Supporting information

Table 1. Optimized geometric data for HBC at B3LYP/6-311+G(d,p) level of theory

Bond lengths (Å)		Bond angles (°)		Dihedral angle (°)	
$C_1 – C_2$	1.404	$C_2 – C_1 – C_3$	121.94	$H_{15} – C_1 – C_3 – H_{16}$	-1.77
$C_2 – C_4$	1.412	$C_2 – C_1 – H_{15}$	118.80	$H_{15} – C_1 – C_3 – C_5$	177.54
$C_4 – C_6$	1.394	$H_{15} – C_1 – C_3$	119.20	$C_1 – C_3 – C_5 – C_6$	-0.48
$C_5 – C_6$	1.392	$C_1 – C_3 – H_{16}$	120.03	$C_1 – C_3 – C_5 – H_{17}$	179.87
$C_3 – C_5$	1.393	$C_1 – C_3 – C_5$	119.60	$H_{16} – C_3 – C_5 – H_{17}$	-0.80
$C_1 – C_3$	1.391	$H_{16} – C_3 – C_5$	118.70	$H_{16} – C_3 – C_5 – C_6$	178.83
$C_4 – O_{14}$	1.366	$C_3 – C_5 – H_{17}$	120.42	$C_3 – C_5 – C_6 – H_{18}$	-179.88
$O_{14} – H_{26}$	0.962	$C_3 – C_5 – C_6$	119.96	$C_3 – C_5 – C_6 – C_4$	0.12
$C_1 – H_{15}$	1.082	$H_{17} – C_5 – C_6$	119.60	$H_{17} – C_5 – C_6 – H_{18}$	-0.24
$C_3 – H_{16}$	1.083	$C_5 – C_6 – H_{18}$	120.25	$H_{17} – C_5 – C_6 – C_4$	179.77
$C_5 – H_{17}$	1.083	$C_5 – C_6 – C_4$	120.15	$C_5 – C_6 – C_4 – C_2$	0.72
$C_6 – H_{18}$	1.086	$H_{18} – C_6 – C_4$	119.48	$C_5 – C_6 – C_4 – O_{14}$	179.87
$C_2 – C_7$	1.464	$C_6 – C_4 – O_{14}$	121.75	$H_{18} – C_6 – C_4 – O_{14}$	-0.11
$C_7 – H_{19}$	1.085	$C_6 – C_4 – C_2$	121.08	$H_{18} – C_6 – C_4 – C_2$	-179.26
$C_7 – C_{13}$	1.351	$C_4 – O_{14} – H_{26}$	109.83	$H_{26} – O_{14} – C_4 – C_6$	4.75
$C_{12} – C_{13}$	1.516	$O_{14} – C_4 – C_2$	117.16	$H_{26} – O_{14} – C_4 – C_2$	-176.06
$C_{12} – H_{24}$	1.092	$C_4 – C_2 – C_1$	117.23	$C_6 – C_4 – C_2 – C_1$	-1.17
$C_{12} – H_{25}$	1.099	$C_4 – C_2 – C_7$	118.93	$C_6 – C_4 – C_2 – C_7$	-177.74
$C_{10} – C_{12}$	1.535	$C_2 – C_7 – H_{19}$	115.22	$O_{14} – C_4 – C_2 – C_1$	179.63
$C_{10} – H_{22}$	1.096	$H_{19} – C_7 – C_{13}$	115.70	$O_{14} – C_4 – C_2 – C_7$	3.06
$C_{10} – H_{23}$	1.094	$C_2 – C_7 – C_{13}$	129.05	$C_4 – C_2 – C_1 – C_3$	0.81
$C_8 – C_{10}$	1.528	$C_7 – C_{13} – C_{11}$	115.90	$C_4 – C_2 – C_1 – H_{15}$	-176.73
