

Chemical shifts (in hertz) of selected proton of
cyclophane **2** at various concentration and temperature

	-20 °C	-10 °C	0 °C	15 °C	25 °C
100 mg/mL	3666.87 Hz 3565.71 Hz	3682.88 Hz 3581.89 Hz	3699.76 Hz 3598.83 Hz	3724.29 Hz 3623.92 Hz	3739.51 Hz 3957.84 Hz
80 mg/mL	3679.05 Hz 3577.86 Hz	3697.70 Hz 3596.31 Hz	3713.58 Hz 3612.38 Hz	3737.94 Hz 3637.57 Hz	3752.61 Hz 3977.06 Hz
60 mg/mL	3688.64 Hz 3587.27 Hz	3704.14 Hz 3603.12 Hz	3721.92 Hz 3620.97 Hz	3746.67 Hz 3646.52 Hz	3760.77 Hz 3989.06 Hz
40 mg/mL	3704.72 Hz 3603.45 Hz	3722.23 Hz 3621.04 Hz	3739.24 Hz 3638.39 Hz	3762.78 Hz 3662.52 Hz	3775.31 Hz 4010.38 Hz
20 mg/mL	3729.35 Hz 3628.14 Hz	3746.17 Hz 3645.13 Hz	3762.83 Hz 3662.20 Hz	3782.06 Hz 3682.03 Hz	3791.65 Hz 4034.26 Hz
12 mg/mL	3746.87 Hz 3645.71 Hz	3764.86 Hz 3664.17 Hz	3777.61 Hz 3677.23 Hz	3793.37 Hz 3693.53 Hz	3800.71 Hz 4047.44 Hz
7.2 mg/mL	3761.29 Hz 3660.24 Hz	3778.13 Hz 3677.55 Hz	3789.01 Hz 3688.24 Hz	3801.29 Hz 3701.59 Hz	3806.57 Hz 4055.96 Hz
4.32 mg/mL	3776.60 Hz 3675.70 Hz	3789.76 Hz 3688.80 Hz	3798.64 Hz 3697.92 Hz	3807.49 Hz 3707.93 Hz	3811.01 Hz 4062.39 Hz
2 mg/mL	3799.89 Hz 3698.82 Hz	3806.50 Hz 3705.55 Hz	3811.09 Hz 3710.57 Hz	3814.54 Hz 3715.11 Hz	3815.80 Hz 4067.83 Hz
Dimerization constant (M ⁻¹)	53.46 51.73 <u>52.60</u>	31.04 31.47 <u>31.26</u>	19.56 23.88 <u>21.72</u>	9.09 9.66 <u>9.37</u>	5.41 5.71 <u>5.52</u>

Chemical shifts (in hertz) of selected proton of

cyclophane **3** at various concentration and temperature

	15°C	20°C	25°C	33°C	40°C
49 mg/mL	3779.49 Hz 3659.58 Hz	3785.50 Hz 3662.13 Hz	3791.09 Hz 3660.20 Hz	3798.05 Hz 3673.80 Hz	3802.67 Hz 3668.37 Hz
39.2 mg/mL	3785.06 Hz 3664.90 Hz	3790.55 Hz 3668.40 Hz	3795.89 Hz 3663.64 Hz	3802.05 Hz 3677.35 Hz	3805.93 Hz 3670.81 Hz
29.4 mg/mL	3792.04 Hz 3670.18 Hz	3796.59 Hz 3673.59 Hz	3801.01 Hz 3676.24 Hz	3806.15 Hz 3680.90 Hz	3809.40 Hz 3673.43 Hz
19.6 mg/mL	3799.74 Hz 3676.69 Hz	3803.57 Hz 3679.54 Hz	3806.76 Hz 3671.27Hz	3810.54 Hz 3684.71 Hz	3812.86 Hz 3675.96 Hz
9.8 mg/mL	3809.29 Hz 3684.76 Hz	3811.56 Hz 3686.34 Hz	3813.40 Hz 3675.97 Hz	3815.51 Hz 3689.05 Hz	3816.82 Hz 3678.91 Hz
4.9 mg/mL	3817.97 Hz 3692.09 Hz	3818.81 Hz 3691.20 Hz	3819.27 Hz 3680.01 Hz	3818.84 Hz 3691.94 Hz	3819.39 Hz 3680.85 Hz
2.94 mg/ mL	3818.33 Hz 3692.38 Hz	3819.01 Hz 3692.70 Hz	3819.80 Hz 3681.51 Hz	3819.91 Hz 3692.87 Hz	3820.18 Hz 3681.42 Hz
0.98 mg/mL	3820.83 Hz 3692.46 Hz	3821.05 Hz 3694.43 Hz	3821.10 Hz 3681.38 Hz	3821.16 Hz 3693.98 Hz	3821.07 Hz 3682.09 Hz
0.49 mg/mL	3820.97 Hz 3694.60 Hz	3821.13 Hz 3694.49 Hz	3821.14 Hz 3681.40 Hz	3821.13 Hz 3693.93 Hz	Data identical with the above cell
Dimerization constant (M ⁻¹)	5.28 5.44 <u>5.36</u>	4.49 4.60 <u>4.55</u>	3,68 3,64 <u>3.66</u>	2.73 2.72 <u>2.72</u>	2.00 2.03 <u>2.02</u>

Chemical shifts (in hertz) of selected proton of
cyclophane **4** at various concentration and temperature

	0 °C	12 °C	33 °C	40 °C
20 mg/mL	3651.09 Hz 3588.51 Hz	3701.50 Hz 3624.22 Hz	3780.80 Hz 3686.46 Hz	
16 mg/mL	3676.99 Hz 3608.02 Hz	3720.54 Hz 3639.84 Hz	3776.05 Hz 3682.23 Hz	3780.11 Hz 3690.71 Hz
14 mg/mL	3678.98 Hz 3610.07 Hz	3724.84 Hz 3643.37 Hz	3777.70 Hz 3683.68 Hz	3789.54 Hz 3692.75 Hz
12 mg/mL	3685.59 Hz 3615.37 Hz	3731.85 Hz 3651.09 Hz	3782.36 Hz 3687.54 Hz	3793.14 Hz 3695.72 Hz
10 mg/mL	3695.72 Hz 3623.41 Hz	3740.65 Hz 3656.32 Hz	3787.41 Hz 3691.71 Hz	3797.75 Hz 3699.47 Hz
6 mg/mL	3736.96 Hz 3656.03 Hz	3772.88 Hz 3682.55 Hz	3806.26 Hz 3707.10 Hz	3813.16 Hz 3712.12 Hz
3.6 mg/mL	3769.86 Hz 3681.68 Hz	3794.50 Hz 3699.85 Hz	3817.03 Hz 3715.82 Hz	3821.27 Hz 3718.76 Hz
2.16 mg/mL	3790.05 Hz 3697.83 Hz	3808.38 Hz 3710.79 Hz	3823.20 Hz 3720.79 Hz	3825.90 Hz 3722.47 Hz
0.86 mg/mL	3815.30 Hz 3716.62 Hz	3823.00 Hz 3722.14 Hz	3829.19 Hz 3725.59 Hz	3830.48 Hz 3726.25 Hz
Dimerization constant (M ⁻¹)	58.93 56.70 <u>57.82</u>	33.01 29.53 <u>31.77</u>	20.88 19.81 <u>20.53</u>	14.75 14.85 <u>14.80</u>