

A top-down approach to crystal engineering of a racemic D²-isoxazoline

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Supplementary Material

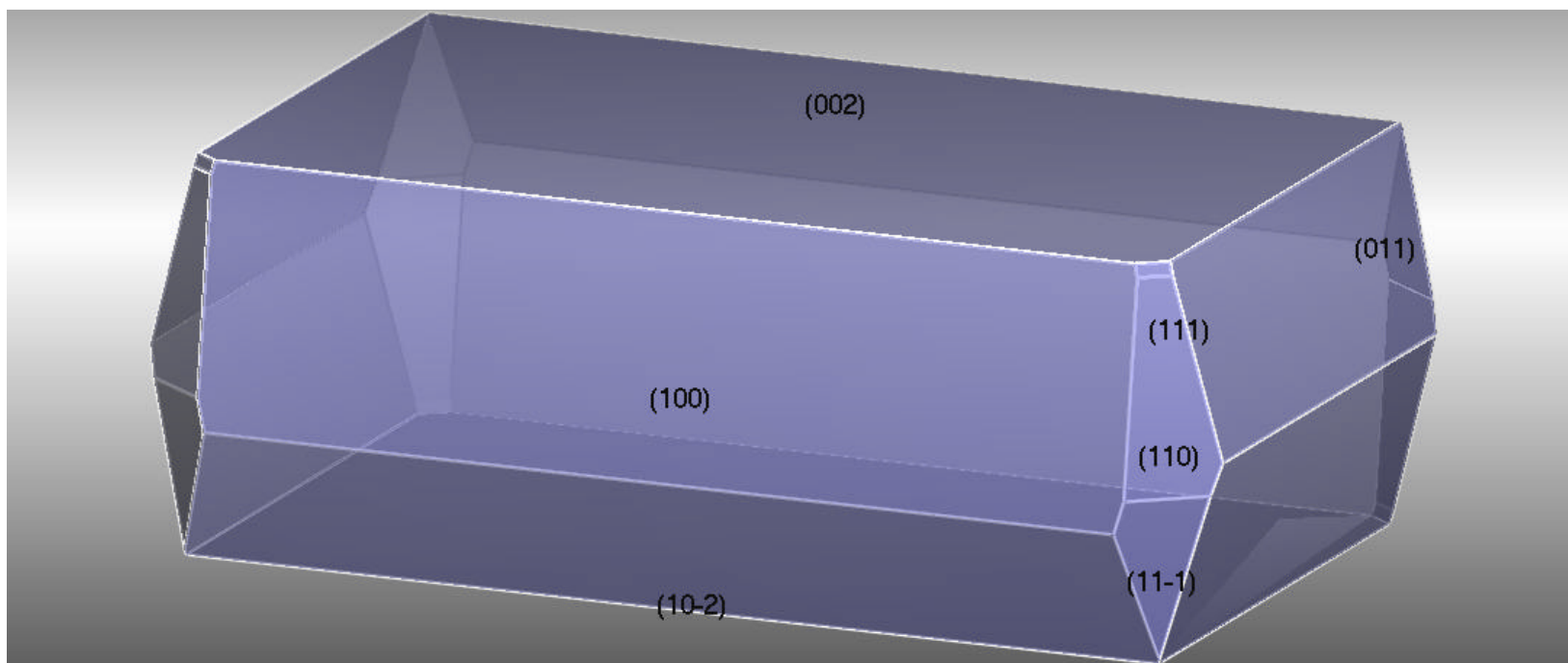


Fig. S1: GM prediction. Miller indices for MI faces are superimposed on each face.

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hkl	multiplicity	d _{hkl} (Å)	E _{att} (Tot) (kcal mol ⁻¹)	% Total Facet Area
(0 0 2)	2	13.7480	-34.07157715	50.44
(1 0 0)	2	7.1982	-71.45698415	16.55
(0 1 1)	4	6.7092	-89.45852399	19.85
(1 0 -2)	2	6.4769	-69.48523156	9.59
(1 1 0)	4	4.9880	-106.96038675	2.24
(1 1 -1)	4	4.9303	-106.68734749	1.27
(1 1 1)	4	4.8858	-110.42861818	0.07

Table S1: MI faces, with their relative Miller indices, reported in descending % of Total Facet Area, calculated as $100 \times (\text{hkl facet area})/(\text{total surface area})$.