2	0.2							18
A1g	7	563.0		2.3		568 w	569 w	569 w	567 w	**32**
A1u	6	570.0								11
Eu	13	575.1	3.6							18
A2u	7	577.3	23.9		581 w		581 vw			18
A2g	6	594.8					599 vw			**36**
A1g	8	616.2		22.5		617 s, br	619 ms	620 vs	618 w+	22

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
Eg	12	618.1		3.9						12
A1g	9	622.0		6.8			623 m	624 w+	623 w, sh	15
Eg	13	623.4		0.1						23
Eg	14	634.5		5.7		637 w	637 w	637 w	637 vw	24
A1u	7	637.1								13
A2g	7	643.2								12
Eg	15	650.1		0.4		654 vw	654 vw	655 vw	654 vw	16
Eu	14	653.1	0.1		656 vw					34
Eu	15	674.6	5.2		662 vw					36
A2u	8	677.5	1.0		668 vw					16
Eu	16	679.7	5.6		678 w					**44**
Eg	16	682.5		0.3		677 vw	679 vw	679 vvw	678 vvw	24
Eg	17	694.1		5.5		683 vw	685 w	685 w	685 vw	29
A1g	10	694.3		0.0		695 w	697 w	697 vw	696 vw	16
Eu	17	696.2	1.2							29
Eg	18	702.6		0.4			701 w+/m	701 vw	701 vw	11
A2u	9	702.8	3.7				708 vw	709 vw	708 vw	11
Eg	19	710.3		0.6			716 w+	716 w	714 vw	07
Eu	18	710.7	1.7							09
A2g	8	724.2								35
A1g	11	728.3		1.0			731 vs	732 vw	731 w	14
Eu	19	728.5	6.3		727/ 732 w					13
Eg	20	737.2		0.1			740 vw	741 vw	740 vw	09
Eg	21	740.4		0.5			745 w	745 vw	744 vw	11
A1u	8	743.5								01
Eu	20	751.8	0.7							09
A1g	12	757.0		0.3			759 w	759 w	758 vw	**39**
A2g	9	759.2								14
Eu	21	759.9	0.0							06
A1u	9	761.9								02
A2u	10	761.9	8.3		756 vw					15
A2g	10	768.3					763 vw			12
A2u	11	770.6	0.0							21
A1u	10	771.2								07
A1u	11	774.6								05
Eu	22	774.8	0.6							08
A2g	11	777.4								05
Eg	22	779.2		0.4			780 vw	781 vw	780 vw	06
Eu	23	779.6	20.1		780 w					11
Eu	24	786.4	10.3							11
A1g	13	797.3		1.1		797 w	798 m	799 m	798 w	04
Eu	25	801.4	0.6		802 vw, br					34
Eg	23	814.7		0.0			814 w	814 vw	813 vw	**53**
A2u	12	820.7	18.1		829 w					**57**
Eu	26	831.2	4.5		834 w					15
Eg	24	838.4		0.1						28
Eg	25	852.5		0.2						28
A2u	13	868.3	1.2							26
A2g	12	875.0								08
A2u	14	882.8	1.2							**37**
A1u	12	895.1					902 vw	903 vw	905 vw	39
Eg	26	923.9		0.7		924 vw	927 w	926 vw	926 w	19
A1g	14	924.4		0.2		924 vw	927 w	926 vw	926 w	06
Eg	27	952.5		0.3		953 vw	955 vw	956 vw	954 vw	15

