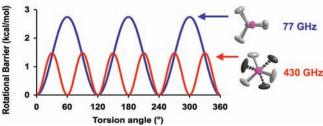


Ultra-fast Rotors for Molecular Machines and Functional Materials via Halogen Bonding: Crystals of 1,4-Bis(iodoethynyl)-bicyclo[2.2.2]octane with Distinct Gigahertz Rotation at Two Sites [Journal of the American Chemical Society 2011, 133, 6371–6379. DOI: 10.1021/ja200503j]. Cyprien Lemouchi, Cortnie S. Vogelsberg, Leokadiya Zorina, Sergey Simonov, Patrick Batail,* Stuart Brown,* and Miguel A. Garcia-Garibay*

The exponents for the frequency factors listed in the abstract (p 6371), in the text (p 6376), and in Table 1 (p 6377) were incorrectly reported due to transcription error of the decimal point. Specifically, the pre-exponential factors (A) for rotation in the ordered and disordered layers of 1,4-bis(iodoethynyl)-bicyclo[2.2.2]octane (BIBCO) were incorrectly listed in the article as 8.00×10^{10} and 5.21×10^{10} s⁻¹, respectively. The correct values for the two layers are 8.00×10^{12} and 5.21×10^{12} s⁻¹. Their corresponding time constants (τ_0) are 1.25×10^{-13} and 1.92×10^{-13} s. Note that the relative magnitude of the values with respect to one another, and their analysis throughout the paper, remains the same. However, the correct pre-exponential factors result in calculated rates of room temperature rotation with values of 77 GHz for BIBCO rotators in the ordered layer and 430 GHz in the disordered layer. This correction affects values reported in the abstract and in the table of contents graphic, which is shown here in its corrected form:

Bicyclo[2.2.2]octane Rotation in 3-Fold and 6-Fold Potentials



DOI: 10.1021/ja2062665 Published on Web 08/03/2011

