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Supporting Information

for

The C=N…C—X σ-Hole Interaction Acts as a Conformational Lock

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X-Ray structure determination

The selected crystal was mounted in inert oil on glass fibers. Data were measured using Mo-Ka radiation on a Bruker SMART 1000 CCD diffractometer. Data collection at 296 K and reduction were performed using SMART and SAINT software.[1]

Absorption correction was applied using the multi-scan method (SADABS).[2] The crystal structures of **1** and **9** were solved by direct methods and refined by full matrix least-squares on F^2 using the SHELXTL program package.[3] All non-hydrogen atoms were subjected to anisotropic refinement and all H atoms were located in difference Fourier maps and their atomic coordinates and isotropic displacement parameters were refined freely. The cyano group in **9** was found to be disordered, the atoms C3 and N3 were therefore modelled over two sets of positions, respectively.

1 SMART 5.0 and SAINT 4.0 for Windows NT, Area Detector Control and Integration Software, Bruker Analytical X-Ray Systems Inc., Madison, WI, 1998.

2 G. M. Sheldrick, SADABS: Program for Empirical Absorption Correction of Area Detector Data, University of Göttingen, Germany, 1996.

3 G. M. Sheldrick, SHELXTL 5.1 for Program for Windows NT: Structure Determination Software Programs, Bruker Analytical X-Ray Systems, Inc., Madison, WI, 1997.