

Supporting Information

Computational and infrared spectroscopic investigations of

***N*-substituted carbazoles**

Jonathan Y. Mane,^{*a} Kirk H. Michaelian,^{*a} Stanislav R. Stoyanov,^{*a} Brant E. Billingham^b and
Jianbao Zhao^b

^a Natural Resources Canada, CanmetENERGY Devon, 1 Oil Patch Drive, Devon, Alberta,
CANADA T9G 1A8

^b Canadian Light Source Inc., 44 Innovation Boulevard, Saskatoon, Saskatchewan, CANADA
S7N 2V3

*E-mail: jonathan.mane@canada.ca ; kirk.michaelian@canada.ca ;
stanislav.stoyanov@canada.ca

Table S1. Calculated bond orders and bond lengths for N9-R at the DFT/ ω B97X-D/6-311++G(d,p) level of theory.

Molecule	R	Bond Order	N9-R Bond Length, Å
carbazole	H	0.81	1.00
9-methylcarbazole	Me	0.95	1.44
9-ethylcarbazole	Et	0.94	1.45
9-vinylcarbazole	Vi	1.01	1.40
9-phenylcarbazole	Ph	0.96	1.42

Table S2. Experimental (exp) and calculated (calc) far-IR band positions (cm⁻¹) for carbazole.

exp ^b	calc ^a		
	monomer	dimer I	dimer II
70 m		59 (1.97) – Monomer rocking	55 (1.58), 78 (0.30) – Monomer rocking
101 w	102 (5.54) – Aromatic ring bending (butterfly motion)	100 (0.51) – Monomer rocking	106 (0.17) – Monomer rocking
124 m		116 (3.94) – Butterfly motion	117 (7.48) – Butterfly motion
145 m	150 (0.00) – Out-of-plane ring twisting	152 (0.24) – Monomer out-of-plane ring twisting	162 (0.45), 174 (0.23) – Bending of rings in one monomer, out-of-plane twisting of other monomer
221 vw	222 (0.38) – In-plane ring rocking	220 (0.37, 0.47) – Monomer in-plane ring rocking	221 (0.40, 0.51) – Monomer in-plane ring rocking
311 vw	344 (61.81) – NH hydrogen out-of-plane wagging	322 (4.82) – Monomer out-of-plane ring bending	313 (0.51), 322 (0.96) – Monomer out-of-plane ring bending 374 (125.93) – NH hydrogen out-of-plane wagging in one monomer
426 ^c vs	434 (11.28) – Out-of-plane ring bending	425 (163.18), 426 (36.70) – Monomer NH hydrogen out-of-plane wagging 430 (73.95), 433 (1.22) – Monomer out-of-plane ring bending	434 (8.93) – Monomer out-of-plane ring bending 437 (0.94) – Out-of-plane ring bending of one monomer, ring breathing of other monomer 439 (1.72) – Monomer ring breathing, NH

			hydrogen wagging in one monomer 440 (6.60) – Monomer out-of-plane ring bending
445° vs	438 (1.44) – In-plane stretching or ring breathing	442 (9.05, 59.13) – Monomer ring breathing and NH hydrogen wagging 452 (2.37), 455 (1.43) – Monomer out-of-plane ring bending	454 (2.26) – Monomer out-of-plane ring bending 459 (99.76), 463 (39.52) – Out-of-plane ring bending of one monomer, NH hydrogen wagging in other monomer
507 w	520 (4.77) – In-plane pyrrole ring stretching	520 (1.97), 521 (3.11) – Monomer in-plane pyrrole ring stretching	520 (0.44), 521 (5.01) – Monomer in-plane pyrrole ring stretching
552 vw 566 vw	569 (0.21) – In-plane benzene ring stretching	567 (0.31), 569 (0.71) – Monomer in-plane benzene ring stretching	569 (0.44, 0.51) – In-plane benzene ring stretching in one monomer
573 s	583 (14.71) – Out-of-plane ring bending	583 (19.71) – Monomer out-of-plane ring bending	585 (23.53) – Monomer out-of-plane ring bending
600 vw	592 (0.00) – Out-of-plane ring bending	592 (0.68) – Monomer out-of-plane ring bending	592 (0.75) – Out-of-plane ring bending of one monomer
619 vw	636 (6.10) – In-plane benzene ring stretching	635 (2.52, 3.82) – Monomer in-plane benzene ring stretching	635 (1.53), 636 (5.86) – Monomer in-plane benzene ring stretching
656 vw	675 (0.49) – In-plane ring stretching	678 (3.70), 679 (1.58) – Monomer in-plane ring stretching	677 (1.33), 678 (2.25) – In-plane ring stretching of one monomer
717 m	749 (102.30) – Out-of-plane aromatic hydrogen wagging	745 (192.66), 758 (2.59), 762 (5.45) – Monomer out-of-plane aromatic hydrogen wagging	746 (152.20), 750 (26.41), 761 (2.95) – Monomer out-of-plane aromatic hydrogen wagging

