Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

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N N 0.0311 0.0180 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0492 0.0322 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cu Cu -1.9646 0.5888 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.3639 0.7018 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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CrysAlisPro, Oxford Diffraction Ltd.,
Version 1.171.34.44 (release 25-10-2010 CrysAlis171 .NET)
(compiled Oct 25 2010,18:11:34)
Analytical numeric absorption correction using a multifaceted crystal
model based on expressions derived by R.C. Clark & J.S. Reid.
(Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)
;

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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^ > 2sigma(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.
;
SQUEEZE RESULTS (APPEND TO CIF)
Note: Data are Listed for all Voids in the P1 Unit Cell
i.e. Centre of Gravity, Solvent Accessible Volume,
Recovered number of Electrons in the Void and
Details about the Squeezed Material
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O1 O 0.4442(6) -0.9702(4) 0.03348(11) 0.130(3) Uani 1 1 d . . .
O2 O 0.4830(5) -0.8886(5) -0.00178(10) 0.117(2) Uani 1 1 d . . .
O3 O 0.4826(5) -0.6291(4) -0.00154(10) 0.1037(18) Uani 1 1 d . . .
O4 O 0.4405(4) -0.5901(4) 0.03280(10) 0.1040(18) Uani 1 1 d . . .
O5 O 0.4415(8) -0.4351(7) 0.05460(9) 0.174(3) Uani 1 1 d . . .
C1 C 0.4531(7) -0.9107(5) 0.02069(15) 0.099(3) Uani 1 1 d . . .
C2 C 0.4299(8) -0.8508(7) 0.03331(16) 0.114(3) Uani 1 1 d . . .
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H3A H 0.4617 -0.7694 0.0031 0.122 Uiso 1 1 calc R . .
C4 C 0.4339(6) -0.7194(6) 0.03198(17) 0.104(3) Uani 1 1 d . . .
C5 C 0.4559(8) -0.6415(7) 0.01935(15) 0.102(3) Uani 1 1 d . . .
C6 C 0.4042(8) -0.7356(8) 0.05909(18) 0.139(4) Uani 1 1 d . . .
H6A H 0.3940 -0.6974 0.0675 0.167 Uiso 1 1 calc R . .
C7 C 0.3917(5) -0.8050(8) 0.07183(11) 0.131(2) Uani 1 1 d . . .
C8 C 0.4027(6) -0.8641(5) 0.05812(17) 0.105(3) Uani 1 1 d . . .
H8A H 0.3911 -0.9134 0.0661 0.127 Uiso 1 1 calc R . .
C11 C 0.3651(5) -0.8243(6) 0.09914(8) 0.161(4) Uani 1 1 d GU . .
C12 C 0.4209(5) -0.8286(6) 0.11592(10) 0.199(5) Uani 1 1 d GU . .
H12A H 0.4678 -0.8286 0.1096 0.239 Uiso 1 1 calc R . .
C13 C 0.4068(5) -0.8329(6) 0.14217(9) 0.227(6) Uani 1 1 d GU . .
C14 C 0.3369(5) -0.8329(5) 0.15164(8) 0.196(4) Uani 1 1 d GU . .
C15 C 0.2810(4) -0.8287(4) 0.13486(12) 0.297(9) Uiso 1 1 d GU . .
C16 C 0.2951(4) -0.8244(5) 0.10861(11) 0.227(5) Uani 1 1 d GU . .
C17 C 0.2392(6) -0.8201(8) 0.09182(16) 0.380(13) Uiso 1 1 d GU . .
H17A H 0.2486 -0.8172 0.0743 0.456 Uiso 1 1 calc R . .
C18 C 0.1692(6) -0.8202(9) 0.1013(2) 0.51(2) Uiso 1 1 d GU . .
C19 C 0.1551(6) -0.8244(9) 0.1275(2) 0.438(16) Uiso 1 1 d GU . .
H19A H 0.1083 -0.8245 0.1339 0.526 Uiso 1 1 calc R . .
C20 C 0.2110(5) -0.8287(7) 0.14432(18) 0.356(9) Uani 1 1 d GU . .
H20A H 0.2015 -0.8316 0.1619 0.427 Uiso 1 1 calc R . .
Cl1 Cl 0.0688(13) -0.8429(12) 0.0834(2) 0.736(14) Uani 1 1 d U . .
O6 O 0.4505(8) -0.8615(8) 0.1601(2) 0.239(4) Uiso 1 1 d U . .

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O2 0.177(7) 0.101(5) 0.071(3) 0.008(3) 0.019(4) 0.068(5)
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O4 0.130(4) 0.132(5) 0.086(3) 0.005(3) 0.000(3) 0.092(4)
O5 0.271(11) 0.184(6) 0.108(3) -0.008(6) 0.062(7) 0.145(5)
C1 0.141(8) 0.060(4) 0.084(5) -0.008(4) -0.004(5) 0.042(4)
C2 0.168(10) 0.099(6) 0.075(5) -0.006(5) -0.021(5) 0.069(6)
C3 0.121(4) 0.120(7) 0.082(3) 0.001(6) 0.003(2) 0.074(7)
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C5 0.153(9) 0.117(7) 0.075(5) 0.006(4) 0.005(5) 0.096(7)
C6 0.200(13) 0.158(9) 0.084(6) -0.002(6) 0.032(7) 0.108(9)
C7 0.190(7) 0.151(9) 0.088(3) 0.043(7) 0.044(4) 0.113(9)
C8 0.147(8) 0.077(5) 0.099(6) 0.003(4) 0.034(5) 0.061(5)
C11 0.299(10) 0.211(9) 0.090(3) 0.022(6) 0.049(5) 0.215(9)
C12 0.326(13) 0.283(12) 0.089(4) 0.009(6) 0.049(6) 0.227(12)
C13 0.333(14) 0.331(15) 0.101(4) 0.053(7) 0.079(7) 0.230(13)
C14 0.310(11) 0.207(10) 0.141(5) 0.116(8) 0.127(6) 0.180(11)
C16 0.339(11) 0.345(14) 0.128(5) 0.101(7) 0.126(7) 0.269(11)
C20 0.400(15) 0.49(2) 0.356(16) 0.248(14) 0.286(13) 0.352(15)
Cl1 0.88(3) 0.96(3) 0.561(14) 0.285(19) -0.130(19) 0.60(3)

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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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Cu1 O5 2.147(4) . ?
Cu1 Cu1 2.6534(10) 4_645 ?
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O2 C1 1.275(10) . ?
O2 Cu1 1.968(7) 6_655 ?
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C2 C3 1.429(15) . ?
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O5 Cu1 Cu1 178.1(4) . 4_645 ?
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C1 O2 Cu1 120.5(7) . 6_655 ?
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C5 O4 Cu1 121.6(6) . . ?
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