Electronic Supplementary Material for CrystEngComm

Predicting Microporous Crystalline Polyimides

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Supplementary information

The networks described were constructed using the Materials studio visualiser. The systems were fully minimised using the Discover minimisation package using the COMPASSS forcefield with no symmetry group constraints imposed. van der Waals interactions were treated using atom based summation whilst coulombic interactions were treated using Ewald summation. A cutoff distance of 9.50 Å was used for all models.

	A	B	C
1	-55.48	352.40	-157.29
2	-52.78	330.03	-138.64
3	-118.33	1061.32	-118.75
4	469.45	2117.03	1537.25
5	-198.60	6467.52	-789.10

Table 1. The absolute energies of the 15 hypothetical porous and non-porous polyimides.