

Demartin\_AM-12-062

data\_argesite

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

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;

\_chemical\_name\_common ?

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'H23.16 Bi3 Br1.42 Cl14.58 K1.21 N5.79'

\_chemical\_formula\_weight 1409.05

loop\_

\_atom\_type\_symbol

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'H' 'H' 0.0000 0.0000

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'N' 'N' 0.0061 0.0033

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Cl' 'Cl' 0.1484 0.1585

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'Bi' 'Bi' -4.1077 10.2566

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'K' 'K' 0.2009 0.2494

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Br' 'Br' -0.2901 2.4595

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting trigonal

\_symmetry\_space\_group\_name\_H-M R-3c

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-y, x-y, z'

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

'-x+y, -x, z'

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

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

'x+2/3, y+1/3, z+1/3'

'-y+2/3, x-y+1/3, z+1/3'

'y+2/3, x+1/3, -z+5/6'

'-x+y+2/3, -x+1/3, z+1/3'

'-x+2/3, -x+y+1/3, -z+5/6'

'x-y+2/3, -y+1/3, -z+5/6'

'x+1/3, y+2/3, z+2/3'

'-y+1/3, x-y+2/3, z+2/3'  
 'y+1/3, x+2/3, -z+7/6'  
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 '-x+1/3, -x+y+2/3, -z+7/6'  
 'x-y+1/3, -y+2/3, -z+7/6'  
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 'y, -x+y, -z'  
 '-y, -x, z-1/2'  
 'x-y, x, -z'  
 'x, x-y, z-1/2'  
 '-x+y, y, z-1/2'  
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\_computing\_molecular\_graphics ?  
\_computing\_publication\_material ?

\_refine\_special\_details

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Refinement of  $F^2$  against ALL reflections. The weighted R-factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional R-factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

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 Cl1 Cl 0.42424(5) 0.53716(5) 0.061762(6) 0.03377(18) Uani 1 1 d . . .  
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 Br4 Br 0.66707(6) 0.79390(6) 0.042206(7) 0.0623(2) Uani 0.2216(15) 1 d P . .  
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 Cl9 Cl 0.19199(7) 0.47653(7) 0.181760(14) 0.0843(4) Uani 1 1 d . . .  
 N1 N 0.3378(4) 0.9918(3) 0.011783(15) 0.0460(4) Uiso 1 1 d . . .  
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 K2 K 0.6667 1.04908(13) 0.0833 0.0426(4) Uiso 0.357(3) 2 d SP . .  
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Bi3 0.01684(6) 0.01684(6) 0.0818(2) 0.000 0.000 0.00842(3)  
Cl1 0.02675(19) 0.0458(2) 0.0356(3) 0.0010(2) 0.0014(2) 0.02329(16)  
Cl2 0.0270(2) 0.0286(2) 0.0325(3) -0.0019(2) -0.0014(2) 0.00514(18)  
Cl3 0.01537(19) 0.0379(2) 0.0571(3) -0.0304(2) 0.0004(2) 0.00786(16)  
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Br7 0.0721(3) 0.0598(2) 0.1442(7) 0.0151(4) 0.0129(4) 0.04556(17)  
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\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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 Cl1 K2 3.2964(8) 15\_444 ?  
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