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Structural Investigation of N-N' Methylenebisacrylamide via X-ray Diffraction Assisted by Crystal Structure Prediction

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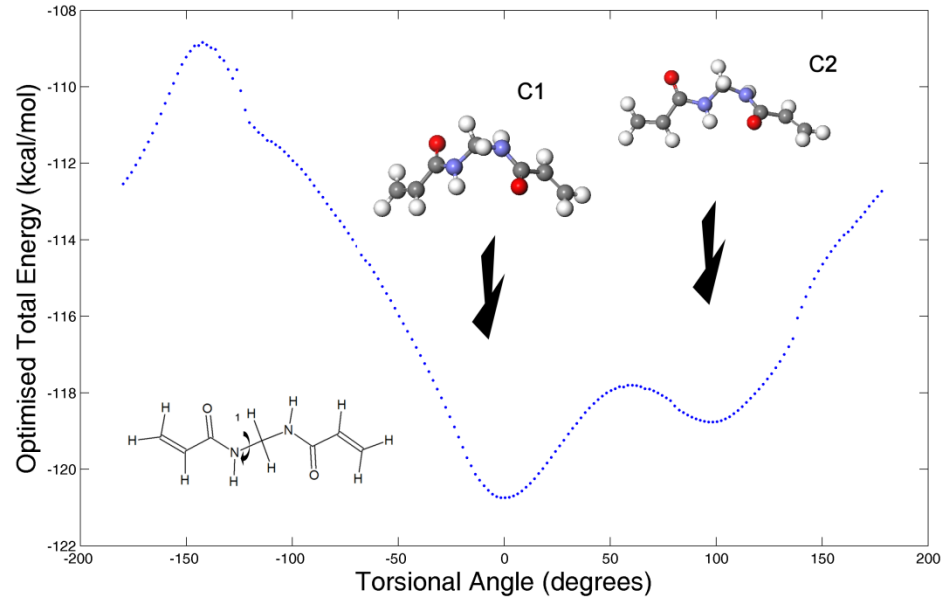
Figure S1 Plots of the optimised total energy of MBA molecule versus the bond torsion angle of the C-N bond 1 and of the C-C bond 2, respectively. The molecule conformers corresponding to the local minima is also displayed. In both cases, the minimum energy configuration corresponds to the ground-state indicated by the DFT optimisation.



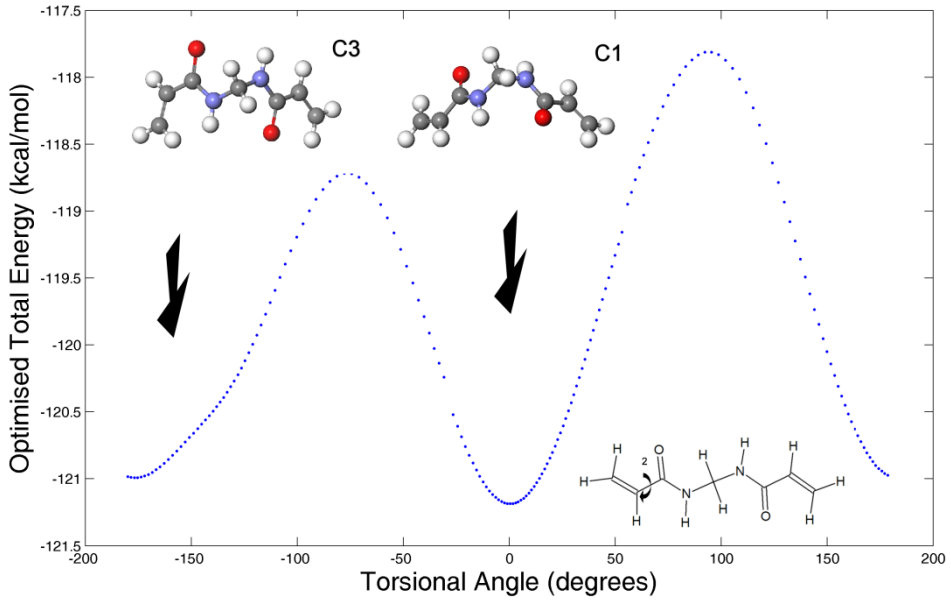


Figure S2 Le Bail analysis of the experimental powder diffraction pattern performed with the monoclinic C2/c cell of the best α-structure suggested by CSP analysis (Rwp = 4.77 %). All the diffraction peaks appear well indexed, indicating an excellent agreement between the model and the observed data.