

## **Stereoselective synthesis of ring C-hexasubstituted trianglamines**

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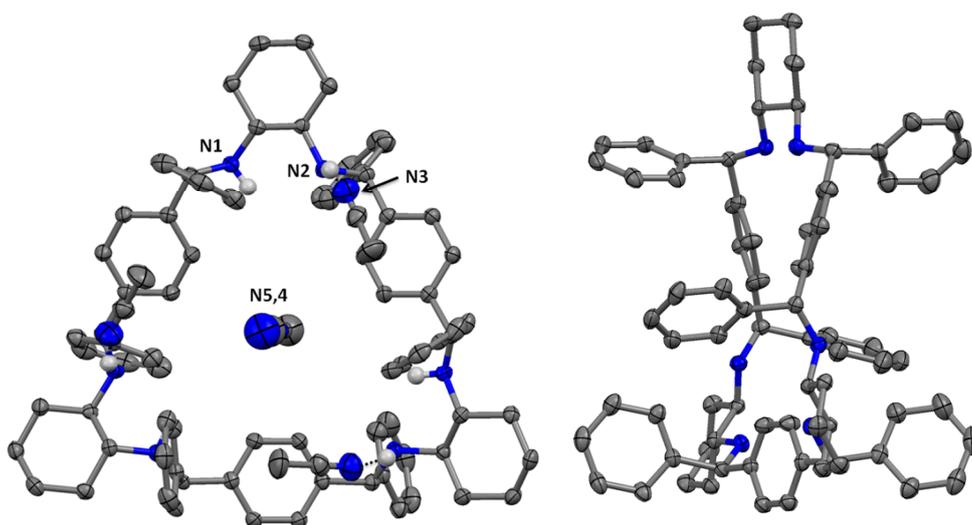
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### **Supplementary Data**

## X-ray crystallography

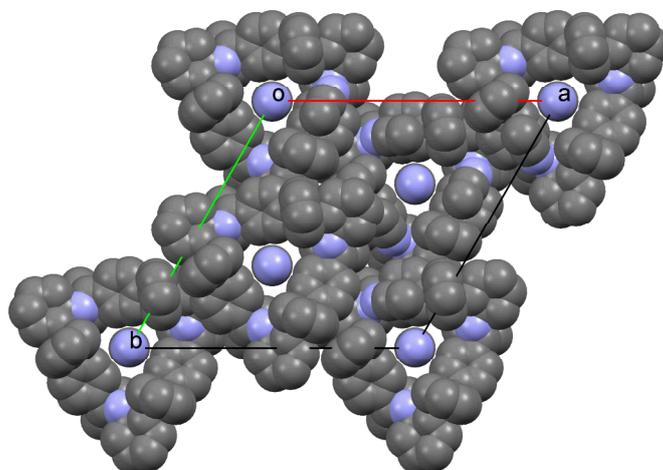
Suitable crystals of **3c•4(CH<sub>3</sub>CN) solvate** were obtained as colourless blocks by slow evaporation of a solution in acetonitrile. The intensity data were collected at 173K (-100°C) on a Stoe Mark II-Image Plate Diffraction System<sup>1</sup> equipped with a two-circle goniometer and using MoK $\alpha$  graphite monochromated radiation. Image plate distance 100 mm,  $\omega$  rotation scans 0 - 180° at  $\phi$  0°, step  $\Delta\omega$  = 1.0°, with an exposure time of 6 mins per image,  $2\theta$  range 2.29 - 59.53°,  $d_{\min}$  -  $d_{\max}$  = 17.779 - 0.716 Å. The structure was solved by Direct methods using the program SHELXS.<sup>2</sup> The refinement and all further calculations were carried out using SHELXL-97.<sup>2</sup> The NH H-atoms were refined with distance restraints N-H = 0.88(2) Å, while the C-bound H-atoms were included in calculated positions and treated as riding atoms using SHELXL default parameters. The non-H atoms were refined anisotropically, using weighted full-matrix least-squares on  $F^2$ . In the final cycles of refinement, in the absence of significant anomalous scattering effects, 3231 Friedel pairs were merged and  $\Delta f'$  set to zero.

The molecule has crystallographic  $C_3$  symmetry, and crystallizes with 4 molecules of acetonitrile. Three acetonitrile molecules are hydrogen bonded to the NH groups, one on each side of the triangle. The fourth molecule is disordered about 2 positions sitting on the threefold axis in the center of the triangle. The molecular structure is illustrated in Figure 1, drawn using the program Mercury.<sup>3</sup>



**Figure 1.** Views of the molecular structure of **3c•4(CH<sub>3</sub>CN) solvate** [the C-bound H-atoms have been omitted for clarity].

In the crystal the molecules stack along [001] creating columns with the channels filled with acetonitrile molecules, see Figure 2.



**Figure 2.** A CPK view, along the *c*-axis, of the crystal packing of compound **3c.4(CH<sub>3</sub>CN) solvate** [the H-atoms have been omitted for clarity].

Crystallographic data (excluding structure factors) for this structure have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 759763. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: (internat.) +44-1223/336-033; E-mail: [deposit@ccds.cam.ac.uk](mailto:deposit@ccds.cam.ac.uk)].

Acknowledgements: We are grateful to the XRD Application LAB, Microsystems Technology Division, Swiss Center for Electronics and Microtechnology, Neuchâtel, for access to the X-ray diffraction equipment.

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