

## Supplementary Information

### Quantitative Determination of Approximate Centrosymmetry in P1 Organic Crystals

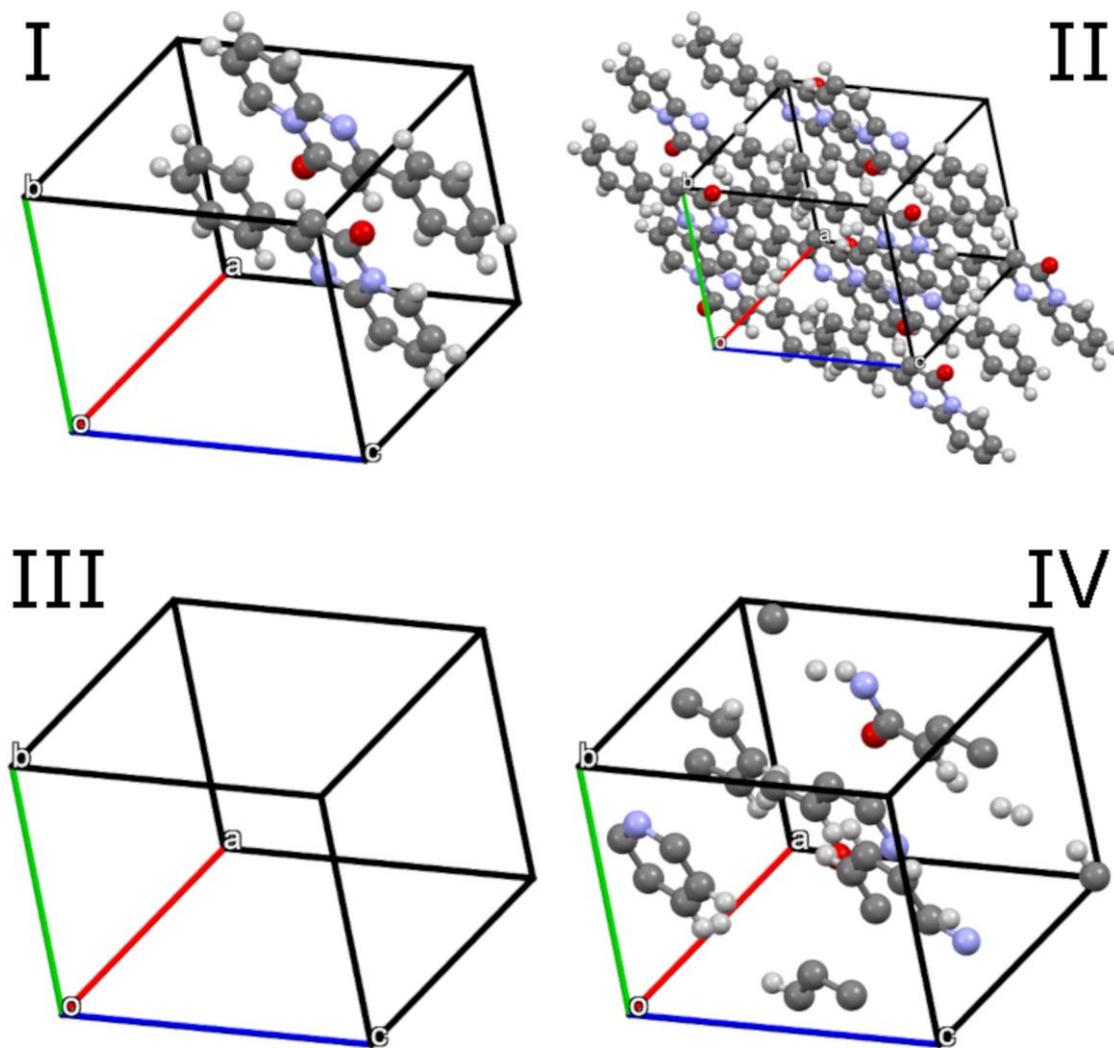
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#### Refcodes that required approximate CSM calculations:

ACEZOX, CIDHAB, COVQEM, DAKBIC, EDOZAB, FIMCUC, GUZVIG, HILQOI, HOCYEG, JUXZUA, KIBKOZ, LAQFIV, LECDUW, LUSCOU, NUPBEI, OBAFUW, ONOWEU, PEHWIM, SIKBAQ, UQIJEM, UVOREF, UWALIP, VEKGUO, VENPOU, WENXIA, XAGMOH, XODGAA, YONVOM, ZENXAV.



**Figure S1.** Four common options to pack a unit cell. I. Molecules whose centroids lie at or within the unit-cell boundaries; II. Molecules for which at least one atom lies at or within the boundaries of the unit cell; III. Molecules for which all atoms lie at or within the unit-cell boundaries; IV. Atoms whose coordinates are at or within the boundaries of the unit cell.

