Electronic Supplementary Material (ESI) for CrystEngComm

Oxalyl Dihydrazide Polymorphism: a Periodic Dispersion-Corrected DFT and MP2 Investigation.

- Electronic Supporting Information -

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A) *k*-points and Energy Cutoff Screening

PBE-TS (NCPP) - cutoff: 750 eV		
k-pt. mesh	*k-pt. dist. (1/Å)*	*Energy (eV/atom)*
1x1x1 (Γ)	-	-167.140499
3x1x1	0.10	-167.310192
3x2x1	0.08	-167.311698
5x2x2	0.06	-167.312090
7x4x3	**0.04**	**-167.312105**

Table 1 Single-point energy of crystalline oxalyl dihydrazide (α phase) as a function of increasing k-points mesh size. Results are reported in eV per atom.

PBE-TS - k-points mesh size: 7x4x3			
Energy cutoff (eV)		*Energy (eV/atom)*	*ΔE (meV/atom)*
NCPP	750	-167.312105	-
	800	**-167.313536**	**-1.431**
	850	-167.314699	-1.163
	900	-167.315604	-0.905

Table 2 Single-point energy (eV) of crystalline oxalyl dihydrazide (α phase) as a function of increasing kinetic energy cutoff. Results for ΔE are reported in meV per atom for convenience.

B) Relative Stability at the Experimental Geometry

Experimental Relative Stability - ΔE		
Phase	**PBE-TS** (kJ/mol)	**PBE-D** (kJ/mol)
α	-	-
β	11.371	4.718
γ	-26.884	-28.821
δ	2.330	0.848
ϵ	66.761	64.121

Table 3 PBE-TS and PBE-D experimental relative stability (per molecule) of crystalline oxalyl dihydrazide. The α-polymorph is taken as reference.