$C_8 – H_{20}$	1.094	$C_{13} – C_{11} – O_{27}$	121.92	$C_4 – C_2 – C_7 – H_{19}$	31.51
$C_8 – H_{21}$	1.097	$O_{27} – C_{11} – C_9$	119.81	$C_4 – C_2 – C_7 – C_{13}$	-146.98
$C_8 – C_9$	1.532	$C_{11} – C_9 – H_{29}$	105.42	$C_2 – C_7 – C_{13} – C_{11}$	-178.75
$C_9 – H_{28}$	1.092	$C_{11} – C_9 – H_{28}$	107.58	$C_2 – C_7 – C_{13} – C_{12}$	3.44
$C_9 – H_{29}$	1.099	$C_{11} – C_9 – C_8$	115.03	$H_{19} – C_7 – C_{13} – C_{12}$	-175.04
$C_9 – C_{11}$	1.524	$C_9 – C_8 – H_{20}$	109.73	$H_{19} – C_7 – C_{13} – C_{11}$	2.75
$C_{11} – O_{27}$	1.218	$C_9 – C_8 – H_{21}$	109.78	$C_7 – C_{13} – C_{12} – H_{24}$	21.79
$C_{11} – C_{13}$	1.504	$C_9 – C_8 – C_{10}$	110.41	$C_7 – C_{13} – C_{12} – H_{25}$	-94.22
		$C_8 – C_{10} – H_{22}$	109.54	$C_7 – C_{13} – C_{12} – C_{10}$	145.43
		$C_8 – C_{10} – H_{23}$	110.70	$C_7 – C_{13} – C_{11} – O_{27}$	19.64
		$C_8 – C_{10} – C_{12}$	110.81	$C_7 – C_{13} – C_{11} – C_9$	-157.69
		$C_{10} – C_{12} – H_{24}$	110.06	$C_{13} – C_{12} – C_{10} – H_{22}$	-68.20
		$C_{10} – C_{12} – H_{25}$	107.91	$C_{13} – C_{12} – C_{10} – H_{23}$	175.11
		$C_{10} – C_{12} – C_{13}$	113.45	$C_{13} – C_{12} – C_{10} – C_8$	52.86
		$C_{12} – C_{13} – C_7$	125.36	$C_{13} – C_{11} – C_9 – C_8$	-28.54
		$C_{13} – C_{12} – H_{24}$	109.82	$H_{24} – C_{12} – C_{10} – H_{22}$	55.29
		$C_{13} – C_{12} – H_{25}$	109.11	$H_{24} – C_{12} – C_{10} – H_{23}$	-61.38
				$H_{25} – C_{12} – C_{10} – H_{22}$	170.77
				$H_{25} – C_{12} – C_{10} – H_{23}$	54.09
				$H_{24} – C_{12} – C_{10} – C_8$	176.36
				$H_{25} – C_{12} – C_{10} – C_8$	-68.15
				$C_{12} – C_{10} – C_8 – H_{20}$	176.92
				$C_{12} – C_{10} – C_8 – H_{21}$	59.72
				$C_{12} – C_{10} – C_8 – C_9$	-61.19
				$H_{22} – C_{10} – C_8 – H_{20}$	-61.93
				$H_{22} – C_{10} – C_8 – H_{21}$	-179.13
				$H_{23} – C_{10} – C_8 – H_{20}$	55.51
				$H_{23} – C_{10} – C_8 – H_{21}$	-61.68
				$H_{22} – C_{10} – C_8 – C_9$	59.94
				$H_{23} – C_{10} – C_8 – C_9$	177.38
				$C_{10} – C_8 – C_9 – C_{11}$	48.84
				$C_{10} – C_8 – C_9 – H_{29}$	-69.39