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
A1u	13	955.8								20
A1g	15	1012.5		3.9		1015 w	1014 ms	1015 w	1014 w+	11
A2g	13	1013.0								11
Eg	28	1035.6		2.4					1037 w, br	34
Eu	27	1052.1	0.3							10
A2u	15	1052.2	4.8		1053 w+	1055 vw				15
Eu	28	1053.6	6.5		1053 w+					12
A2u	16	1092.7	3.6							35
A1u	14	1096.1								34
Eg	29	1121.5		6.2		1125 vw	1126 vw	1126 vw	1125 vw	15
A1g	16	1135.4		4.5		1137 w, br	1138 vw	1138 w+	1137 vw	13
Eu	29	1145.8	23.4		1147 m					23
A1g	17	1151.6		0.6			1146 w+	1147 w		08
Eg	30	1152.1		0.2		1152 vw	1152 vw, sh	1153 vw	1152 w	11
Eu	30	1155.0	27.1		1160 m					17
A2g	14	1158.3								17
A2u	17	1176.2	27.0		1176 w					21
A1u	15	1192.9								18
Eu	31	1209.3	23.1		1208 m					09
Eu	32	1215.4	0.0							11
Eg	31	1216.5		1.3		1222 vw	1221 vw	1222 vw	1220 vw	30
A2g	15	1228.4								27
A2u	18	1233.0	8.9							10
A1g	18	1236.2		2.1		1242 w+	1241 m	1242 w	1242 w+	24
Eg	32	1240.0		2.3		1242 w+	1241 m	1242 w	1242 w+	12
Eu	33	1242.6	0.0							21
Eg	33	1251.8		0.6				1250 vw	1248 w, sh	28
Eg	34	1254.2		0.4				1262 vw	1260 vw	12
Eg	35	1278.0		4.9			1284 vw			11
A2g	16	1278.4								18
A2u	19	1280.9	0.1							03
Eu	34	1281.7	1.8							37
A1g	19	1289.4		22.9		1299 vs	1301 m	1302 w+	1300 m	28
A1u	16	1291.3								17
A1u	17	1304.0								24
Eu	35	1305.6	0.0							20
Eu	36	1309.1	0.0							**37**
Eg	36	1313.0		1.3		1314 sh	1316 w	1316 vw	1315 w	**38**
A2g	17	1317.5								09
A1g	20	1321.9		59.8		1326 vs	1329 s	1330 m	1327 vs	**40**
Eg	37	1323.0		1.3			1336 vw			15
A1u	18	1327.0								07
Eu	37	1328.0	2.3							19
Eu	38	1332.6	0.1							06
Eg	38	1340.4		1.0			1342 vw			30
Eu	39	1353.6	0.4							27
A2g	18	1357.3								07
Eg	39	1357.3		1.1			1350 w	1350 w+	1350 w	11
A1g	21	1363.2		2.4			1375 w+	1374 w	1373 w	16
A2u	20	1365.8	95.4		1375 w					01
A1u	19	1372.9								**60**
A2u	21	1386.6	1.7							**42**
Eg	40	1398.5		3.9						31
A2g	19	1399.3								34
A1u	20	1400.4								30
Eu	40	1404.1	14.7		1420 w+ ?					24

sym	N	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %
A1g	22	1419.5		3.1		1415 w, br		1418 vw	1416 w	**33**
Eu	41	1423.6	13.6		1420 w+ ?					38
Eg	41	1426.0		2.5			1434 w	1434 w, sh	1433 w+	**36**
A2u	22	1433.7	108.0		1436 m, br					03
A1g	23	1435.7		22.6		1435 ms, br	1440 w, sh	1440 w+	1439 w	01
Eg	42	1456.8		0.8						02
Eu	42	1458.0	2.7							03
Eu	43	1461.1	100.0		1466 s, br					02
A2g	20	1463.1								23
A1u	21	1464.1								19
Eg	43	1466.3		6.6		1465 w		1467 vw	1466 w	07
A2u	23	1471.9	7.2					1478 vw	1477 vw	06
Eg	44	1494.7		0.7					1487 vw	20
Eu	44	1519.4	0.6					1515 vw	1513 vw	19
A1g	24	1520.2		8.4				1536 vw, br	1536 vw	12
A1g	25	1542.1		30.8		1549 w+	1552 w	1552 w+	1551 w+	03
Eu	45	1544.0	8.4							13
A2u	24	1547.1	16.6		1558 w?					01
A2g	21	1550								00
Eg	45	1550.1		1.5			1567 vw	1566 w, br	1566 w	10
A1u	22	1563.3								03
A2u	25	1567.1	43.4		1558 w?					25
Eg	46	1570.8		5.8				1582 vw		21
Eu	46	1576.9	5.7		1586 w			1590 vw	1590 vw	29
A1g	26	1580.9		10.3		1599 m	1602 w	1602 w+	1602 w+	**52**
Eu	47	1583.6	0.3							06
Eg	47	1585.3		8.3		1599 m	1602 w	1602 w+	1602 w+	02

Red – IR-active modes, purple – Raman-active modes, grey – silent modes (neither IR nor Raman active), green – weak experimental features tentatively assigned to inactive modes.

Table S3. Computed vibrational frequencies, relative IR and Raman intensities, and experimental IR and Raman features of C_{100}-D_{5d}(1) and description of its normal modes in terms of CNT and C_{60} modes.

