Supplementary Material (ESI) for Chemical Communications

Supporting Information

Conformational Control in the Regioselective Synthesis of N-2 Substituted-1,2,3-Triazoles

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X-ray Crystal Analysis:

Single crystal X-ray diffraction data collection was carried out on the four-circle of a Siemens P4 diffractometer equipped with a graphite monochromator, a monocap collimator, a Mo Kα radiation source (λ = 0.71073 Å), and a SMART CCD detector held at 5.082 cm from the crystal. The program SMART (version 5.6)[1] was used for diffractometer control, frame scans, indexing, orientation matrix calculations, least-squares refinement of cell parameters, and the data collection. All 1650 crystallographic raw data frames were read by program SAINT (version 5/6.0)[1] and integrated using 3D profiling algorithms. An semi-empirical absorption correction was applied using the SADABS routine available in SAINT.[1] The crystal structure was solved by a The structure was solved by a combination of direct methods and difference Fourier analysis with the use of SHELXTL 6.1.[2] Idealized positions for the hydrogen atoms were included as fixed contributions using a riding model with isotropic temperature factors set at 1.2 (aromatic and olefinic protons) or 1.5 (methyl protons) times that of the adjacent carbon atom. The linear absorption coefficient, atomic scattering factors, and anomalous dispersion corrections were calculated from values found in the International Tables of X-ray Crystallography.[4]

Reference:

1. SMART, SAINT and XPREP programs are part of Bruker crystallographic software package for single crystal data collection, reduction and preparation.
2. Sheldrick, G. M., SHELXTL6.1 (2000), Crystallographic software package, Bruker AXS, Inc. Madison, Wisconsin, USA.
3. International Tables for X-ray Crystallography (1974). Vol. IV, p. 55. Birmingham: Kynoch Press. (Present distributor, D. Reidel, Dordrecht.).