			766 (2.86) – Monomer ring breathing 767 (2.68, 3.86) – Ring breathing in one monomer, out-of-plane aromatic hydrogen wagging in other monomer
742 m	776 (65.00) – Out-of-plane aromatic hydrogen wagging	766 (19.24) – Monomer ring breathing 776 (139.72) – Monomer out-of-plane aromatic hydrogen wagging	776 (137.54), 779 (15.75) – Monomer out-of-plane aromatic hydrogen wagging
759 m		791 (1.29) – Monomer out-of-plane ring bending	793 (1.41) – Out-of-plane ring bending in one monomer
774 w	795 (0.00) – Out-of-plane aromatic hydrogen wagging, ring bending	796 (1.11) – Monomer out-of-plane ring bending	797 (4.91) – Out-of-plane ring bending in one monomer

^a Intensities in (km/mol)

^b vs = very strong; s = strong; m = medium; w = weak; vw = very weak

^c broad, overlapping

Table S3. Experimental (exp) and calculated (calc) far-IR band positions (cm⁻¹) for 9-methylcarbazole.

exp ^b	9-methylcarbazole , calc ^a		
	monomer	dimer I	dimer II
66 vw			67 (0.02) – Monomer rocking
80 vw		79 (0.24) – Monomer rocking	79 (0.07) – Monomer rocking
100 vw	105 (4.64) – Aromatic ring bending (butterfly motion)	115 (6.91) – Butterfly motion	106 (0.29) – Butterfly motion in one monomer, methyl rotation in other monomer
129 s	111 (0.12) – Butterfly motion	141 (0.75) – Butterfly motion in one monomer, methyl rotation in other monomer 150 (0.41) – Out-of-plane ring twisting in one monomer, methyl rotation in other monomer	112 (1.60) – Monomer butterfly motion
163 ^c m		161 (1.07) – Out-of-plane ring twisting and methyl wagging in one monomer 166 (0.46) – Monomer out-of-plane ring twisting	157 (0.89), 164 (0.42) – Monomer out-of-plane ring twisting
175 ^c m		192 (3.12) – Monomer methyl wagging	170 (5.51), 177 (5.82) – Out-of-plane ring twisting in one monomer, methyl wagging in other monomer
223 w	223 (0.19) – In-plane ring rocking	222 (0.17), 223 (0.14) – Monomer in-plane ring rocking	214 (0.77) – Methyl rotation in one monomer 222 (0.23), 223 (0.15) – Monomer in-plane ring rocking