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E2g	1	131.6	132.5		100.0		144 s	154	154 w	154 w	80	78 E2g(1)	20	18 Hg(1)
E1u	1	208.4	208.7	0.5			212 vw				46	40 E1u(1)	55	27 Tr, 20 Hu(1)
E1g	1	219.0	218.9		32.5		223 w	222 w	222 w	222 w	34	26 E1g(1)	67	56 Hg(1)
A1u	1	220.1	220.1								16	14 A2g(1)	83	68 Hu(1)
E2u	1	228.4	228.9				234 vw				83	82 E3u(1)	17	09 Gu(1)
A1g	1	237.7	237.7		28.7		243 ms	243/ 245 vs	243/ 245 s	243/ 245 w	12	08 A1g(1)	87	68 Hg(1), 09 Ag(1)
E2u	2	238.3	238.3								32	26 E2g(1)	68	38 F2u(1), 12 Gu(1)
A2u	1	290.8	290.9	0.6				261 w			30	16 A1g(1), 10 A2u(1)	71	51 F2u(1), 12 F1u(1)
E2g	2	305.6	305.8		1.3		298 vw				36	27 E3u(1)	63	33 Hg(2), 13 H1g(1)
E2g	3	317.9	318.0		11.9		312 w			309 vw	25	08 E2g(1), 08 E3u(1)	75	59 Hg(1), 11 Gg(1)
E1u	2	318.8	318.7	0.7							23	14 E1u(2)	77	40 Gu(1), 17 F1u(2)
A1g	2	323.2	323.1		12.6		325 m	325 w	325 w	325 w	76	64 A1g(1), 12 B2u(1)	23	14 Hg(1)
E1g	2	328.1	328.3		2.4		333 w, sh	333 m	333 m	333 w	40	28 E1u(1), 08 E1u(2)	59	21 Hg(1), 18 Hg(2)
E1g	3	361.6	362.7		0.0		363 w	367 vw	367 vw	367 w	88	84 E4g(1)	12	06 Hg(2)
A2u	2	373.6	374.3	0.1							54	50 A1g(1)	46	36 F2u(1), 10 F1u(1)
A1g	3	374.7	374.5		57.4		379 vs	380 vs	380 s	379 w	26	18 A1g(1)	74	43 Ag(1)
E2u	3	377.4	377.7								40	24 E2u(1), 10 E2g(1)	59	29 F2u(1), 23 Hu(1)
E1u	3	389.1	389.3	0.5							32	13 E4g(2), 12 E1u(2)	68	48 Gu(1)
E2u	4	394.2	394.6								30	13 E2u(1)	71	51 Gu(1), 12 Hu(1)
E2u	5	410.3	410.5								42	30 E2g(1)	59	20 Hu(1), 18 Gu(1), 10 F2u(1)
E1u	4	410.0	410.8	0.0							54	44 E4g(1)	49	23 F1u(1), 10 Hu(1)
A2g	1	412.1	412.1				414 w, br	414 vw	414 w		42	36 A2g(1) rot	58	36 Rot, 18 F2g(1)
E1g	4	420.8	421.0		1.1		422 sh	422 vw	422 w	422 w	34	16 E1g(1)	66	25 Gg(2), 16 Hg(2), 09 Rot
A1g	4	425.4	426.2		8.4		427 m	430 m	430 m	429 w	32	30 B2u(1)	69	65 Hg(2)
E1g	5	443.1	443.9		0.8		446 w			446 vw	52	34 E1u(2), 12 E1u(1)	48	41 Hg(2)
A1u	2	448.9	451.0								88	86 B1u(1)	12	09 Hu(2)
E2g	4	451.5	452.2		0.2		455 w	457 m	457 w	456 w	18		81	42 Hg(2), 26 Gg(1)
A2u	3	475.2	477.0	15.1		480 ms					34	30 A1g(1)	66	60 F1u(1)
A2g	2	475.3	477.2				474 vw				42	34 B1u(1)	58	46 F1g(2), 11 F2g(2)
E1u	5	479.7	479.4	20.3		480 ms					46	36 E1u(2)	54	35 F1u(2), 14 Hu(1)
E2g	5	480.3	481.0		0.0		483 vw	487 ms	487 m	486 w	40	32 E3u(1)	59	28 Gg(1), 16 Hg(2)
E1g	6	489.7	490.4		1.3		493 vw	493 sh	494 sg	493 sh	18	–	82	73 Gg(1)