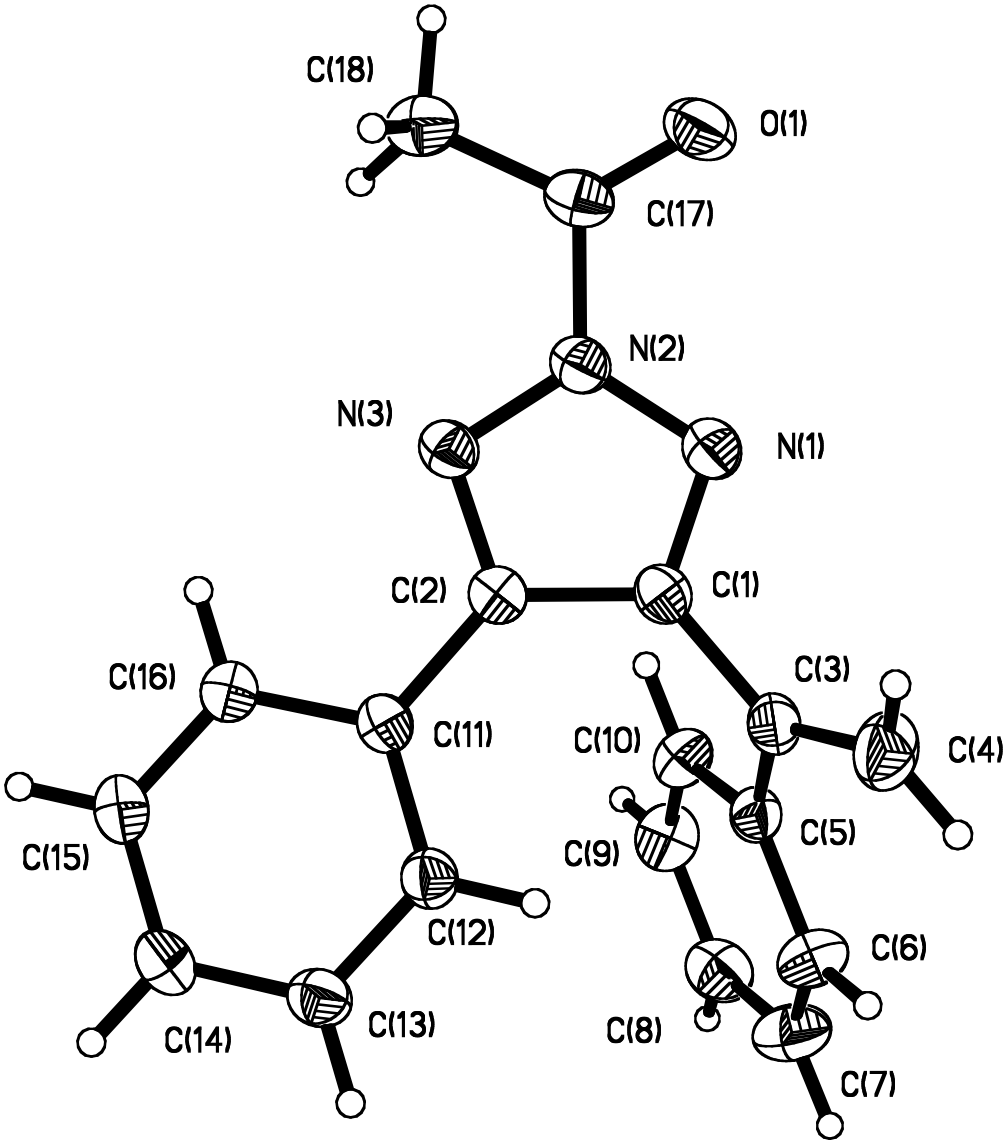

Figure 1. Perspective view of the molecular structure of **2a** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

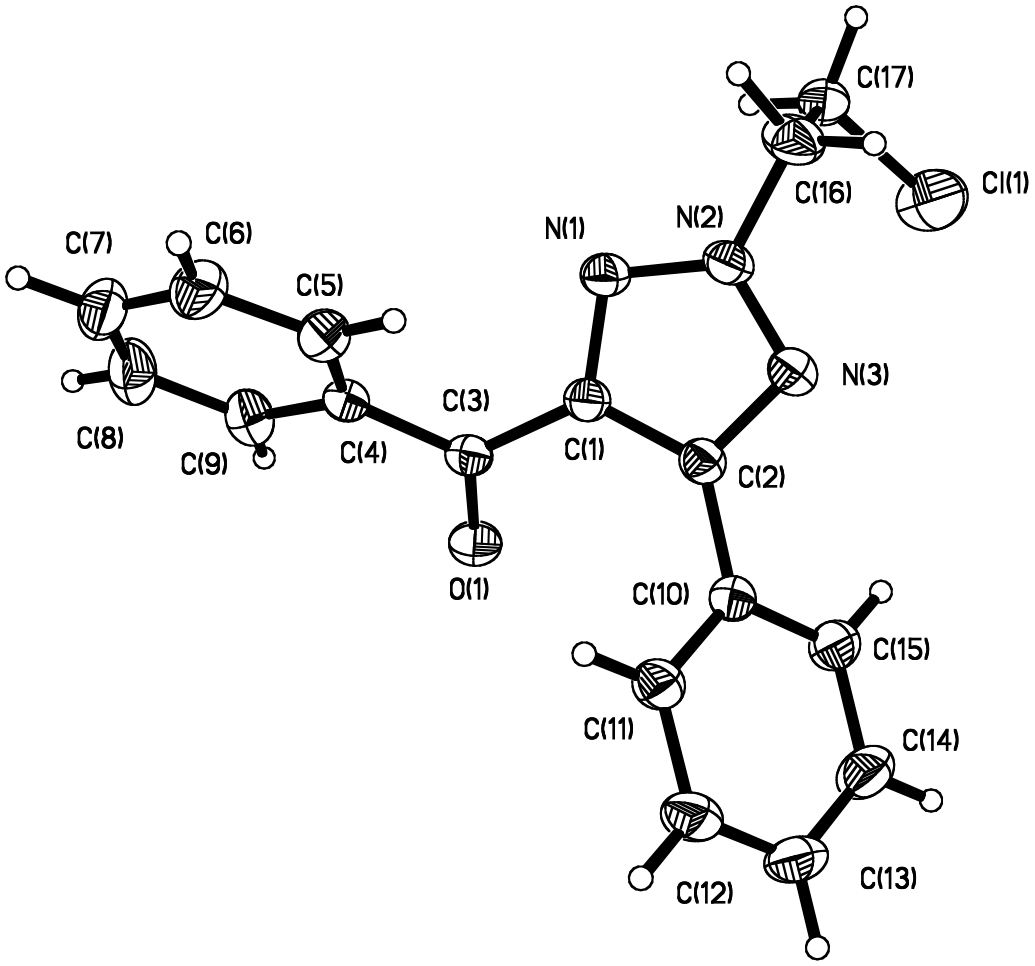

Figure 2. Perspective view of the molecular structure of **7d** with the atom labeling scheme. The positions of atoms C(16), C(17), and Cl(1) exhibit a 2:1 conformational disorder within the lattice. The thermal ellipsoids are scaled to enclose 30% probability.

