Supporting Information

Local Ordering at Mobile Sites in Proteins from NMR Relaxation: the Role of Site Symmetry

Oren Tchaicheeyan,[1] Jack H. Freed[2,*] and Eva Meirovitch[1,*]

[1]The Mina and Everard Goodman Faculty of Life Sciences, Bar-Ilan University, Ramat-Gan 52900 Israel; [2]Baker Laboratory of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853-1301, U.S.A

*Corresponding authors: eva.meirovitch@biu.ac.il, phone: 972-3-531-8049; jhf3@cornell.edu, phone: 1-607-255-3647.

Table S1. Relevant Part of the D_{2h} Point Group Character Table. [a]

	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	linear	quadratic
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

[a] The symmetry operations are E (identity), C_2 (two-fold rotation), i (inversion) and σ (reflection). x, y and z are the Cartesian coordinates.[1]

Table S2. The Functions $D^{L}_{00}(0, \theta, 0)$ for L = 1–4.[2]

L	$D^{L}_{00}(0, \theta, 0)$
1	$\cos\ \theta$
2	$\left(\frac{1}{2}\right)[3\ cos^2\ \theta - 1]$
3	$\left(\frac{1}{2}\right)\cos\theta\ [5\ cos^2\ \theta - 3]$
4	$\left(\frac{1}{8}\right)\{[35\ cos^2\ \theta - 30]\ cos^2\ \theta + 3\}$

Table S3. Real Spherical Harmonics.[1,3]

real spherical harmonics	corresponding atomic orbitals	definition in terms of Cartesian coordinates	D_{2h} point group symmetry
Y_{10}	p_z	$\sqrt{\frac{3}{4\pi}} \cdot \frac{z}{r}$	B_{1u}
$\sqrt{\frac{1}{2}}\ (Y_{1-1} - Y_{11})$	p_x	$\sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r}$	B_{3u}
$i\sqrt{\frac{1}{2}}\ (Y_{1-1} + Y_{11})$	p_y	$\sqrt{\frac{3}{4\pi}} \cdot \frac{y}{r}$	B_{2u}
Y_{20}	d_{z^2}	$\frac{1}{4}\sqrt{\frac{5}{\pi}} \cdot \frac{2z^2 - x^2 - y^2}{r^2}$	A_g
$\sqrt{\frac{1}{2}}\ (Y_{2-2} + Y_{22})$	$d_{x^2-y^2}$	$\frac{1}{4}\sqrt{\frac{15}{\pi}} \cdot \frac{x^2 - y^2}{r^2}$	A_g

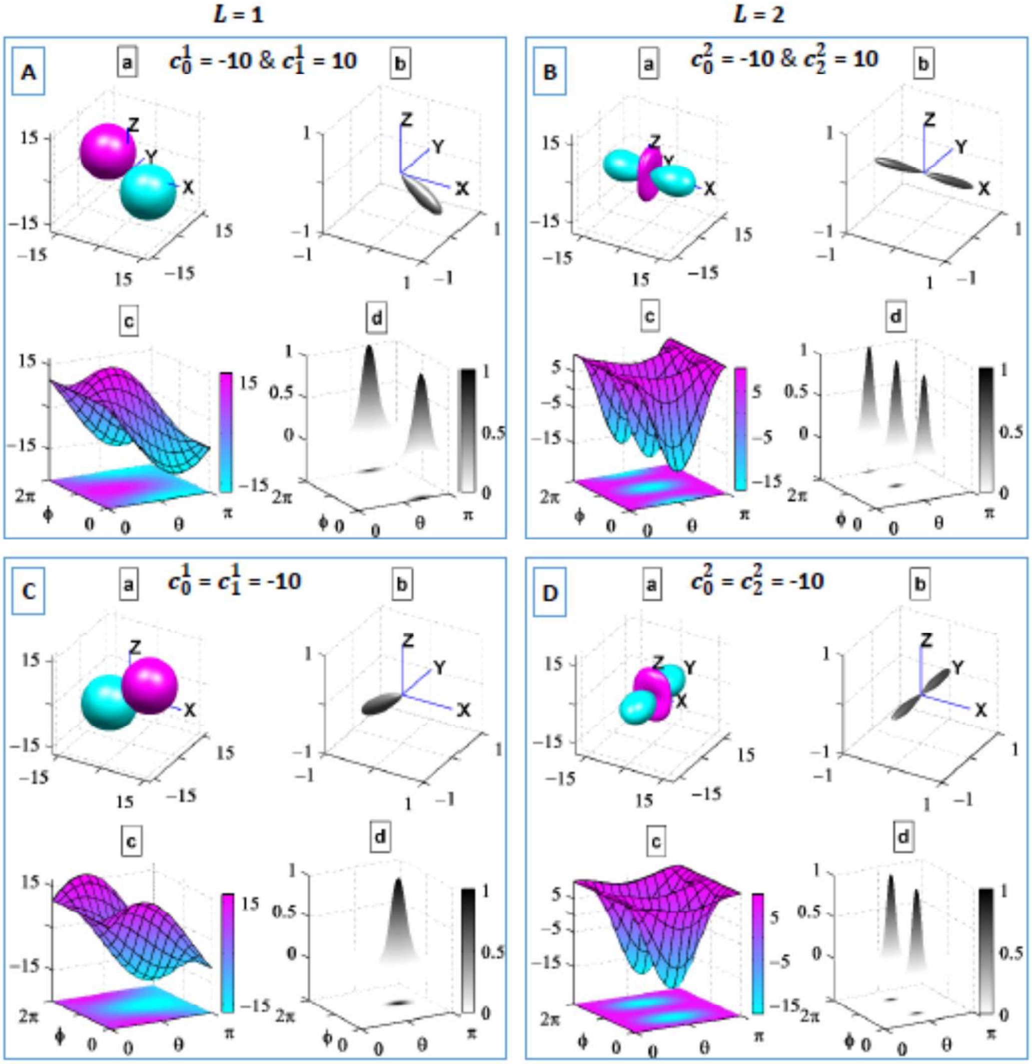

Figure S1. 4-panel representations of the scenarios L = 1, K = 0, 1 $c_0^1 = -10$ and $c_1^1 = 10$ (part *A*); L = 2, K = 0, 2, $c_0^2 = -10$ $c_2^2 = 10$ and (part *B*). 4-panel representations of the scenarios L = 1, K = 0, 1 $c_0^1 = -10$ and $c_1^1 = -10$ (part *C*); L = 2, K = 0, 2, $c_0^2 = -10$ $c_2^2 = -10$ and (part *D*). The potential, u, is represented in Cartesian coordinates in panels *a* and in spherical coordinates in panels *c*. The probability density function, exp(–u), is represented in Cartesian coordinates in panels *b* and in spherical coordinates in panels *d*. Further details are given in the text.

References

1. *e-Chemical Portal, D_{2h} point group*, http://www.webqc.org/printable-symmetrypointgroup-d2h.html.
2. de Gennes, P. G.; Prost, J. The Physics of Liquid Crystals, Oxford Universiy Press, **1993**.
3. Zare, R. N. *Angular Momentum*, Wiley, Ch. 5, Application 13, p.226, **1988**.