306 vw	294 (0.33), 297 (0.10) – In-plane methyl wagging	297 (0.11), 302 (0.24), 306 (0.21) – Monomer out-of-plane ring bending	303 (0.23) – In-plane methyl wagging in one monomer 309 (0.22) – Monomer out-of-plane ring bending
311 vw	307 (0.20) – Out-of-plane ring bending	316 (0.28) – Monomer out-of-plane ring bending	313 (0.56) – Monomer out-of-plane ring bending 320 (0.25) – In-plane methyl wagging in one monomer
423 s	434 (5.92) – Out-of-plane ring bending, ring breathing	435 (0.46, 12.56) – Monomer out-of-plane ring bending	432 (13.48), 436 (1.17) – Monomer out-of-plane ring bending
440 vw	440 (1.94) – Out-of-plane ring bending, ring breathing	440 (3.02), 441 (0.91) – Monomer ring breathing	440 (0.90), 441 (2.26) – Monomer ring breathing
474 vw	454 (0.01) – Out-of-plane ring bending	455 (0.28), 456 (0.11) – Monomer out-of-plane ring bending	454 (0.42), 460 (0.52) – Monomer out-of-plane ring bending
530 m	541 (4.29) – In-plane pyrrole ring stretching	541 (3.35, 3.70) – In-plane pyrrole ring stretching in one monomer	541 (1.88), 542 (4.64) – In-plane pyrrole ring stretching in one monomer
562 s	575 (8.24), 582 (5.78) – Out-of-plane ring bending	576 (3.21, 8.18), 582 (6.11), 583 (2.11), 593 (0.47) – Monomer out-of-plane ring bending	576 (6.36), 577 (6.13) – Out-of-plane ring bending in one monomer 582 (7.02) – Monomer out-of-plane ring bending
593 vw	614 (0.02) – In-plane benzene ring stretching	614 (0.06) – Monomer in-plane benzene ring stretching	614 (0.05) – Monomer in-plane benzene ring stretching
615 m	636 (4.69) – In-plane benzene ring stretching	635 (2.78, 2.86) – In-plane benzene ring stretching in one monomer	634 (0.71), 635 (4.72) – Monomer in-plane benzene ring stretching
721 vs	746 (11.68, 67.89) – Out-of-plane	742 (153.30), 744 (4.90) – Monomer out-of-plane	741 (140.19), 745 (16.69) –

	aromatic hydrogen wagging	aromatic hydrogen wagging 746 (7.62) – Monomer ring breathing 758 (1.00), 761 (3.61) – Monomer out-of-plane aromatic hydrogen wagging	Monomer out-of-plane aromatic hydrogen wagging
745 vs	775 (82.83) – Out-of-plane aromatic hydrogen wagging, ring bending	773 (171.06), 775 (2.83) – Monomer out-of-plane aromatic hydrogen wagging	763 (5.88), 775 (174.06), 778 (2.66) – Monomer out-of-plane aromatic hydrogen wagging
771 m	794 (1.12) – In-plane ring stretching, N9-methyl C stretching	792 (0.30) – Monomer out-of-plane aromatic hydrogen wagging, monomer ring bending 794 (0.24, 1.21), 795 (0.67) – In-plane ring stretching and N9-methyl C stretching in one monomer, out-of-plane ring bending in other monomer	792 (2.35) – Monomer out-of-plane aromatic hydrogen wagging, monomer ring bending 794 (1.10, 2.16), 795 (0.65) – In-plane ring stretching and N9-methyl C stretching in one monomer, out-of-plane ring bending in other monomer

^a Intensities in (km/mol)

^b vs = very strong; s = strong; m = medium; w = weak; vw = very weak

^c broad, overlapping

Table S4. Experimental (exp) and calculated (calc) far-IR band positions (cm⁻¹) for 9-ethylcarbazole.

exp ^b	9-ethylcarbazole, calc. ^a		
	monomer	dimer I	dimer II
109 w	108 (1.16) – Aromatic ring bending (butterfly motion)	74 (2.72), 79 (1.10) – Ethyl bending with rings in one monomer 86 (0.50) – Monomer rocking	92 (1.20) – Ethyl bending with monomer aromatic rings
131 m		130 (1.06) – Butterfly motion	117 (3.78) – Butterfly motion
216 w	214 (0.39) – In-plane ring rocking	211 (0.25), 213 (0.23) – In-plane ring rocking and ethyl CH ₃ rotation in one monomer 215 (0.43) – Monomer in-plane ring rocking and ethyl CH ₃ rotation 216 (0.21) – In-plane ring rocking and ethyl CH ₃ rotation in one monomer, in-plane ring rocking in other monomer	217 (0.17, 0.64) – In-plane ring rocking and ethyl CH ₃ rotation in one monomer, in-plane ring rocking in other monomer 219 (0.22, 0.40) – In-plane aromatic ring rocking and ethyl CH ₃ rotation in one monomer
269 m	265 (1.51) – Ethyl rocking, out-of-plane ring bending	270 (2.00) – Monomer ethyl rocking and out-of-plane ring bending	273 (2.69) – Monomer ethyl rocking and out-of-plane aromatic ring bending in both monomers
410 m	412 (2.82) – Ethyl bending, out-of-plane ring bending	413 (8.79), 416 (1.89) – Monomer ethyl bending and out-of-plane ring bending	416 (8.84) – Monomer ethyl bending and out-of-plane ring bending
424 m	434 (6.14) – Out-of-plane ring bending	436 (6.47), 437 (4.19) – Out-of-plane ring bending in one monomer	434 (12.86), 438 (0.25) – Monomer out-of-plane ring bending