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E2g	6	506.6	506.9		0.0		510 vw	513 w	513 w	513 vw	36	14 E3u(2)	65	16 Gg(2), 15 Gg(1), 13 F2g(1), 12 Hg(4)
E1u	6	507.2	507.9	1.9							40	14 E1u(2)	60	35 Hu(2), 14 Hu(1)
E2u	6	514.1	515.3				518 vw	520 vw	520 vw	520 vw	28	14 E2g(1)	72	66 Hu(2)
A2u	4	518.3	518.0	23.7		511 w					22	18 A2u(1)	79	56 F1u(2)
A1u	3	517.8	518.1								26	10 A2g(1), 10 A2g(2)	73	47 Hu(2), 16 Hu(1)
E1u	7	530.8	531.2	0.0							31	14 E1u(2)	69	37 Hu(2), 18 Hu(1)
E2g	7	536.6	536.9		0.0						48	46 E3g(1)	53	27 Gg(2), 25 F2g(1)
E1g	7	545.0	545.3		0.0						12	–	88	74 F1g(1)
E1u	8	545.4	545.6	27.0		548 vs					24	18 E4g(1)	75	65 F1u(1)
A1u	4	549.5	549.5								22	16 A2g(1)	77	27 Hu(2), 24 Hu(3), 13 Hu(1)
A1g	5	550.4	550.9		4.2		551 m	552 s	552 vs	551 w	64	56 B2u(1)	36	20 Hg(2)
E2u	7	561.4	561.6								62	31 E2g(2), 16 E2u(1)	38	16 Hu(1), 12 Hu(3)
A2g	3	592.4	592.7								54	44 B1u(2)	47	42 F1g(1)
A1g	6	599.9	599.3		38.1		599 m	600 m	600 m	602 w	16	12 A2u(1)	79	34 Hg(4), 32 Ag(1)
E2g	8	599.2	600.1		0.0						53	16 E3u(3), 14 E2u(1)	50	26 F2g(1), 12 Hg(4)
A2g	4	602.6	602.8								18	–	81	65 F2g(1)
E1g	8	606.7	607.2		3.9						28	10 E1g(1)	69	51 Gg(2)
A2u	5	613.9	614.6	1.5							90	88 B2u(1)	10	09 F1u(1)
E2u	8	619.0	619.3								12	–	87	61 Hu(3)
E1u	9	626.2	626.4	0.9		628 w		624 w, br	624 w, br		66	36 E4g(2), 12 E4u(1)	35	17 Hu(3)
E1g	9	634.4	634.0		16.6		634 w			636 vw	34	14 E1u(2)	61	32 Hg(4)
E1u	10	643.1	643.2	5.2		648 m					58	37 E4u(1), 13 E4g(2)	43	20 Hu(3)
E2u	9	661.2	661.7								48	12 E2g(1), 12 E3g(1), 12 E2g(3)	52	20 F2u(2), 13 Gu(2)
A1u	5	664.8	664.7								40	24 A2g(2), 16 A2g(1)	59	45 Hu(3)
E1g	10	666.7	666.9		0.0	670 w, br		668 w	668 w	668 vw	70	41 E4g(2), 20 E1u(3)	31	21 Hg(3)
E2g	9	677.6	677.2		0.2			679 m		679 w	48	36 E3u(2)	52	40 Hg(3)
E2u	10	683.4	683.3								56	24 E2g(3), 15 E2g(2)	44	13 F2u(2), 11 Hu(3), 11 Hu(4)
E1g	11	690.0	689.9		0.3						58	38 E4g(2), 14 E1u(3)	43	37 Hg(3)
E2g	10	694.4	693.8		1.1			692 w	692 vw	691 vw	62	18 E3u(2), 14 E3u(3)	38	11 F2g(1), 10 Hg(4)
E2g	11	702.4	701.5		0.9			698 w	698 vw	698 vw	74	53 E2g(2)	26	15 Hg(4)
A2u	6	706.7	706.0	0.9							2	–	99	98 F2u(2)
A2g	5	706.3	706.3								58	52 B2g(1)	42	11 F2g(2), 11 F2g(3), 11 F1g(3)
A1g	7	707.8	707.1		0.1			706 m	706 w	706 w+	2	–	99	97 Hg(3)