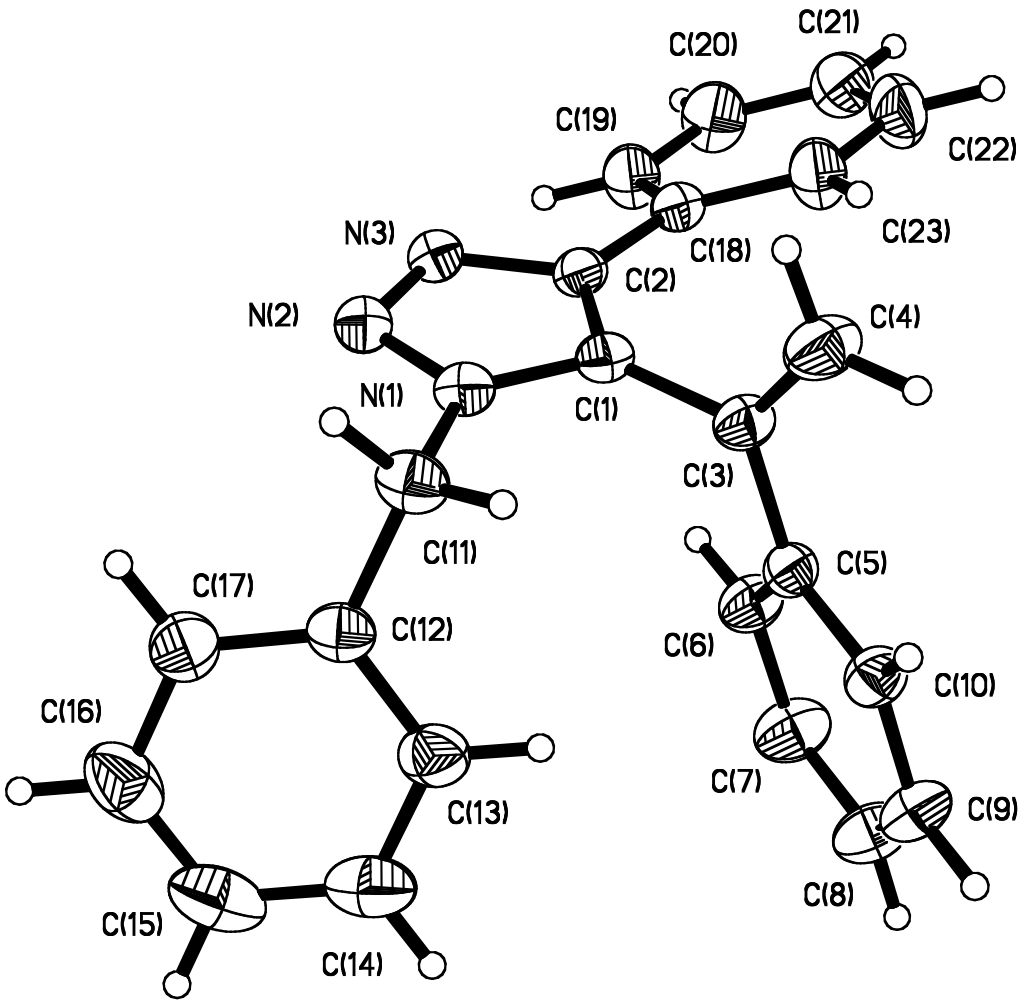

Figure 3. Perspective view of the molecular structure of **N-1-3a** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