435 w	445 (1.67) – Ethyl bending, ring breathing	446 (1.62, 2.29) – Ethyl bending, ring breathing in one monomer	447 (3.46), 449 (0.27) – Monomer ethyl bending and ring breathing
449 vw	453 (0.04) – Out-of-plane ring bending	457 (0.25), 459 (0.29) – Out-of-plane ring bending in one monomer	456 (0.41), 462 (0.32) – Monomer out-of-plane ring bending
529 m	541 (4.26) – In-plane pyrrole ring stretching	541 (3.14, 3.83) – Monomer in-plane pyrrole ring stretching	541 (1.22, 5.17) – Monomer in-plane pyrrole ring stretching
561 s	575 (6.11) – Ethyl rocking, out-of-plane ring bending	575 (5.02), 576 (3.32) – Ethyl rocking, out-of-plane aromatic ring bending in one monomer	575 (0.44, 7.05) – Monomer ethyl rocking and out-of-plane ring bending
578 s	595 (4.89) – Ethyl bending/scissoring, out-of-plane ring bending	597 (0.57), 598 (3.87) – Monomer ethyl bending/scissoring and out-of-plane ring bending	592 (0.20, 0.43) – Out-of-plane ring bending in one monomer 597 (5.01) – Monomer ethyl bending/scissoring and out-of-plane ring bending
616 m	636 (4.20) – In-plane ring stretching	634 (2.70), 635 (2.38) – In-plane ring stretching in one monomer	634 (0.53), 635 (4.30) – Monomer in-plane ring stretching
725 vs	746 (76.82) – Aromatic hydrogen wagging	744 (143.44), 746 (27.07) – Monomer aromatic hydrogen wagging	745 (141.90), 748 (6.80) – Monomer aromatic hydrogen wagging
754 vs	776 (82.25) – Aromatic hydrogen wagging	760 (2.07), 774 (154.60), 775 (8.00) – Monomer aromatic hydrogen wagging	763 (4.91), 775 (180.56), 778 (0.75) – Monomer aromatic hydrogen wagging
784 m	788 (0.42) – In-plane ring stretching, N9-ethyl C and ethyl C-C stretching	788 (1.67) – Monomer in-plane ring stretching and N9-ethyl C stretching 788 (4.85) – Monomer in-plane ring stretching,	787 (0.64) – Monomer in-plane ring stretching and N9-ethyl C stretching 794 (4.06) – Out-of-plane ring bending, aromatic

	792 (6.92) – Ethyl hydrogen rocking	ethyl hydrogen rocking in one monomer	hydrogen wagging in one monomer, ethyl hydrogen rocking in other monomer
	797 (0.33) – Out-of-plane ring bending, aromatic hydrogen wagging	795 (1.60) – Monomer out-of-plane ring bending and aromatic hydrogen wagging 796 (3.21), 798 (2.74) – Out-of-plane aromatic ring bending, aromatic hydrogen wagging in both monomers, ethyl hydrogen rocking in one monomer	796 (3.17) – Monomer out-of-plane ring bending and aromatic hydrogen wagging, ethyl hydrogen rocking in one monomer 804 (2.71), 812 (6.24) – Ethyl hydrogen rocking in one monomer

^a Intensities in (km/mol)

^b vs = very strong; s = strong; m = medium; w = weak; vw = very weak

^c broad, overlapping

Table S5. Experimental (exp) and calculated (calc) far-IR band positions (cm⁻¹) for 9-vinylcarbazole.

