

Corrigendum

Rotational Isomerism in 1,1'-Dinitrobicyclopentyl, 1,1'-Dinitrobicyclohexyl and 1,1'-Dinitrobicycloheptyl

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Page 2035: *Delete* Table 5 and *replace* with the following.

Table 5 Comparison between 1,1'-dinitro- and 1,1'-dicyano-bicycloalkanes

Compound	ΔE^+ /kJ mol ⁻¹		Torsion angle of <i>gauche</i> rotamer/°		% <i>gauche</i> population		Barrier height/kJ mol ⁻¹ between <i>gauche</i> and <i>trans</i> forms AM1
	Experimental ^d	AM1	Experimental	AM1	Experimental	AM1	
1,1'-Dinitrobicyclopentyl ^a	-2.25	-1.69	67	58	83	80	21.82
1,1'-Dinitrobicyclohexyl ^b	2.59	1.44	90	59	42	53	32.68
1,1'-Dinitrobicycloheptyl ^b	5.99	5.82	64	57	16	16	49.92
	Experimental	MMP2	Experimental	MMP2	Experimental	MMP2	MMP2
1,1'-Dicyanobicyclopentyl ^c	9.28	10.71	85	61	4.5	2.5	22.34
1,1'-Dicyanobicyclohexyl ^c	6.60	11.17	86	60	11	2	27.48
1,1'-Dicyanobicycloheptyl ^c	3.05	3.51	67	52	38	33	30.25

^a AM1 calculations with full geometry optimization. ^b AM1 calculations using fixed geometries. ^c MMP2 calculations with full geometry optimization. ^d Experimental values are based on the Lennard-Jones-Pike method of calculation using data from measurements on CCl₄ solutions. ΔE^+ is defined as $E(\textit{gauche}) - E(\textit{trans})$.

Non-linear Brønsted Correlations: Evidence for a Levelling Off in the Reactivity of Oximate Ions in Aqueous Solution

François Terrier,* Patricio MacCormack, Elyane Kizilian, Jean-Claude Hallé, Pierre Demerseman, Frédéric Guir and Claude Lion

J. Chem. Soc., Perkin Trans. 2, 1991, 153

Page 157: *Delete* eqn. (13) and *replace* with

$$k_{\text{app}} = \frac{1}{[\text{PNPA}]_0} \left(\frac{d[\text{PNP}^-]}{dt} \right)_0 = \frac{k_0 + \frac{k_1 B + k_2 C}{A} [\text{Ox}]_0}{1 + 10^{7.05 - \text{pH}}} \quad (13)$$

Page 158: *Delete* eqn. (17) and *replace* with

$$k_{\text{app}} = \frac{1}{[\text{PNPA}]_0} \left(\frac{d[\text{PNP}^-]}{dt} \right)_0 = k_0 + k_2 [\text{Ox}]_0 \quad (17)$$