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E1u	11	711.0	711.1	5.6		716 w		712/716 vw	712/716 vw	712/716 w	22	–	78	30 Gu(2), 22 Hu(3), 20 Hu(4)
E2u	11	714.0	713.5								18	–	81	55 Hu(4), 20 F2u(2)
A1u	6	719.4	719.4								34	18 A2g(2), 14 A2g(1)	65	45 Hu(4), 10 Hu(3)
E2g	12	725.7	725.2		0.0			727 w	727 w	727 w	20		79	66 Gg(3)
A2u	7	733.7	732.9	2.3							30	20 A2u(1)	70	39 F1u(2), 13 Tr, 12 F2u(3)
E2g	13	735.7	735.3		0.4						28	14 E3u(2)	72	50 Hg(3)
E1g	12	736.8	736.2		2.2		737 w, br	740 m	740 vw	740 w	17	–	84	56 Gg(3), 10 F1g(2)
E1u	12	737.5	737.2	0.6							24	10 E4g(3)	77	60 Hu(4), 11 Gu(2)
A2g	6	752.3	751.5								18	14 B1u(1)	81	66 F2g(2)
E2u	12	753.8	753.1								61	58 E3u(2)	40	15 Gu(3), 13 Hu(4)
E1g	13	757.1	756.9		0.7						12		89	54 F1g(2), 16 Gg(3)
E1u	13	760.4	759.3	4.5		761 m					16		83	69 Gu(3), 10 Hu(4)
E2u	13	762.5	761.8								41	25 E2g(3), 12 E3u(2)	59	29 F2u(2), 19 Gu(3)
E2g	14	763.2	763.7		0.1						10		89	44 F2g(2), 31 F2g(3)
E1u	14	772.3	771.6	11.4		771 w					28	18 E1g(1)	72	31 Gu(4), 28 F1u(2)
E2u	14	773.2	772.6								28	12 E2g(3), 10 E3u(2)	72	31 Gu(2), 25 Gu(3), 09 F2u(2)
E2g	15	775.1	773.3		0.2			796 w	797 w		8	–	92	42 F2g(3), 40 F2g(2)
E2u	15	782.0	781.3								16	–	83	38 Gu(3), 29 Gu(2)
E1g	14	790.3	789.1		0.7		788 vw, br	790 vw	790 vw	790 vw	46	40 E1u(3)	53	22 Hg(3), 22 Gg(3)
A1u	7	792.0	790.9								48	42 A2g(2)	52	36 Hu(4)
E2g	16	804.4	803.7		0.0			802 m	802 w	802 vw	86	84 E2g(3)	15	08 Gg(3)
E2u	16	809.9	808.8								38	20 E2u(1), 11 E2g(2)	62	19 Gu(4), 13 Hu(1), 10 F2u(3)
A2g	7	815.9	815.6								46	30 B1u(2), 10 A2g(2)	53	33 F1g(2), 17 F2g(3)
E1u	15	821.6	820.7	0.8		818 w					88	88 E1u(3)	11	10 Gu(3)
A2g	8	821.8	820.9						817 vw	817 vw	86	82 A2g(2)	16	06 F2g(3)
E1g	15	831.1	830.9		0.7						56	24 E4u(1), 10 E1u(1)	44	13 Fg(2), 11 Hg(5)
A1u	8	843.4	843.2								28	22 B2g(1)	72	43 Au(1), 14 Hu(7)
E1u	16	852.4	851.9	0.0				857 vw			54	22 E4g(3), 18 E4u(1)	46	27 Hu(3)
A1g	8	890.4	888.7		0.5		887 vw	887 w	887 w	887 w	44	38 A2u(1)	56	40 Hg(4)
E1g	16	903.5	902.8		2.9		903 vw			905 vw	30	10 E1g(1), 10 E4u(2)	73	52 Hg(4)
E2u	17	920.3	918.4								78	74 E3u(3)	22	10 F2u(3)
A1u	9	924.1	923.7					933 vw	933 w		40	22 A2g(1), 14 B2g(1)	59	42 Au(1), 11 Hu(5)
E2g	17	947.3	945.6		0.3					947 w	33	20 E2u(1)	70	34 Hg(4), 21 Gg(4)
A2g	9	946.9	946.5								38	16 B2g(1), 14 B1u(2)	62	43 F1g(2)