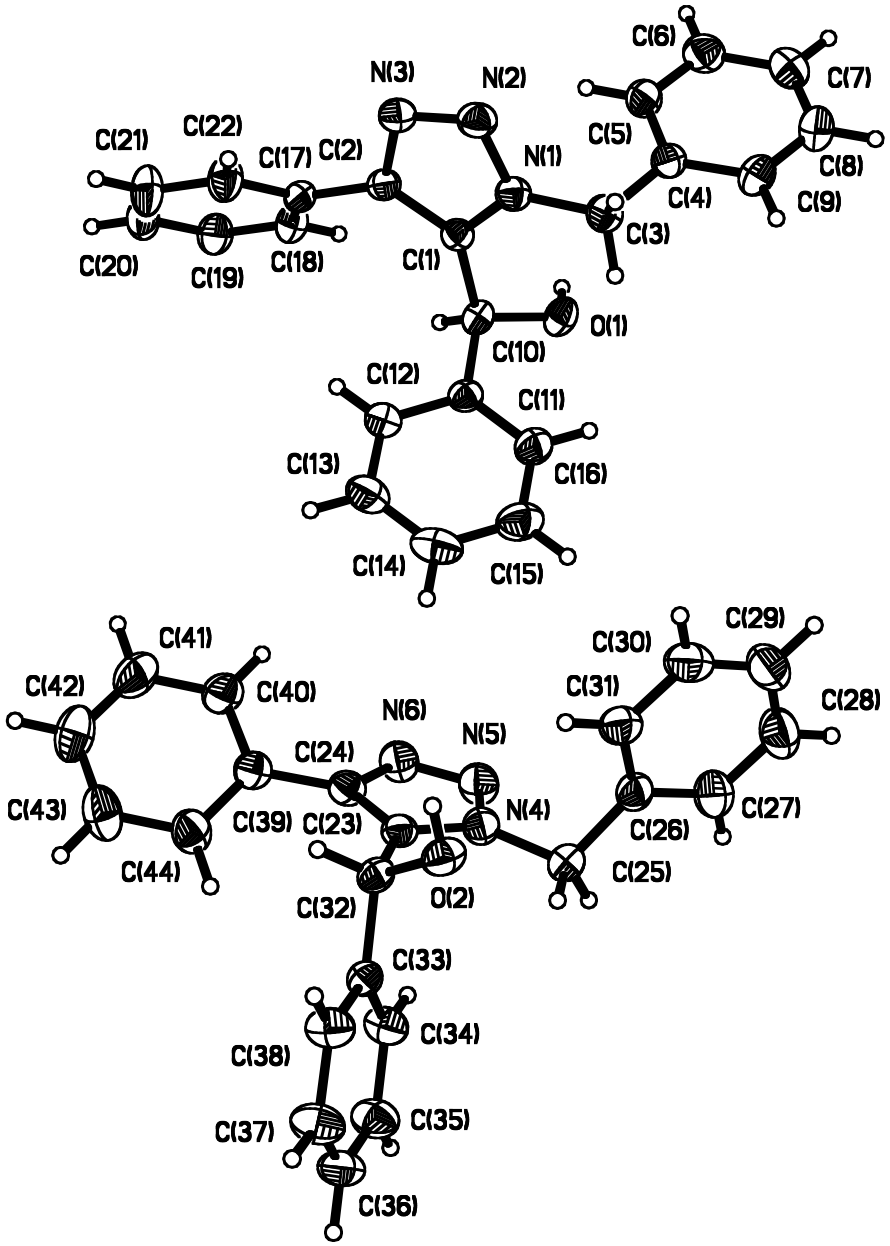

Figure 4. Perspective view of the molecular structures of the two independent molecules of $C_{22}H_{19}N_3O$ with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

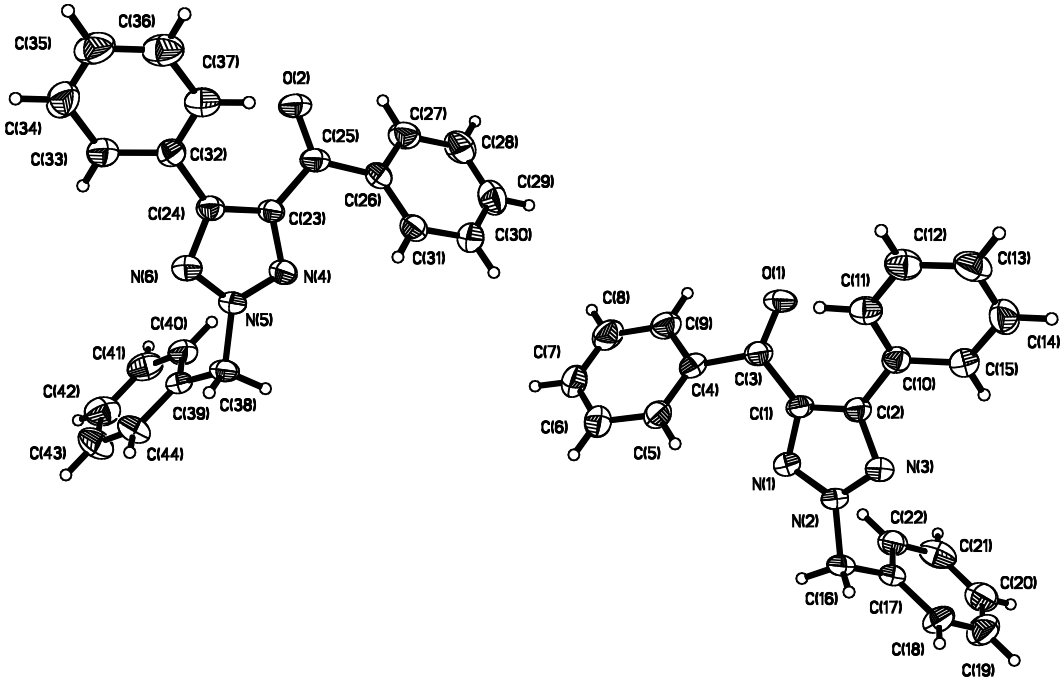

Figure 5. Perspective view of the two independent molecules of **N-2-4a (7a)** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.