**Table S1.** Pairs of related crystals – group A.

<b>Refcode</b>	<b>Stereochemistry</b>	<b>Related Crystal</b>	<b>Space Group</b>
DOCKUB	Meso	DOCKUB01	P-1
ABORER	Achiral	ABORER01	P-1
YUFVAX	Racemic	YUFVAX01	P-1
ISECOZ	Achiral	ISECOZ01	P-1
TUFTUK	Achiral	TUFTUK01	P-1
DCHPHA01	Achiral	DCHPHA	P-1
JUXLIX	Achiral	JUXLIX01	P-1
EKOKOE	Racemic	EKOKOE01	P-1
FRANAC03	Achiral	FRANAC	P-1
SIDXUY	Achiral	SIDXUY01	P-1
HIGHAH	Achiral	HIGHAH01	P-1
EGAXOZ01	Achiral	EGAXOZ	P-1
DISHIX	Achiral	DISHIX01	P-1
CEBZAM	Achiral	CEBZAM01	P-1
MEYYEU	Achiral	MEYYEU01	P-1
QETTEO	Achiral	QETTEO01	P-1
DISHOD	Achiral	DISHOD01	P-1
QANCEP	Achiral	QANCEP01	P-1
WEQHEF	Achiral	WEQHEF01	P-1
GIPTAA	Achiral	GIPTAA01	P-1
FURGAA02	Achiral	FURGAA	P-1
HIDJUA	Achiral	HIDJUA01	P-1
GIXPAE	Achiral	GIXPAE01	P-1
KETCAN	Achiral	GALWIZ10	C2/c
HUXBOR	Achiral	HUXBOR01	P-1
XUBPUF	Achiral	XUBPUF01	P-1
XECJEU	Achiral	XECJEU01	P-1
HITNED	Achiral	HITNED01	P-1
GIXREK	Achiral	GIXREK01	P-1
FEPZOP	Achiral	FEPZOP01	P-1
WEPWUJ	Racemic	WEPWUJ01	P-1
DUNION01	Chiral	DUNION	P-1
HOFVED	Achiral	HOFVED01	P-1
ZOWFAS	Achiral	ZOWFAS01	P-1
KAYXUD	Chiral	GACVEL10	P21/c
VADGUC01	Chiral	VADGUC	P-1
MIQQUZ	Achiral	MIQQUZ01	P-1
UVAKUY03	Achiral	UVAKUY	P-1
PUBTUC	Achiral	PUBTUC01	P-1
DIXYUE01	Achiral	DIXYUE	P-1
QUDQUB	Achiral	QUDQUB01	P-1
YEBQUR	Achiral	YEBQUR01	P-1

**Table S2.** Pairs of related crystals – group B.

Refcode	Stereochemistry	Related Refcode	Space Group
BAZHAM	Achiral	BAZHAM01	Pna2 <sub>1</sub>
CEPKOY	Achiral	CEPKOY01	Cc
CIDHAB	Achiral	CIDHAB01	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
CUNBET	Chiral	CUNBET01	P2 <sub>1</sub>
GULPUY	Chiral	GULPUY01	R3
JORMIM	Chiral	JORMIM01	C2
KEGBAZ	Chiral	KEGBAZ01	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
LEZLEI	Achiral	LEZLEI01	P2 <sub>1</sub>
MBDARP	Chiral	MBDARP01	C2
MUTYOP01	Chiral	MUTYOP	I4
NIXQAM	Achiral	NIXQAM01	Fdd2
NOQBUQ	Achiral	NOQBUQ01	Cm <sub>c</sub> 2 <sub>1</sub>
PABYIA	Achiral	PABYIA01	Cc
POTBAC	Chiral	POTBAC01	P2 <sub>1</sub>
SARZOA02	Achiral	SARZOA	P2 <sub>1</sub> 2 <sub>1</sub> 2
TOQJAK	Racemic	TOQJAK01	Cc
VEMSAH	Chiral	VEMSAH01	C2
VENPOU	Achiral	VENPOU01	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
VOZMAY	Chiral	VOZMAY01	P2 <sub>1</sub>
WENVIY	Achiral	WENVIY01	P2 <sub>1</sub>
WENVUK	Achiral	WENVUK01	P2 <sub>1</sub>
YAHYIP	Racemic	YAHYIP01	Cc
ZIMLOA	Chiral	ZIMLOA01	P2 <sub>1</sub>

**Table S3.** Stereochemical classification of the molecules with related crystals.

Classification	Group A	Group B
	Related crystal has inversion point	Related crystal does not have an inversion point
Achiral	35	11
Chiral	3	10
Meso	1	
Racemate		2

**Table S4.** CSM before and after origin shift for structures with related measurements

Refcode	S(C) <sub>i</sub> – original Cell	Origin Shift Vector	S(C) <sub>i</sub> – After Origin Shift	Related Refcode and SG
GIXREK	26.7037	(0.0, 0.1, 0.0)	0.0149	GIXREK01 (P-1)
GIXPAE	25.8935	(0.0, 0.1, 0.4)	0.069	GIXPAE01 (P-1)
HOFVED	15.7503	(0.7, 0.0, 0.0)	0.0267	HOVFED01 (P-1)