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E2g	18	982.0	980.5		0.1		982 vw	982 w	983 w	983 w+	38	18 E3u(3), 12 E3g(1)	62	21 Hg(5), 13 Gg(2), 12 F2g(3)
A2u	8	1013.0	1011.0	2.7		1023 vw					32	28 B1g(1)	69	66 F2u(3)
E1u	17	1024.9	1023.5	0.6							38	26 E1g(1)	62	53 Gu(4)
E2u	18	1058.6	1055.8								22	10 E3g(2)	78	37 F2u(3), 26 Gu(4)
E2u	19	1082.0	1080.5								28	–	73	25 Gu(4), 20 F2u(3), 12 Hu(5)
A1g	9	1094.2	1092.3		2.6		1095 w, br	1096 w	1096 vw	1096 w	32	18 A2u(1), 12 B2u(2)	69	67 Hg(5)
E1g	17	1096.8	1094.0		2.2				1102, 1107 vw	1102 vw, sh	88	84 E4g(3)	11	–
E1u	18	1100.5	1098.4	2.0		1099 vw					48	30 E4g(3)	51	19 Gu(2), 10 F1u(3)
E1g	18	1125.2	1123.1		5.9		1123 w			1124 w	36	26 E4u(2)	64	39 Hg(5), 19 Gg(4)
E2g	19	1143.8	1140.0		1.0		1138 w	1137 vw		1140 w	26	18 E2u(1)	75	67 Gg(4)
A2u	9	1155.4	1152.8	20.4		1156 w					42	24 B1g(1), 12 A1g(2)	58	41 F2u(4)
E2g	20	1168.7	1167.2		1.8			1173 w	1173 w	1171 w	18	–	83	68 Hg(5)
E1g	19	1175.1	1172.2		0.1						22	14 E4u(1)	78	50 Gg(4), 10 Hg(5)
A1g	10	1197.4	1192.8		22.3		1195 m	1198 w	1199 w+	1198 w+	64	52 B2u(2)	35	14 Hg(5)
E1u	19	1195.5	1193.0	0.6		1196 vw					24	12 E1g(1)	76	68 Hu(5)
A2g	10	1195.6	1194.0								46	34 B1u(2)	54	27 F2g(3), 13 F2g(4)
A2u	10	1217.7	1211.8	8.8		1196 vw					24	16 A1g(2)	76	72 F2u(4)
A1u	10	1218.5	1215.8								62	30 B1u(2), 24 B2g(1)	38	19 Hu(5)
E2u	20	1220.1	1216.6								24	18 E3g(2)	76	41 F1u(3), 29 Hu(5)
E2u	21	1234.9	1231.9								20	14 E3g(1)	79	43 Hu(5), 29 F1u(4)
E1g	20	1238.0	1234.4		6.5						34	16 E1u(4)	66	30 F1g(3), 27 Hg(6)
E1u	20	1238.2	1234.5	4.4		1237 w					12	–	88	66 F1u(3)
A1g	11	1240.7	1235.6		44.1		1232 s	1233 m	1233 s	1233 m	12	–	88	80 Hg(6)
A2u	11	1247.3	1242.4	1.4							86	82 B2u(2)	14	14 F2u(4)
A1u	11	1255.7	1253.6								54	50 B1u(2)	47	44 Hu(5)
E2g	21	1271.7	1267.6		0.0						26	16 E3u(4)	74	60 Hg(6), 12 Gg(5)
E1g	21	1275.1	1271.3		6.1			1276 w. br		1276 w. br	14	–	85	52 Hg(6), 28 F1g(3)
E1u	21	1278.7	1273.8	0.1							64	54 E4g(4)	37	12 Gu(5)
E1g	22	1301.5	1297.0		0.8						38	20 E4u(2)	61	53 Gg(5)
E1u	22	1302.4	1298.2	1.2							36	20 E4u(2)	64	43 Gu(5), 13 Hu(6)
E2u	22	1306.7	1301.2								56	44 E2g(4)	43	22 Hu(6), 18 Gu(5)
A1g	12	1311.6	1304.9		94.0		1301 vs	1304 w+	1304 m	1303 s	82	32 B1g(1), 28 B2u(2), 14 A2u(1)	17	10 Hg(7)
E2g	22	1308.8	1305.4		0.1					1319 w	40	19 E3u(4), 15 E2u(2)	60	39 Gg(5), 16 Hg(6)
A2g	11	1312.5	1309.2								14	12 A1u(1)	87	76 F1g(3), 10 F2g(4)
A2u	12	1319.4	1314.8	3.2							60	**34 B1g(1), 16 A1g(2)**	40	17 F2u(4), 10 F2u(3)

