

Supplementary information for “Effects of hydrogen dissociation on the infrared emission spectra of naphthalene: theoretical modeling”

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In this supplementary material, we summarize the spectral characteristics of the three most stable didehydronaphthalene radicals grouped by their symmetry and computed at the DFT/B3LYP/cc-pVDZ level.

TABLE I. Harmonic and fundamental frequencies and harmonic intensities for IR active modes (with $\mathcal{I} \geq 1.5 \text{ km.mol}^{-1}$) for the three most stable isomer 1,2-didehydronaphthalene, 1,3-didehydronaphthalene and 2,3-didehydronaphthalene in the S_0 electronic state calculated at the DFT/B3LYP/cc-pVDZ level and grouped according to their symmetry

1,2-didehydronaphthalene				1,3-didehydronaphthalene				2,3-didehydronaphthalene			
	Harm. freq.	Fund. freq.	Harm. intensity		Harm. freq.	Fund. freq.	Harm. intensity		Harm. freq.	Fund. freq.	Harm. intensity
A'	367.9	364.1	28.66	A'	354.1	344.0	12.97	A ₁	632.6	623.7	5.35
	405.7	400.0	69.16		462.1	361.2	72.28		1045.5	1028.5	2.43
	515.1	508.6	1.62		523.4	506.3	19.52		1093.3	1076.1	27.04
	558.6	552.2	13.90		546.9	536.7	27.37		1218.6	1198.1	2.64
	698.4	688.5	5.27		627.1	618.6	19.76		1481.4	1450.9	5.46
	789.5	779.8	2.32		747.0	732.8	3.37		3199.0	3065.1	18.52
	869.3	857.6	4.16		865.4	853.3	2.33	B ₁	358.8	352.1	3.76
	1042.2	1025.9	4.68		1028.0	1011.4	4.70		465.8	455.5	9.87
	1103.0	1087.4	18.44		1155.5	1140.4	7.33		757.3	735.6	20.64
	1110.8	1094.8	5.85		1213.4	1192.6	4.65		853.7	828.0	35.29
	1172.7	1159.0	1.88		1338.5	1309.4	16.21	B ₂	360.9	356.7	40.67
	1221.7	1203.4	2.97		1363.2	1329.6	19.19		404.3	399.9	43.75
	1237.1	1213.0	3.97		1435.9	1405.8	37.31		601.1	592.4	25.83
	1351.3	1324.2	3.96		1490.1	1458.8	7.86		892.4	879.3	9.26
	1392.1	1357.3	2.24		1548.6	1513.3	2.61		1248.9	1227.2	24.83
	1428.3	1398.4	4.51		1599.5	1559.7	20.52		1452.2	1421.6	5.96
	1529.9	1495.0	10.09		1654.2	1612.4	39.96		1656.0	1615.5	1.65
	1576.2	1537.3	7.76		1841.3	1796.9	27.58		3168.2	3023.9	1.69
	1659.1	1617.9	11.29		3169.1	3039.2	5.84		3186.0	3055.4	11.42
	3172.1	3033.6	1.83		3169.8	3033.3	8.95		3189.6	3052.5	36.65
	3181.3	3051.9	8.80		3184.2	3054.1	3.64				
	3194.5	3194.5	18.94		3191.4	3063.1	20.28				
	3205.3	3073.5	13.09		3203.1	3064.0	16.65				
	3208.3	3076.0	16.37		3212.1	3071.6	11.06				
A''	170.9	168.0	1.95	A''	156.5	153.0	3.52				
	423.7	414.8	2.29		380.5	374.0	3.35				
	510.9	499.8	1.82		469.7	458.3	2.53				
	584.9	572.3	4.69		565.8	550.9	2.24				
	735.7	713.6	4.55		615.3	596.9	1.52				
	768.9	750.2	29.91		751.4	731.9	7.00				
	820.6	798.2	32.75		775.5	752.5	44.39				
	888.5	858.9	1.83		806.5	778.3	23.69				
					882.2	850.9	3.62				