$C_{10} – C_8 – C_9 – H_{28}$	172.60
$H_{20} – C_8 – C_9 – H_{28}$	-64.80
$H_{20} – C_8 – C_9 – H_{29}$	53.19
$H_{21} – C_8 – C_9 – H_{28}$	51.91
$H_{21} – C_8 – C_9 – H_{29}$	169.91
$H_{21} – C_8 – C_9 – C_{11}$	-71.84
$H_{20} – C_8 – C_9 – C_{11}$	171.43
$C_{10} – C_{12} – C_{13} – C_{11}$	-32.31
$C_8 – C_9 – C_{11} – O_{27}$	154.04
$H_{28} – C_9 – C_{11} – O_{27}$	27.66
$H_{29} – C_9 – C_{11} – O_{27}$	-85.62
$C_9 – C_{11} – C_{13} – C_{12}$	20.25

Table 2. Computed vibrational bands for HBC and their assignments

$\nu_{cal}(cm^{-1})$	IR intensity	Assignment
3687	79,8	$O_{14} – H_{26}$ stretch
3081	6,8	$C_1 – H_{15}$ and $C_3 – H_{16}$ symmetric stretch
3066	15,8	$C_3 – H_{16}$ and $C_5 – H_{17}$ symmetric stretch
3052	4,3	$C_3 – H_{16}$ and $C_5 – H_{17}$ asymmetric stretch
3044	0,5	$C_7 –H_{19}$ stretch
3028	14,3	$C_6 – H_{18}$ stretch
2967	21,6	$C_9 – H_{28}$ stretch
2949	17,1	$C_{12} – H_{24}$ stretch
2941	46,2	$H_{22} – C_{10} – H_{23}$ asymmetric stretch
2938	61	$H_{20} – C_8 – H_{21}$ asymmetric stretch
2899	41,1	$H_{22} – C_{10} – H_{23}$ and $H_{20} – C_8 – H_{21}$ symmetric stretch
2893	21,5	$C_8 – H_{21}$, $C_9 – H_{29}$, $C_{10} – H_{22}$ stretch
2884	3,6	$C_9 – H_{29}$ stretch
2864	16	$C_{12} – H_{25}$ stretch
1672	166,3	$C_{11} – O_{27}$ stretch
1578	20,7	phenyl ring stretch
1573	205,9	$C_7 – C_{13}$ stretch
1554	26,9	phenyl ring stretch
1467	20,9	$C_{ar} – H$ stretch
1447	2,5	$H_{20} – C_8 – H_{21}$ scissoring
1437	6,5	$H_{22} – C_{10} – H_{23}$ scissoring
1427	9,6	$H_{24} – C_{12} – H_{25}$ scissoring
1424	61,1	$C_{ar} – H$ stretch
1400	8,3	$H_{28} – C_9 – H_{29}$ scissoring
1326	2,5	H – cyclohexanone wagging
1314	1,1	H – cyclohexanone wagging
1309	23,4	CH_2 wagging
1300	15,7	CH_2 wagging
1292	16,7	CH_2 wagging
1276	53,9	C – H ipb in the phenyl ring
1248	10,2	CH_2 twisting (C_{12} and C_{10})
1233	56,2	CH_2 twisting (C_9)
1228	83,5	C – O ipb in phenyl ring
1213	61,6	CH_2 twisting (C_{12}, C_{10}, C_8, C_9)
1178	21,7	H_{26} and H_{19} ipb
1147	48,7	C – H ipb in the phenyl ring
1137	5	C – H ipb in the phenyl ring
1109	106,9	CH_2 twisting (C_{12}, C_{10}, C_8, C_9)
1100	34,1	CH_2 twisting (C_{12}, C_{10}, C_8, C_9)
1069	54,3	C – H ipb in the phenyl ring
1058	10,3	CH_2 wagging

1050	20,9	CH_2 twisting (C_{12}, C_{10}, C_8, C_9)
1037	1,8	CH_2 wagging
1023	6,8	C – H ipb in the phenyl ring
947	0,8	C – H opb in the phenyl ring
944	9,8	C – H opb in the phenyl ring and C – H ipb in cyclohexanone
926	9,2	C – H opb in the phenyl ring and C_7 – H_{19} opb
911	5,2	C – H opb in the phenyl ring and C_7 – H_{19} opb
899	4,2	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
867	4,6	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
845	7,5	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
825	5,5	C – H opb in the phenyl ring
821	18,3	C – H opb in the phenyl ring
800	20,9	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
773	2	C – H opb in the phenyl ring
731	67,3	C – H opb in the phenyl ring
719	1,5	C – H opb in the phenyl ring
691	7,7	C – H opb in the phenyl ring
632	3,8	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
598	0,6	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
583	11,1	CH_2 rocking (C_{12}, C_{10}, C_8, C_9)
542	28,9	C – H ipb in the phenyl ring and CH_2 rocking
502	10,3	C – H opb in the phenyl ring
472	3,6	O_{14} – H_{26} ipb and CH_2 rocking (C_{10}, C_8, C_9)
466	2,5	CH_2 rocking (C_{10}, C_8, C_{12})
413	6,6	O_{14} – H_{26} ipb and CH_2 rocking (C_{10}, C_8, C_9)
408	1,2	C – H opb in the phenyl ring and CH_2 rocking
393	93,6	O_{14} – H_{26} opb

Table 3. Experimental and calculated absorption wavelength (nm), excitation energies E(eV), oscillator strengths (f) and number of states (n) for singlet (s) and triplet (t) states

Exp.	TD-DFT				TD-DFT/I-PCM			
λ(nm)	λ(nm)	E(eV)	f	n	λ(nm)	E(eV)	f	n
	314(54→55)	3.9511	0.3034	6, s	309(54→55)	4.0139	0.3454	6, s
330	278(52→55)	4.4519	0.2224		275(52→55)	4.4995	0.1855	
284	314(54→55)	3.9512	0.3033	8, s	309(54→55)	4.0139	0.3454	8, s
	278(52→55)	4.4518	0.2225		275(52→55)	4.4994	0.1855	
	314(54→55)	3.9511	0.3033	10, s	309(52→55)	4.0119	0.3442	10, s
	278(52→55)	4.4518	0.2224		275(52→55)	4.4976	0.1866	
	314(54→55)	3.9511	0.3033	20, s	309(52→55)	4.0139	0.3454	20, s
	278(52→55)	4.4518	0.2223		275(52→55)	4.4994	0.1855	