

data\_global

\_publ\_contact\_author\_name 'Leslaw Sieron'  
\_publ\_contact\_author\_email 'lsieron@p.lodz.pl'

loop\_

\_publ\_author\_name

"L.Sieron"

"J.Kobylecka"

"A.Turek"

\_chemical\_name\_systematic

;

(+)-2-(4-Chloro-2-methylphenoxy)propanoic acid

;

\_chemical\_name\_common 'MCPD'  
\_chemical\_formula\_moiety 'C10 H11 Cl O3'  
\_chemical\_formula\_sum 'C10 H11 Cl O3'  
\_chemical\_formula\_weight 214.64

\_symmetry\_cell\_setting monoclinic

\_symmetry\_space\_group\_name\_Hall '-P 2ybc'

\_symmetry\_space\_group\_name\_H-M 'P 21/c'

\_symmetry\_Int\_Tables\_number 14

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\_symmetry\_equiv\_pos\_site\_id

\_symmetry\_equiv\_pos\_as\_xyz

1 x,y,z

2 -x,1/2+y,1/2-z

3 -x,-y,-z

4 x,1/2-y,1/2+z

\_cell\_length\_a 4.2261(3)

\_cell\_length\_b 6.8196(5)

\_cell\_length\_c 35.176(3)

\_cell\_angle\_alpha 90

\_cell\_angle\_beta 91.801(1)

\_cell\_angle\_gamma 90

\_cell\_volume 1013.28(13)

\_cell\_formula\_units\_Z 4

\_cell\_measurement\_temperature 90

\_exptl\_crystal\_colour 'colorless'

\_exptl\_crystal\_preparation 'ethanol/water'

\_exptl\_crystal\_density\_diffn 1.407

\_exptl\_crystal\_F\_000 448

\_exptl\_absorpt\_coefficient\_mu 0.354

\_exptl\_special\_details 'herbicide agent'