

data\_mcpa

\_publ\_contact\_author\_name 'Leslaw Sieron'  
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loop\_  
\_publ\_author\_name  
"L.Sieron"  
"J.Kobylecka"  
"A.Turek"

\_chemical\_name\_systematic '4-Chloro-2-methylphenoxyacetic acid'  
\_chemical\_name\_common MCPA  
\_chemical\_formula\_moiety 'C9 H9 Cl O3'  
\_chemical\_formula\_sum 'C9 H9 Cl O3'  
\_chemical\_formula\_weight 200.61

\_symmetry\_cell\_setting triclinic  
\_symmetry\_space\_group\_name\_Hall '-P 1'  
\_symmetry\_space\_group\_name\_H-M 'P -1'  
\_symmetry\_Int\_Tables\_number 2

loop\_  
\_symmetry\_equiv\_pos\_site\_id  
\_symmetry\_equiv\_pos\_as\_xyz  
1 x,y,z  
2 -x,-y,-z

\_cell\_length\_a 5.0867(3)  
\_cell\_length\_b 7.7824(4)  
\_cell\_length\_c 12.2134(7)  
\_cell\_angle\_alpha 73.933(1)  
\_cell\_angle\_beta 84.610(1)  
\_cell\_angle\_gamma 77.009(1)  
\_cell\_volume 452.45(4)  
\_cell\_formula\_units\_Z 2  
\_cell\_measurement\_temperature 90

\_exptl\_crystal\_colour 'colorless'  
\_exptl\_crystal\_preparation 'ethanol/water'  
\_exptl\_crystal\_density\_diffn 1.472  
\_exptl\_crystal\_F\_000 208  
\_exptl\_absorpt\_coefficient\_mu 0.391  
\_exptl\_special\_details 'herbicidal agent'

\_diffrn\_ambient\_temperature 90  
\_diffrn\_radiation\_wavelength 0.71073  
\_diffrn\_radiation\_probe 'x-ray'  
\_diffrn\_radiation\_type 'MoK $\alpha$ '