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E2u	23	1322.5	1319.1								18	14 E3g(2)	82	41 Hu(6), 38 Gu(5)
E2g	23	1325.3	1320.7		0.0				1336 w	1335 m, sh	26	10 E3u(4)	74	67 F2g(4)
E2g	24	1331.3	1326.4		5.1		1339 w	1341 w	1342 w	1341 s	72	24 E3u(4), 16 E3g(2), 15 E2u(1), 10 E2u(2)	29	10 Gg(5), 10 F2g(4)
E1u	23	1333.5	1329.2	1.7							42	19 E1g(2)	59	47 Hu(6)
A1u	12	1334.7	1330.9								10	–	90	90 Hu(6)
E1g	23	1347.4	1343.0		1.0						68	23 E4g(4), 22 E4u(2), 20 E1u(4)	32	08 F1g(3), 08 Gg(5)
E1u	24	1357.8	1353.9	0.7							63	37 E4u(2), 10 E1g(2)	37	26 Gu(5)
A2g	12	1358.4	1354.7								32	26 A1u(1)	68	67 F2g(4)
A1g	13	1360.5	1355.8		10.3		1366 w	1362 w			66	48 B1g(1), 14 A1g(2)	34	20 Hg(7), 09 Hg(6)
E2u	24	1362.5	1357.8								60	24 E2g(4), 10 E2u(2), 10 E3u(4)	40	17 Gu(5), 11 Gu(6)
E1g	24	1361.8	1357.9		0.3						70	60 E4g(4)	30	15 Gg(5)
E2u	25	1385.5	1382.1								58	26 E3g(2), 26 E3u(4)	41	13 Gu(5)
E1u	25	1386.9	1382.6	0.4							54	26 E4u(2), 18 E1u(4)	46	20 Gu(6), 16 Hu(6)
E2g	25	1404.8	1400.8		0.0						62	36 E2g(4)	39	16 Gg(6)
E2g	26	1411.8	1407.4		0.1					1413 w	74	63 E3g(2)	26	13 F2g(4)
E1g	25	1414.7	1411.2		2.5					1424 w	38	14 E1u(4), 10 E1g(2)	62	21 Hg(7), 14 Gg(6)
E2u	26	1421.6	1418.3								68	26 E3u(4), 18 E3g(1), 10 E2u(2)	31	17 F2u(5)
A2u	13	1424.9	1421.3	0.0							44	40 A1g(2)	57	28 F2u(4), 18 F1u(4)
E1u	26	1429.4	1427.5	100.0		1430 vs					4	–	96	51 F1u(4), 42 Gu(6)
E1g	26	1432.4	1430.0		16.6		1434 sh			1434 vw	14	–	86	67 Hg(7)
E2g	27	1437.3	1435.1		1.5						36	22 E2u(2)	63	41 Hg(7), 11 Hg(6)
A1g	14	1450.3	1448.0		32.2		1447 m	1450 w	1451 w	1450 vs	14	**14 A1g(2)**	85	46 Hg(7), 37 Ag(2)
E2u	27	1456.9	1453.9								50	46 E2u(2)	51	49 Gu(6)
A2u	14	1462.1	1460.1	47.4		1459 w					10	08 A1g(2)	89	74 F1u(4)
E1u	27	1468.4	1464.9	0.1							52	38 E1u(4), 12 E1g(2)	48	20 Gu(6), 17 F1u(4)
A1u	13	1477.9	1475.1								52	32 B2g(1), 16 A1u(1)	48	44 Hu(7)
E1g	27	1485.7	1483.2		2.0						42	22 E4u(1), 10 E1u(4)	59	28 Hg(8), 16 Gg(6)
A1g	15	1495.8	1492.8		2.6						50	**48 A1g(2)**	50	42 Ag(2)
E2u	28	1504.1	1501.7								48	20 E3u(4), 12 E2g(4)	52	12 Hu(6), 10 F2u(5)
E1g	28	1508.7	1505.8		28.0		1506 w, br	1508 vw	1508 vw	1508 w+	64	64 E1g(2)	36	35 Gg(6)
E2g	28	1506.9	1507.1		0.9			1516 vw	1516 w	1516 m	14	–	86	65 Gg(6), 11 Hg(7)
E2u	29	1511.0	1510.9								24	18 E2u(2)	76	54 F2u(5), 12 Gu(6)
E2g	29	1531.7	1529.4		0.1		1524 w				60	32 E2g(4)	40	12 Gg(5)
E1u	28	1545.1	1543.4	0.4							44	18 E1g(2), 22 E1u(4)	55	37 Hu(7)
A1u	14	1548.1	1544.9								76	76 A1u(1)	23	23 Hu(7)

sym	N	PBE/PAW cm^{-1}	PBE/Λ2 cm^{-1}	Int-IR %	Int-R %	IR	Raman 785 nm	Raman 656 nm	Raman 620 nm	Raman 532 nm	d_{CNT} %	% CNT modes	d_{C60} %	% C_{60} modes
E2g	30	1551.5	1551.8		0.0			1550 vw	1549 w	1548 w+	9	–	93	85 Hg(8)
E2u	30	1551.5	1551.9								9	–	91	80 Hu(7)
A2g	13	1555.6	1554.1								58	48 A1u(1), 10 B2g(1)	43	14 F2g(3), 0,14 F1g(3), 10 F2g(4)
E1u	29	1557.9	1558.5	2.1							26	20 E1g(2)	75	44 Hu(7), 11 F1u(4)
A2u	15	1556.8	1559.0	6.2							2	–	98	91 F2u(5)
E1g	29	1560.4	1561.1		24.1			1570 w, sh	1570 w, sh	1571 s, sh	18	–	82	47 Hg(8), 22 Gg(6)
A1g	16	1561.5	1563.2		27.7		1574 m	1576 w+	1576 w+	1575 vs	8	–	92	83 Hg(8)

Red – IR-active modes, purple – Raman-active modes, grey – silent modes (neither IR nor Raman active), green – weak experimental features tentatively assigned to inactive modes.

