Electronic supplementary information for Journal of Materials Chemistry

Ring Effect on Helical Twisting Power of Optically Active Mesogenic Esters Derived from Benzene, Bicyclo[2.2.2]octane and *p*-Carborane Carboxylic Acids.

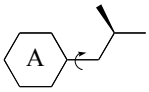
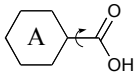
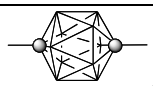
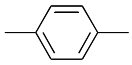
Adam Januszko, Piotr Kaszynski*, and Witold Drzewinski§

Organic Materials Research Group

Department of Chemistry, Vanderbilt University, Nashville, TN 37235

§ *Military Technical University, Warsaw, Poland*

Table S1. Computed Barriers to Internal Rotation at T = 298K.

A	Method [a]	 **3**			 **4**		
		$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
		[kcal/mol]			[kcal/mol]		
 **A**	B3LYP	1.4	0.9	2.3	0.0	-0.6	1.2
	MP2	2.1	1.6	3.0	0.0	-0.6	1.2
 **B**	B3LYP	3.3	2.8	4.2	0.6	0.0	1.9
	MP2	4.3	3.8	5.2	0.9	0.3	2.2
 **C**	B3LYP	3.6	3.0	4.6	7.5	7.1	8.2
	MP2	4.5	3.9	5.5	6.2	5.8	6.8
		CH_3–CH_3 [b]					
	B3LYP	2.6	2.3	2.7			
	MP2	2.9	2.6	3.1			

[a] Calculations at the B3LYP/6-31G(d) or MP2/6-31G(d) (with B3LYP/6-31G(d) thermodynamic corrections) level of theory. $\Delta E^{\ddagger}$ is a difference in SCF energies corrected for ZPE. $E_a = \Delta H^{\ddagger} + RT$. The calculated negative enthalpy of activation reflects a general deficiency of the DFT methods in precise calculations of low frequency vibrational modes.

[b] Experimental torsional potential is 2.9 kcal (Hirota, E.; Saito, S.; Endo, Y. *J. Chem. Phys.* 1979, **71**, 1183-1187)

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Computational Details

Quantum-mechanical calculations were carried out using Gaussian 98 suite of programs. Geometry optimizations were undertaken at the B3LYP/6-31G(d) and MP2/6-31G(d) levels of theory using appropriate symmetry constraints and tight convergence limits. The rotational transition states were located using the QST2 keyword. Thermodynamic correction parameters were obtained at the B3LYP/6-31G(d). Zero-point energy (ZPE) corrections were scaled by 0.9806.

Gaussian 98, Revision A.7, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 1998.