exp ^b	9-vinylcarbazole, calc. ^a		
	monomer	dimer I	dimer II
71 m	76 (0.67) – Vinyl and carbazole aromatic ring scissoring	76 (0.30), 80 (0.31), 84 (1.50) – Monomer rocking	59 (1.10) – Monomer rocking
136 s	106 (2.21) – Aromatic ring bending (butterfly motion) 128 (5.39) – Vinyl rotation, butterfly motion	110 (0.38) – Monomer rocking, vinyl and carbazole ring scissoring in one monomer 118 (4.00) – Monomer butterfly motion	110 (1.32), 122 (3.54) – Butterfly motion in one monomer, vinyl and carbazole ring scissoring in other monomer 130 (1.04) – Butterfly motion), vinyl rotation in one monomer, vinyl and carbazole ring scissoring in other monomer 139 (0.93) – Butterfly motion, vinyl rotation in one monomer, butterfly motion in other monomer
168 w	153 (2.98) – Vinyl rotation, out-of-plane ring twisting	161 (0.73) – Monomer out-of-plane ring twisting 173 (1.09) – Monomer out-of-plane ring twisting and vinyl rotation 186 (3.84) – Monomer in-plane ring rocking and vinyl rotation	153 (5.80) – Monomer butterfly motion and vinyl rotation 175 (0.55) – Monomer out-of-plane ring twisting and vinyl rotation
224 w	204 (1.49) – Vinyl wagging	212 (0.67), 216 (1.96) – Vinyl wagging in one monomer	211 (0.39), 214 (0.79) – Vinyl wagging in one monomer

	228 (0.24) – Vinyl rotation, in-plane ring rocking	232 (0.25), 241 (2.61) – Vinyl, aromatic ring wagging in one monomer	
300 vw	296 (0.74) – Out-of-plane benzene ring bending	297 (0.86), 304 (0.19) – Monomer out-of-plane benzene ring bending	300 (1.31), 306 (0.27) – Monomer out-of-plane benzene ring bending
318 m	314 (1.07) – Out-of-plane ring bending	325 (1.80) – Monomer out-of-plane ring bending	322 (0.61), 328 (0.38) – Monomer out-of-plane ring bending
422 vw	434 (6.05) – Out-of-plane ring bending 439 (0.98) – Vinyl bending, ring breathing	407 (0.59), 411 (0.62) – Vinyl bending, in-plane ring stretching in one monomer	435 (13.00, 1.47) – Monomer out-of-plane ring bending 439 (0.75), 440 (1.24) – Monomer vinyl bending and ring breathing
430 vs	458 (1.65) – Out-of-plane ring bending	431 (12.46), 435 (0.40) – Monomer out-of-plane ring bending 438 (1.29), 439 (0.32) – Monomer vinyl bending and ring breathing 456 (2.78), 459 (0.52) – Monomer out-of-plane ring bending	457 (1.88), 460 (0.98) – Monomer out-of-plane ring bending
529 s	540 (3.08) – In-plane pyrrole ring stretching	540 (1.80, 2.94) – In-plane pyrrole ring stretching in one monomer	540 (1.44, 3.11) – In-plane pyrrole ring stretching in one monomer
546 s	561 (12.53) – Vinyl bending/scissoring, in-plane ring stretching	560 (0.38), 562 (17.92) – Monomer vinyl bending/scissoring, in-plane ring stretching	560 (5.27), 561 (12.92) – Monomer vinyl bending/scissoring, in-plane ring stretching
564 s	577 (3.69) – Out-of-plane ring bending	576 (7.40) – Monomer out-of-plane ring bending	577 (7.19) – Monomer out-of-plane ring bending