Table S4. DFT-computed vibrational frequencies of C60 and their experimental values

		PBE/Λ2	PBE/PAW	Δ	exp-I	exp-II
Ag	1	487.6	488.1	-0.5	496	498
	2	1474.4	1476.8	-2.4	1468	1470
Au	1	945.0	944.6	0.4	973	951
F1g	1	561.7	561.2	0.5	565	569
	2	821.2	821.3	-0.1	827	834
	3	1265.6	1269.9	-4.3	1275	1282
F1u	1	525.8	525.2	0.6	526	525
	2	577.0	577.8	-0.8	575	577
	3	1183.5	1188.4	-4.9	1182	1189
	4	1432.5	1434.9	-2.4	1429	1428
F2g	1	549.7	549.2	0.5	553	555
	2	760.1	761.0	-0.9	757	770
	3	787.3	787.1	0.2	796	797
	4	1320.8	1326.4	-5.6	1345	1345
F2u	1	336.0	335.5	0.5	342	340
	2	710.0	710.3	-0.3	712	710
	3	964.1	968.1	-4	956	970
	4	1181.7	1188.5	-6.8	1168	1191
	5	1520.9	1519.4	1.5	1525	1530
Gg	1	478.7	477.8	0.9	485	484
	2	563.3	562.0	1.3	567	569
	3	754.4	755.0	-0.6	757	759
	4	1079.4	1085.1	-5.7	1079	1082
	5	1297.1	1299.6	-2.5	1311	1320
	6	1489.0	1489.2	-0.2	1499	1498
Gu	1	347.3	346.8	0.5	353	352
	2	743.2	742.2	1	753	757
	3	774.8	776.4	-1.6	775	782
	4	959.4	961.2	-1.8	962	961
	5	1296.3	1300.8	-4.5	1308	1313
	6	1420.3	1422.7	-2.4	1418	1432
Hg	1	258.4	257.8	0.6	272	266
	2	425.9	424.7	1.2	433	429
	3	706.3	706.2	0.1	709	707
	4	770.8	772.0	-1.2	772	774
	5	1097.2	1099.2	-2	1099	1106
	6	1239.8	1244.9	-5.1	1252	1248
	7	1420.4	1422.3	-1.9	1425	1440
	8	1560.4	1559.7	0.7	1575	1576
Hu	1	397.8	397.5	0.3	403	402
	2	530.3	528.6	1.7	533	531
	3	661.7	661.3	0.4	668	667

	PBE/Λ2	PBE/PAW	Δ	exp-I	exp-II
4	735.1	735.4	-0.3	739	740
5	1205.7	1208	-2.3	1214	1217
6	1327.3	1331.9	-4.6	1342	1352
7	1549.8	1549.3	0.5	1567	1574

PBE/Λ2 and PBE/PAW are calculations with molecular code (Priroda) and periodic code (VASP), respectively. Red – IR-active modes, purple – Raman-active modes, grey – silent modes (neither IR nor Raman active). Experimental assignments for a complete set of fundamentals are based on the analysis of IR/Raman/inelastic neutron scattering/single oxygen photoluminescence/fluorescence/HREELS spectra and DFT calculations. **Exp-I** is from (A. Popov, "*Vibrational spectra of fullerenes and their derivatives*", PhD thesis, 2003), **exp-II** is from *Phys. Chem. Chem. Phys.* **2011,** *13*, 7789

Table S5. DFT-computed (PBE/PAW) Γ-point vibrational frequencies of (5, 5) CNT

sym	freq	exp
A2u(1)	0.0 (-1.0)	
E1u(1)	0.0 (0.8)	
A2g(1)	0.0 (12.2)	
E2g (1)	69.0	
E3u(1)	188.1	
E1g(1)	207.3	
A1g(1)	333.5	338
E4g(1)	335.5	
E2u(1)	384.4	
B1u(1)	432.6	
E1u(2)	456.4	
E3g(1)	512.9	
E4u(1)	588.3	
B2g(1)	612.7	
B2u(1)	627.2	
E2g(2)	692.7	
E4g(2)	692.8	
E3u(2)	764.6	
E2g(3)	809.3	
E1u(3)	824.7	
A2g(2)	825.1	
E3u(3)	935.1	
E4g(3)	1143.4	
B1u(2)	1301.0	
B2u(2)	1324.0	
B1g(1)	1381.3	
E4u(2)	1393.5	
E3g(2)	1427.8	
E4g(4)	1436.3	
E2u(2)	1475.8	
E3u(4)	1514.1	
E1g(2)	1520.5	
A1u(1)	1526.3	
A1g(2)	1544.9	1573
E1u(4)	1545.0	
E2g(4)	1547.4	

Red – IR-active modes, purple – Raman-active modes