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The D-ring, Not the A-ring, Rotates in *Synechococcus* OS-B' Phytochrome

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Table 2. FWHM line-widths ($\nu_{1/2}$) of ^{13}C and ^{15}N resonances of the chromophore in SyB.Cph2(GAF). ^{13}C and ^{15}N experimental line-shapes were simulated by the Voigt function (convolution of a Lorentzian with a Gaussian at an equal ratio). The $\nu_{1/2}$ values listed (mean \pm standard deviation) were extracted from the Voigt profile (fitting spectra not shown). $\Delta\nu_{1/2}$ are reported as P690 – P630 and listed at the right-most column.

chromophore carbon	P630		P690		$\Delta\nu_{1/2}^{(P690-P630)}$ (Hz)	
	δ^{C} (ppm)	$\nu_{1/2}$ (FWHM, in Hz)	δ^{C} (ppm)	$\nu_{1/2}$ (FWHM, in Hz)		
1	182.0	168.3 \pm 22.0	183.3	177.0 \pm 22.5	+8.7	
2	35.2	433.7 \pm 45.7	36.4	1013.5 \pm 187.2	+579.8	
2'	17.2 (2 ^{1a})	341.6 \pm 44.6	17.6 (2 ^{1a})	523.1 \pm 58.7	+181.5	
	18.1 (2 ^{1b})	742.2 \pm 118.0	18.0 (2 ^{1b})	920.9 \pm 143.1	+178.7	
3	53.3 (3 ^a)	146.2 \pm 34.2	50.0 (3 ^a)	523.1 \pm 141.8	+376.9	
	53.6 (3 ^b)	691.8 \pm 43.3	52.7 (3 ^b)	1046.3 \pm 97.4	+354.5	
3'	47.4	316.7 \pm 12.3	48.4	568.2 \pm 35.8	+251.5	
3'	20.6	707.9 \pm 79.2	19.3	1207.3 \pm 84.7	+499.4	
4	156.9 (4 ^a)	271.7 \pm 58.7	156.6	173.6 \pm 33.1	-98.1	
	157.4 (4 ^b)	174.6 \pm 47.8			-1.0	
	157.9 (4 ^c)	114.6 \pm 43.1			+59.0	
A-B	85.4 (5 ^a)	151.4 \pm 54.9	86.1	274.3 \pm 27.8	+122.9	
	86.5 (5 ^b)	219.7 \pm 49.3			+54.6	
6	151.4 (6 ^a)	118.7 \pm 35.5	151.8	174.4 \pm 28.2	+55.7	
	152.1 (6 ^b)	147.6 \pm 17.5			+26.8	
7	127.4	207.2 \pm 17.1	127.2	304.3 \pm 19.7	+97.1	
7'	8.3	98.6 \pm 11.7	9.9	253.1 \pm 66.5	+154.5	
Ring B	8	147.5	121.5 \pm 20.1	146.7	196.1 \pm 16.7	+74.6
	8'	20.9	449.9 \pm 55.9	20.1	632.9 \pm 29.9	+183.0
	8'	38.5	393.4 \pm 10.0	39.1	762.4 \pm 15.1	+369.0
	8'	180.2	261.0 \pm 17.9	179.7	367.6 \pm 24.4	+106.6
9	126.4	173.6 \pm 19.5	126.6	282.9 \pm 19.4	+109.3	
B-C	112.9	148.6 \pm 19.5	113.1	210.8 \pm 28.4	+62.2	
11	130.0	152.0 \pm 8.1	129.7	352.4 \pm 27.8	+200.4	
12	138.5	149.2 \pm 20.5	138.3	294.1 \pm 36.2	+144.9	
Ring C	12'	21.3	221.0 \pm 63.6	22.3	779.3 \pm 66.5	+558.3
	12'	37.3	419.9 \pm 42.6	38.2	870.7 \pm 154.9	+450.8
	12'	177.6	188.7 \pm 7.3	177.0	475.4 \pm 28.4	+286.7
	13	123.6	121.2 \pm 20.3	124.3	144.0 \pm 8.6	+22.8
	13'	11.2	191.2 \pm 5.3	11.3	405.2 \pm 65.9	+214.0
14	140.4	192.1 \pm 9.7	140.3	225.8 \pm 12.0	+33.7	
C-D	94.7	131.1 \pm 21.1	94.6	144.4 \pm 29.7	+13.3	
16	143.6	145.5 \pm 13.1	143.4	320.1 \pm 20.9	+174.6	
17	140.9	200.6 \pm 22.2	141.3	231.6 \pm 26.1	+31.0	
Ring D	17'	8.5	207.1 \pm 4.9	8.8	392.6 \pm 25.2	+185.5
	18	132.7	128.0 \pm 10.5	132.6	215.3 \pm 22.2	+87.3
	18'	15.0	450.0 \pm 17.6	15.4	756.6 \pm 45.1	+306.6
	18'	11.3	167.3 \pm 9.4	12.3	328.7 \pm 29.1	+161.4
	19	171.7	288.7 \pm 18.0	171.0	521.5 \pm 28.6	+232.8
pyrrole nitrogen	δ^{N} (ppm)	$\nu_{1/2}$ (FWHM, in Hz)	δ^{N} (ppm)	$\nu_{1/2}$ (FWHM, in Hz)	$\Delta\nu_{1/2}^{(P690-P630)}$ (Hz)	
Ring A	21	156.6	255.0 \pm 13.3	156.0	152.7 \pm 8.8	-102.3
Ring B	22	161.7	156.4 \pm 9.8	161.7	191.5 \pm 11.0	+35.1
Ring C	23	145.4	180.5 \pm 7.3	145.6	145.5 \pm 8.2	-35.0
Ring D	24	131.9	236.9 \pm 14.4	132.0	154.9 \pm 9.0	-82.0