576 vw	–	578 (0.47) – Monomer out-of-plane ring bending	–
615 s	635 (3.48) – In-plane ring stretching	634 (4.51) – Monomer in-plane ring stretching	634 (3.99) – Monomer in-plane ring stretching
646 s	656 (3.46) – Vinyl scissoring, in-plane ring stretching	658 (0.95), 659 (4.82) – Monomer vinyl scissoring and in-plane ring stretching	658 (3.10), 660 (2.10) – Monomer vinyl scissoring and in-plane ring stretching
685 w	716 (9.75) – Vinyl wagging, in-plane ring stretching	715 (2.84), 719 (9.72) – Monomer vinyl wagging and in-plane ring stretching	712 (7.12), 713 (6.17) – Monomer vinyl wagging and in-plane ring stretching
724 vs	743 (2.28) – N9-vinyl C stretching, ring breathing 751 (85.17) – Vinyl and aromatic hydrogen wagging	742 (29.46), 743 (21.98) – N9-vinyl C stretching and aromatic ring breathing in one monomer 747 (148.12), 749 (0.30) – Monomer vinyl and aromatic hydrogen wagging	746 (80.04), 748 (11.14) – Monomer vinyl and aromatic hydrogen wagging
750 vs	764 (2.94), 779 (74.01) – Aromatic hydrogen wagging	756 (7.08), 762 (5.85) – Monomer aromatic hydrogen wagging 773 (124.66), 776 (8.57) – Monomer aromatic hydrogen wagging and out-of-plane ring bending	777 (130.87), 779 (12.86) – Monomer aromatic hydrogen wagging and out-of-plane ring bending

^a Intensities in (km/mol)

^b vs = very strong; s = strong; m = medium; w = weak; vw = very weak; sh = shoulder

Table S6. Experimental (exp) and calculated (calc) far-IR band positions (cm⁻¹) for 9-phenylcarbazole.

exp ^b	9-phenylcarbazole, calc. ^a		
	monomer	dimer I	dimer II
62 w	75 (0.21) – Phenyl and carbazole ring scissoring	71 (0.70) – Monomer carbazole ring bending and phenyl wagging	62 (1.30) – Monomer phenyl and carbazole ring scissoring
129 vw	110 (1.26) – Carbazole ring bending (butterfly motion)	122 (0.30) – Monomer phenyl rotation about N9-phenyl C bond	114 (3.13) – Monomer butterfly motion
139 w	151 (0.32) – Out-of-plane aromatic ring twisting about N9-phenyl C bond	129 (2.77) – Monomer butterfly motion	
167 vw		166 (0.98) – Monomer out-of-plane aromatic ring twisting about N9-phenyl C bond	160 (0.99) – Monomer out-of-plane aromatic ring twisting about N9-phenyl C bond
196 vw	197 (0.11) – In-plane carbazole ring rocking	202 (0.02, 0.04) – Monomer in-plane carbazole ring rocking	203 (0.14) – Monomer in-plane carbazole ring rocking
243 m	241 (0.67) – Out-of-plane carbazole and phenyl ring bending	249 (0.94) – Monomer out-of-plane carbazole and phenyl ring bending	245 (0.75) – Monomers out-of-plane carbazole and phenyl ring bending
252 m		257 (0.18) – Monomer out-of-plane carbazole and phenyl ring bending	249 (0.45) – Monomer out-of-plane carbazole and phenyl ring bending
263 w	264 (0.68) – Out-of-plane carbazole and phenyl ring bending	270 (0.80) – Monomers out-of-plane carbazole and phenyl ring bending	273 (0.30, 0.22) – Monomer out-of-plane carbazole and phenyl ring bending
293w	293 (0.64) – Out-of-plane carbazole benzene rings bending	300 (0.22), 301 (1.19) – Monomer out-of-plane carbazole benzene rings bending	295 (0.97), 301 (0.51) – Monomer out-of-plane carbazole benzene rings bending

