

Exploitation of pseudo-symmetry in the Cambridge Structural Database for molecular ferroelectric discovery

Sam Y. Thompson,^a Harold T. Stokes,^b Branton J. Campbell,^b Elliot D. Goldberg^a and John S. O. Evans^{*a}

^aDepartment of Chemistry, Science Site, Durham University, Durham DH1 3LE, United Kingdom

^bDepartment of Physics & Astronomy, Brigham Young University, Provo, Utah 84602, United States

Supplementary information

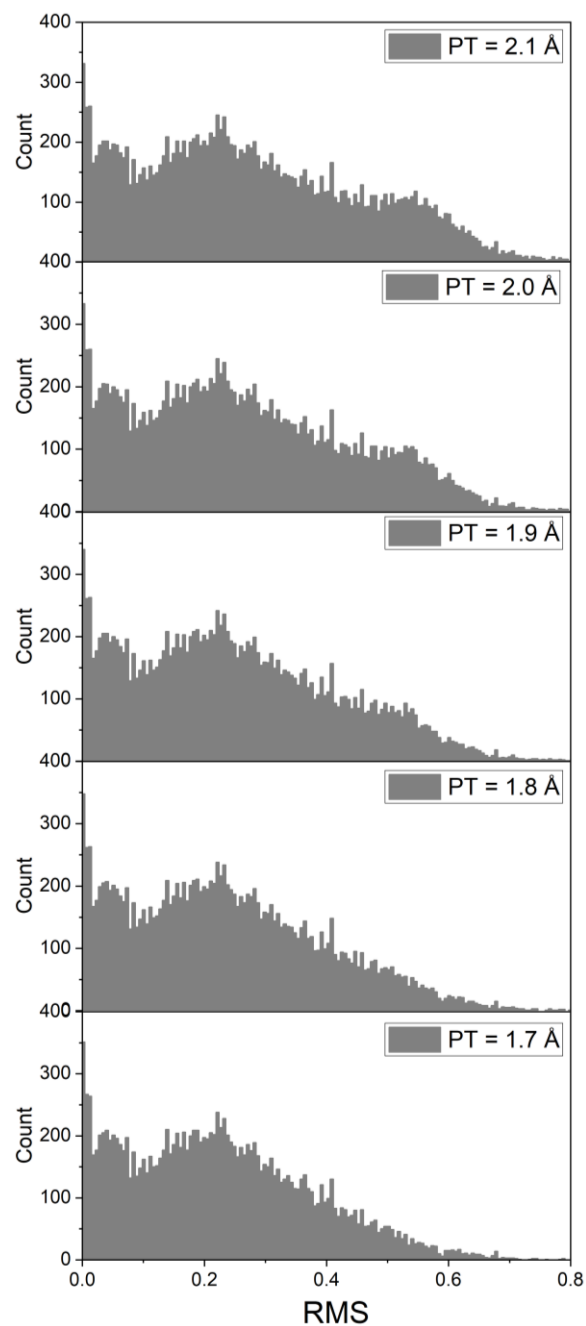


Figure S1 - Reduction of Peak 4 (centred at RMS = 0.54 Å) with decreasing PT.

