Supporting Information

Concise Synthesis of an Amide-Functionalized [7]Helicene-like Molecule via Intramolecular Amidation

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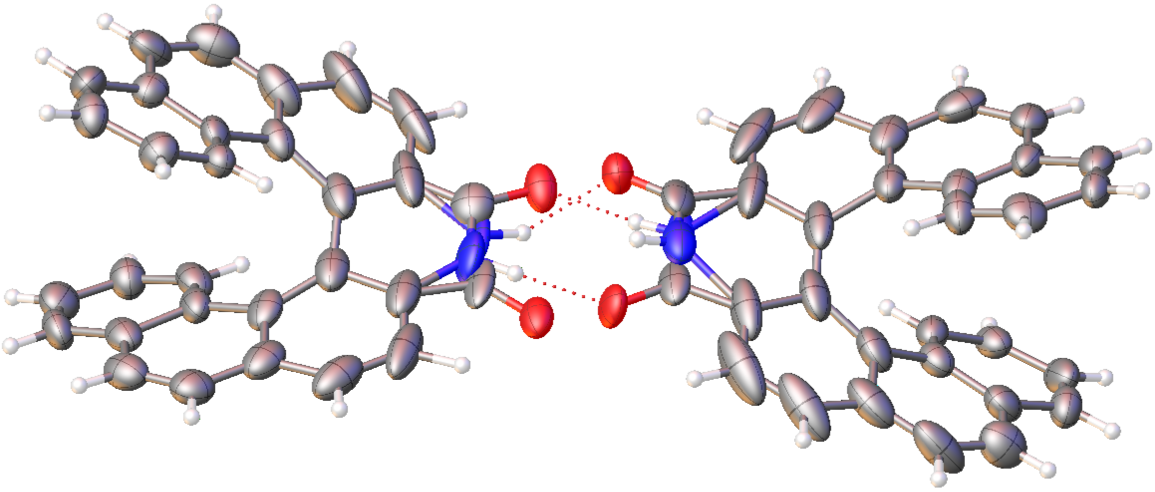
Content:

Crystal structure of (*dl*)-**5**

(full disordered structure, 50% probability)



Crystallographic data for the single crystal of (*dl*)-**5** obtained by recrystallization from *n*-hexane-toluene: $C_{29}H_{17}NO$, M = 395.43, monoclinic, $P2_1$, $a = 9.0465(2)$, $b = 11.3071(3)$, $c = 19.1900(5)$ Å, $\alpha = 90°$, $\beta = 95.411(2)°$, $\gamma = 90°$, $V = 1954.19(8)$ Å^3, $Z = 4$, $\rho_{\mathrm{calcd}} = 1.317$ gcm^{-3}, $T = 103$ K, 22156 reflections measured, 7194 unique. The final R_1 and wR were 0.0587 and 0.1787 (all data). These data have been deposited with the Cambridge Crystallographic Data Center as CCDC 2031916.

Computational details for an estimation of the racemization barrier of 5

Density functional theory (DFT) calculations were performed using the Gaussian 16 software package. 1) The molecular geometries for the transition states (TS) were first estimated with the *Reaction plus* software package, based on the nudged elastic band method,2) and were subsequently re-optimized using the Gaussian 16 software package. Once the stationary points were obtained at B3LYP/6-31G (d,p) level,3) the harmonic vibrational frequencies were calculated at the same level to estimate the Gibbs free energy. The nature of the stationary points was characterized via vibrational analysis. All of the Gibbs free energy values reported in this paper were calculated for a temperature of 298.15 K. All of the transition structures reported were optimized without constraints and the intrinsic reaction coordinate (IRC) routes were calculated in both directions toward the corresponding minima for the transition-state structure. For each gas-phase optimized structure (potential energy minimum or transition state computed at B3LYP/6-31G (d,p) level of theory), additional single-point energy calculations were performed at ωB97XD/6-311+G(d,p) level of theory,4) in which solvent effects were also taken into account by estimating the solvation free energies (for chlorobenzene as solvent).

References

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