323 s	330 (1.30) – Phenyl ring breathing, carbazole benzene rings rocking	330 (2.63) – Monomer phenyl ring breathing, carbazole benzene rings rocking	331 (3.58) – Monomer phenyl ring breathing, carbazole benzene rings rocking
401 vw	412 (0.65) – Out-of-plane carbazole rings and phenyl ring bending	401 (1.04) – Monomer out-of-plane carbazole rings and phenyl ring bending	407 (3.51) – Monomer out-of-plane carbazole rings and phenyl ring bending
418 vw, 421 s	424 (1.10) – Phenyl ring bending	425 (3.20) – Monomer phenyl ring bending	426 (2.60) – Monomer phenyl ring bending
434 vw	437 (5.48) – Out-of-plane carbazole ring bending 445 (2.79) – Out-of-plane carbazole rings bending, phenyl ring breathing	437 (11.24) – Monomer out-of-plane carbazole rings bending	440 (14.06) – Monomer out-of-plane carbazole rings bending
444 s	457 (2.76) – Out-of-plane carbazole rings bending	445 (1.02, 6.15) – Monomer out-of-plane carbazole rings bending 463 (2.47) – Monomer out-of-plane carbazole rings and phenyl ring bending	445 (3.51) – Monomer out-of-plane carbazole rings bending 460 (4.70, 0.89) – Monomer out-of-plane carbazole rings and phenyl ring bending
489 m	508 (4.92) – Phenyl ring bending	511 (8.82) – Monomers phenyl ring bending	511 (4.88), 512 (2.52) – Monomers phenyl ring bending
531 m	542 (6.13) – In-plane carbazole rings stretching	541 (9.80) – Monomer in-plane carbazole rings stretching	542 (0.56, 8.33) – Monomer in-plane carbazole rings stretching
568 m	585 (6.21) – Phenyl ring stretching, out-of-	583 (13.45) – Monomer phenyl ring stretching and out-of-plane carbazole rings bending	586 (1.76, 13.44), 590 (0.89) – Monomer phenyl ring stretching and out-of-

	plane carbazole rings bending		plane carbazole rings bending
617 w	633 (0.52) – Phenyl ring bending, in-plane carbazole benzene rings stretching 636 (3.80) – Phenyl ring stretching and bending, in-plane carbazole benzene rings stretching	635 (8.34) – Monomer in-plane phenyl ring and carbazole benzene rings stretching	635 (6.47, 3.54) – Monomer in-plane phenyl ring and carbazole benzene rings stretching
628 m	649 (7.63) – Phenyl ring stretching and bending, in-plane carbazole benzene rings stretching	649 (8.79) – Monomer phenyl ring stretching and bending, and in-plane carbazole benzene rings stretching	649 (0.78), 650 (7.89) – Monomer phenyl ring stretching and bending, and in-plane carbazole benzene rings stretching
637 m	656 (10.04) – In-plane phenyl and carbazole rings stretching	654 (13.83) – Monomer in-plane phenyl and carbazole rings stretching	655 (13.53) – Monomer in-plane phenyl and carbazole rings stretching
698 m	722 (48.23) – Out-of-plane phenyl ring bending	722 (127.14) – Monomer out-of-plane phenyl ring bending	721 (79.60), 722 (37.00) – Monomer out-of-plane phenyl ring bending 739 (5.63) – Monomer aromatic rings breathing
725 m	751 (60.81) – Carbazole ring hydrogens wagging	750 (108.25) – Monomer carbazole ring hydrogens wagging	745 (109.70), 747 (1.02) – Monomer carbazole ring hydrogens wagging
747 sh	763 (0.40) – Carbazole ring hydrogens wagging	757 (2.49), 760 (14.31) – Monomer carbazole ring hydrogens wagging	758 (3.13), 763 (4.96) – Monomer carbazole ring hydrogens wagging

753 m	776 (72.34) – Carbazole rings bending, hydrogens wagging 782 (0.30) – Phenyl and carbazole rings breathing	771 (126.23), 774 (4.46) – Monomer carbazole rings bending, hydrogens wagging	774 (133.82) – Monomer carbazole rings bending, hydrogens wagging
762 sh	789 (35.93) – Phenyl hydrogens wagging 801 (0.69) – Carbazole rings bending	781 (6.43) – Monomer phenyl and carbazole rings breathing 785 (86.15) – Monomer phenyl hydrogen wagging	782 (1.14) – Monomer phenyl and carbazole rings breathing 787 (21.33, 71.93) – Monomer phenyl hydrogens wagging 796 (2.26, 6.24) – Monomer out-of-plane carbazole ring bending

^a Intensities in (km/mol)

^b vs = very strong; s = strong; m = medium; w = weak; vw = very weak; sh = shoulder