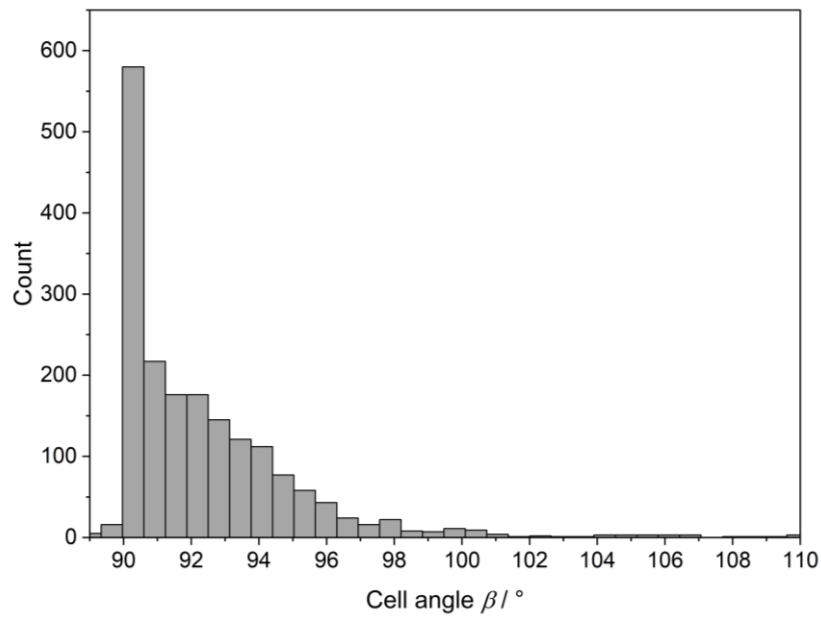


Figure S2 – Histogram of FERROSCOPE HSS that are predicted to transition with a Γ mode distortion. The shape of the graph is a half-Gaussian centred at 90°. A spike at 90° is further evidence of PSTG structures.

The following CSD structures are known ferroelectric materials and were used to optimise FERROSCOPE:

UBOTIQ01
 TUTKUR
 CLCOPB11
 JAWQUT01
 FIBZOH01
 HORFAV
 FIGNER
 YOCVAP
 CATXED01
 MAPJUI
 ESAPOG01
 DADTUY02
 JAKQAA
 RIDFOA01
 NOQLEN
 GEFLOV
 REZBOP01
 KOWYEA02
 GUMMUW
 MIGQOJ02
 HEYNOR
 COJCOV
 JUJFEC
 DOHDAI
 NIWJUA02
 IHIWON
 XEGDUL
 XEGFIB
 VEFWAH01
 WOLYUR01

ABIQOU
ABIRAH
SIYWUT
UHAGAM04
ATENIY
YIBCIY
FAWSAZ01
UXIXAB02
EWAJUK
JEXWOZ02
ELUQIM
JEXWUF02
CAJHUS01
RUJBAC
RUJBIK
AMBACO07
NONYUK02
LIFCIM02
KAVKIE01
TEJKUO
JAYPUU01
KIVFIH
OROWAV
UFODEB
IGEDUW
IGEKOX
TMAMNC
DANFAC
FOSGID
THIOUR14
SIWKEP
KASXUY
RIJVIS01
AMHCLA01
MEGJEP
QODZER
QIXKEQ01
QIXKIU
QODGUM04
XOLXEE01
XOMQUO01
TIVDAF
TIVFEL
MUZCER
BUJQIJ
BUJQOP
OHAMIW
OHAMOC
OHAMUI
OHANAP
CBUDCX
PROLON
TAPZIT
WIZNAX01
WERZUR
BILHUC
BILJOY
BILNES

BILNOC
BILNUI
BILPOE01
BILGAH
BILHAI
BILKEP
BILLEQ
BILLOA
BILLUG
BILMER
BILKIT
BILHIQ
BILLIU
KAVJUP05
LOTBAA01
BEFWOB01
PIKDOC
FINTAZ
FINTIH
TMPPIO03
WULSAY
IGEWID
MIHTEE01
QIVQIY
LOLHIG04
KNATAR05
MUPDAF
HEJGOV01
WUKROM
SOMDOO
SOMDUU
ANPHPR01
LEQWAF
YASKIP
SUGJOW01
AQAVIA01
QUSTIK
QUTFUJ
GUALSU10
GUCRSU
MAMPUM02
ZIYYOX
ZIYYUD
ZIYZAK
FOXNUB07
BOLDIP11
QQQFAD03
FUWWOL02
WIVDUA05
BIKREV
SARCAC01
HAXGOE01
UZIWOQ
JOJYOY
JOJZAL
XEMQIS
JOPZUM
POXQUR

AVUPIT
AVUPUF
CUYGIO
QUKBIJ06
TAKZUE
NIXCOP
JOYDOT
JOYLUH
DUNNUX
DUNPAF