Table S1. Twinning statistics for the crystal selected for full data collection

Domain/Number of domains	Number of reflections'	Unique reflections	I/σ
domain 1 only	2052	1144	18.3
domain 2 only	1914	967	6
domain 3 only	2976	1636	7.7
domain 4 only	2710	1372	4.5
2 domains	19700	9520	9
3 domains	354	347	7.1
4 domains	12874	5158	8.2

Table S2. Twin matrix transformations

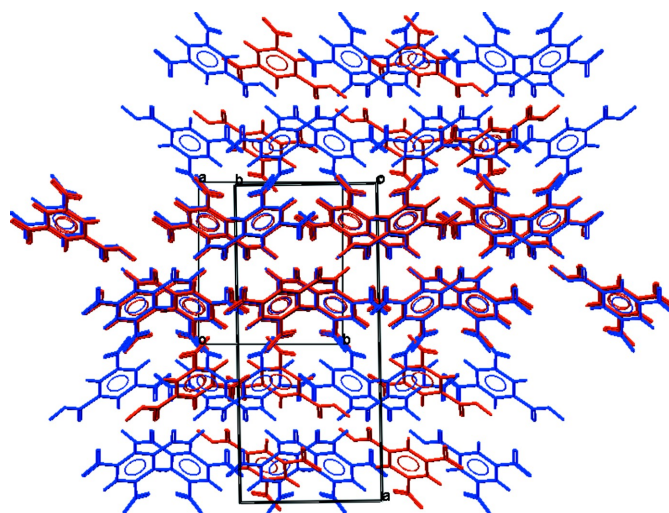|	to Domain 2	to Domain 3	to Domain 4
Domain 1	-0.99989 -0.00095 0.00067 -0.32126 0.99985 -0.00581 -0.00337 -0.00068 -0.99995	-1.00041 0.00201 0.00133 -0.00646 -0.99968 0.00212 -0.13575 -0.00595 1.00010	0.99979 0.00125 0.00014 0.32245 -0.99980 0.00213 0.14492 -0.00342 -0.99998
Domain 2		0.99956 0.00296 -0.00068 0.32759 -0.99952 0.00391 0.14122 -0.00650 -1.00002	-0.99999 0.00030 -0.00082 -0.00122 -0.99996 0.00369 -0.14738 -0.00287 0.99995
Domain 3			-0.99956 -0.00327 0.00148 -0.32884 0.99946 0.00045 -0.00924 0.00935 -0.99989

Fig. S1. Overlay of the two polymorphs of the 3,5 isomer of dinitrobenzoic acid. Blue: CUKCAM01 in $P2_1/c$ (Prince *et al.*, 1991). Red: CUKCAM02 in $C2/c$ (Kanters *et al.*, 1991; Domenicano *et al.*, 1990).
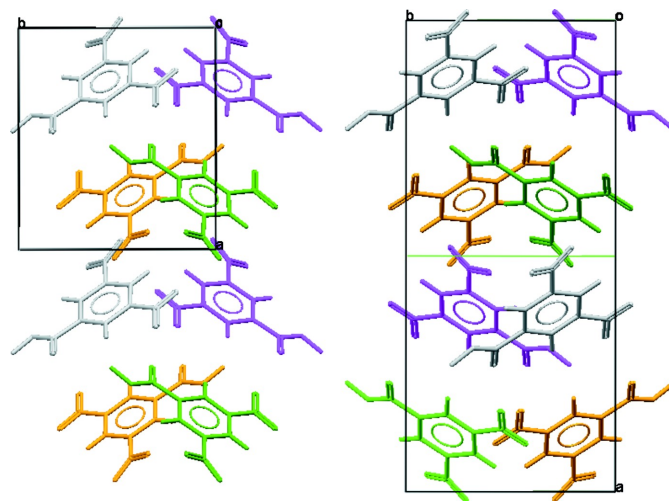

Fig. S2. Comparison of the packing of the two polymorphs of the 3,5 isomer of dinitrobenzoic acid (CUKCAM01 in $P2_1/c$ (Prince *et al.*, 1991) and CUKCAM02 and in $C2/c$ (Kanters *et al.*, 1991; Domenicano *et al.*, 1990). Left: CUKCAM01 in $P2_1/c$; right: CUKCAM02 and in $C2/c$. Molecules are colour coded as a guide to the eye relating equivalent molecules in the two structures with each other. The twofold axis only present in CUKCAM02 is symbolized by a thin green line at $a = 1/2$.