A Theoretical Prediction on the Shear-induced Phase Transformation of TKX-50

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Electronic Supplementary Information (ESI)

Table S1. Fractional Coordinates of the BCPs and Symmetry Multiplicity of TKX-50.

HB kind	D-H…A	Fraction coordinate	Symmetry Multiplicity
Intralayered	O2-H2···O1	(0.0980, 0.6366, 0.8555)	4
	N5-H4···O1	(0.5208, 0.3856, 0.1074)	4
	N5-H1···O1	(0.2279, 0.0210, 0.3905)	4
	N5-H3···N3	(0.4340, 0.3461, 0.8217)	4
	N5-H1···N4	(0.0511, 0.0790, 0.3554)	4
Interlayered	N5-H3···N2	(0.4111, 0.2539, 0.4467)	4
	N5-H3···O2	(0.2212, 0.2277, 0.2821)	4