Reply to the comment "Trimorphs of 4-bromophenyl 4-bromobenzoate. Elastic, brittle, plastic" by J. J. Whittaker, A. J. Brock, A. Grosjean, M. C. Pfrunder, J. C. McMurtrie and J. K. Clegg, Chem. Commun., 2021, 57, DOI: 10.1039/D0CC07668F

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Supporting Information

List of contents

S1: Synthesis of 3: 2-chloro-4-chlorophenyl 4-chlorobenzoate

Compound **3** was synthesized using a reported procedure.[1]

S2: SCXRD experiment

Single crystal X-ray diffraction (SCXRD) data of **3** were collected on a Rigaku Mercury 375R/M CCD (XtaLAB mini) diffractometer using graphite monochromator Mo Kα radiation. The data were processed with the Rigaku CrystalClear 2.0 software.[2,3] Using Olex2,[4] the structure was solved with the SHELXT[5] and was refined with the ShelXL.[6] All the non-hydrogen elements were refined anisotropically and hydrogen atoms were refined isotropically. The crystallographic data are given in the supplementary information, (S3).

S3: Crystallographic information table

Compound	**3**
Formula	$C_{13}H_7Cl_3O_2$
Molecular weight	301.54
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a (Å)	3.927(4)
b (Å)	11.665(12)
c (Å)	27.84(3)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	1275(2)
Z	4
ρ_{calc} (g/cm^3)	1.571
F(000)	608.0
Temp. (K)	293
R_1	0.0623
wR_2	0.1294
Goodness-of fit	1.083
CCDC No.	2053205

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