Electronic Supplementary Material (ESI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2019

Ferromagnetic Interactions in a 1D Heisenberg Linear Chain of 1-Phenyl-3,7-bis(trifluoromethyl)-1,4-dihydro-1,2,4-benzotriazin-4-yls

Electronic Supporting Information

Christos P. Constantinides,*[a] Daniel B. Lawson,[a] Andrey A. Berezin,[b] Georgia A. Zissimou,[b] Maria Manoli,[b] Gregory M. Leitus,[c] Panayiotis A. Koutentis[b]

[a] Department of Natural Sciences, University of Michigan – Dearborn, 4914 Evergreen Road, Dearborn, MI 48128-1491, United States. E-mail: cconst@umich.edu Fax: +01 3135934937 Tel: +01 3135836728

[b] Department of Chemistry, University of Cyprus, P.O. Box 20537, 1678 Nicosia, Cyprus

[c] Department of Organic Chemistry, Weizmann Institute of Science, 76100 Rehovot, Israel

Table of Contents

Fig. S1. ORTEP diagrams (ellipsoids shown at 50% probability level) of radical **2** showing both components of disorder.

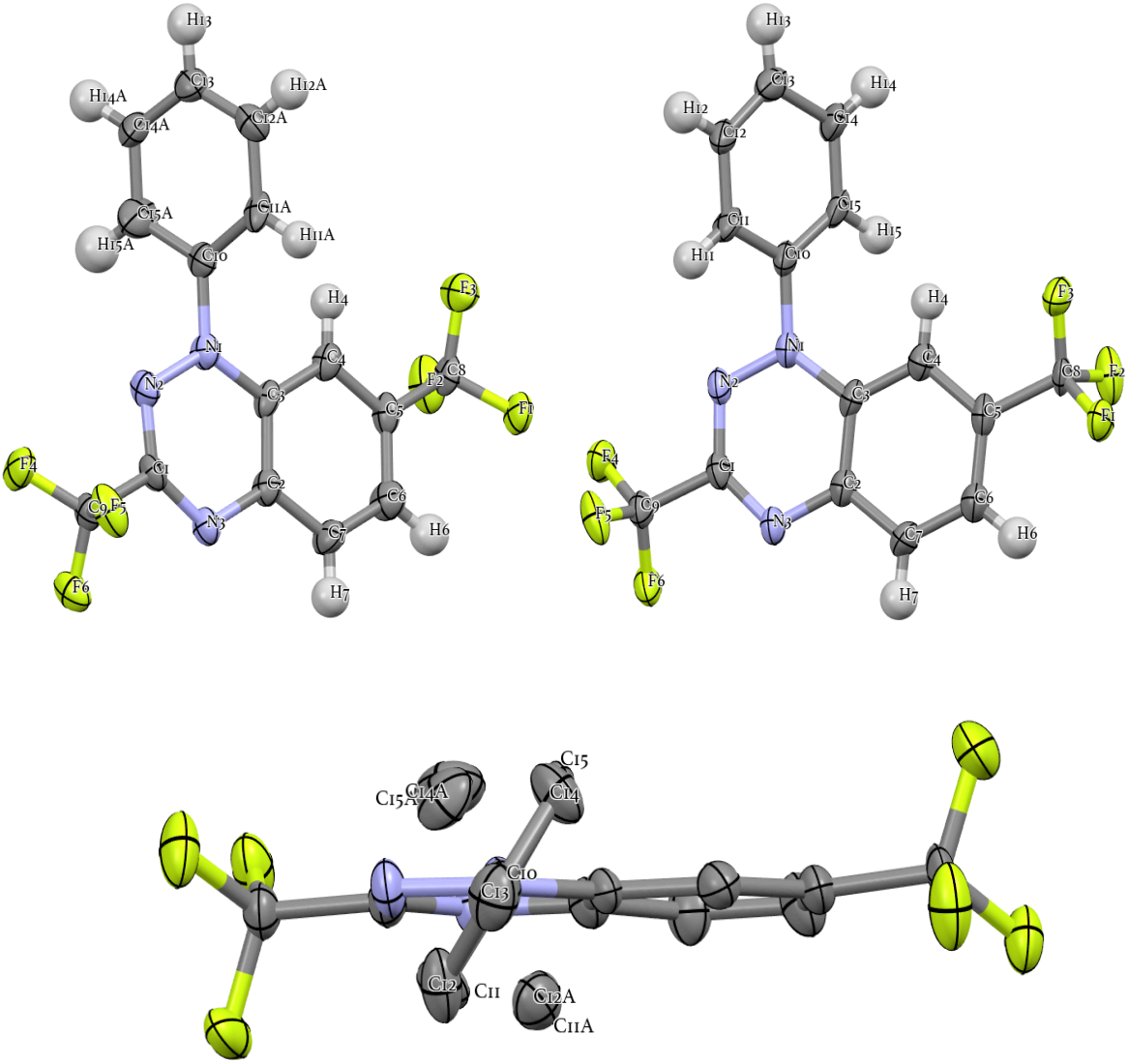

Fig S2. Parameters used to define the degree of longitudinal and latitudinal slippage. Top: the longitudinal slippage is defined as the angle between the plane formed by the central C atoms of two benzotriazinyl rings (4 atoms) and the plane defined by benzotriazinyl ring (10 atoms). Bottom: the latitudinal slippage is defined as the angle between the plane linking atoms N(2) and C(5) on each of the two neighbouring benzotriazinyl radicals (4 atoms) and the benzotriazinyl ring plane (10 atoms).

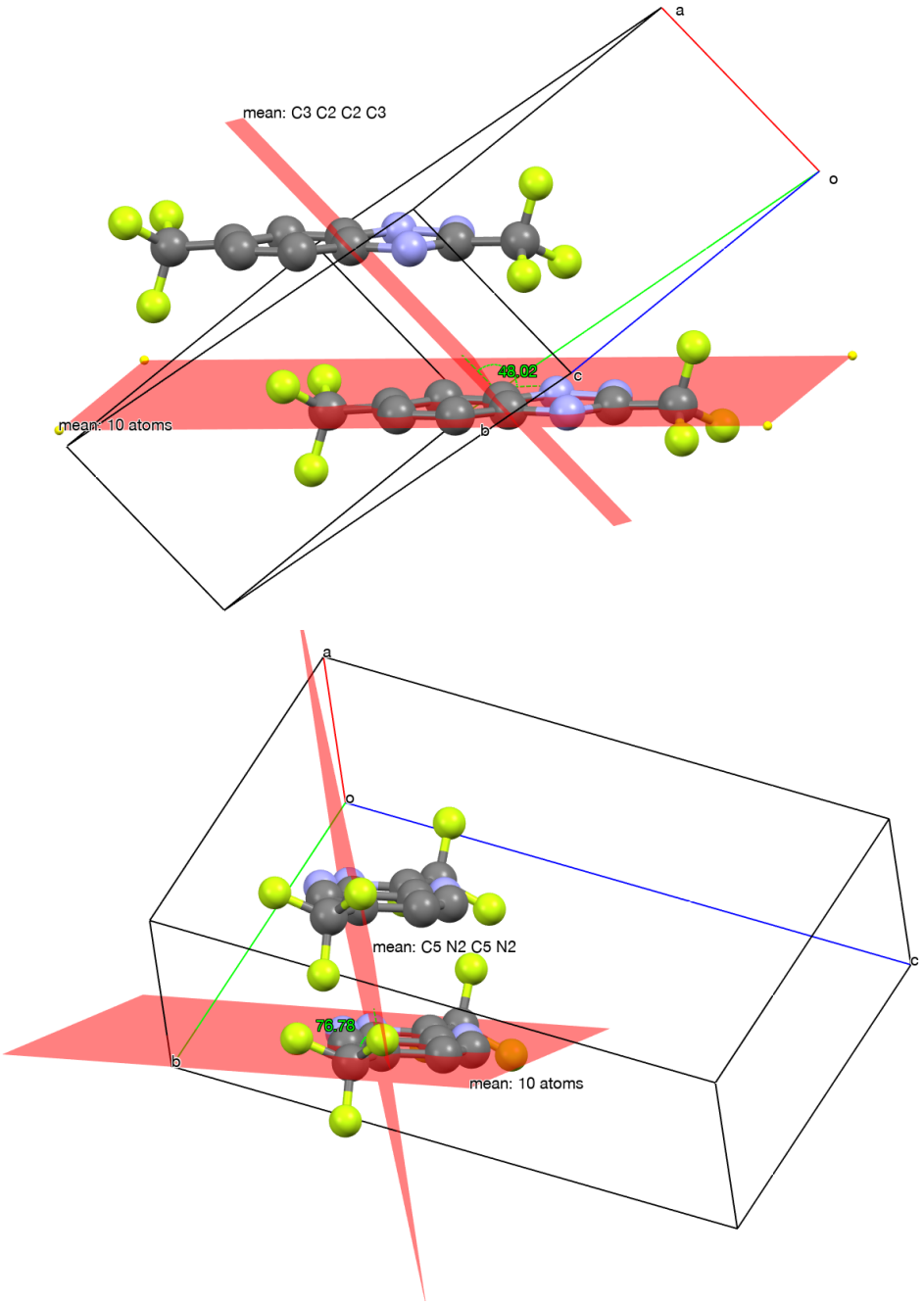

Fig S3. Packing of radical **2** along the α-axis showing both components of disorder.