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


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#                           CCDC
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#  to carry out CIF format checking respectively.
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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-
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 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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O2 O 0.62863(17) 0.10934(15) -0.00239(8) 0.1007(9) Uani 1 1 d . . .
O3 O 0.43644(18) -0.1271(4) 0.08185(15) 0.174(2) Uani 1 2 d S . .
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C2 C 0.77847(19) 0.22153(19) 0.03237(14) 0.0906(16) Uani 1 2 d S . .
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C7 C 0.7963(9) 0.0960(7) 0.1633(2) 0.165(5) Uani 0.50 1 d P A 1
H7A H 0.7760 0.0525 0.1454 0.198 Uiso 0.50 1 calc PR A 1
C8 C 0.8031(8) 0.0799(7) 0.2027(2) 0.162(5) Uani 0.50 1 d P A 1
H8A H 0.7868 0.0270 0.2124 0.194 Uiso 0.50 1 calc PR A 1
C7' C 0.8381(6) 0.2441(6) 0.1762(2) 0.122(3) Uani 0.50 1 d P A 2
C8' C 0.8394(6) 0.2220(6) 0.2171(2) 0.121(4) Uani 0.50 1 d P A 2
C9 C 0.8405(4) 0.1595(4) 0.2282(2) 0.160(3) Uani 1 2 d S . .
C10 C 0.8508(11) 0.2848(10) 0.2500 0.131(6) Uani 0.50 2 d SP . .
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C3 0.101(3) 0.086(3) 0.063(2) -0.0078(19) 0.0005(19) 0.023(2)
C4 0.109(3) 0.093(3) 0.072(2) -0.002(2) 0.001(2) 0.016(2)
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C6 0.118(3) 0.118(3) 0.067(3) 0.003(2) -0.003(2) 0.024(4)
C7 0.234(13) 0.113(8) 0.062(5) 0.004(5) -0.003(6) 0.023(8)
C8 0.239(13) 0.128(8) 0.061(4) -0.003(5) 0.007(6) 0.049(9)
C7' 0.140(8) 0.128(7) 0.063(4) -0.018(5) -0.005(5) 0.040(6)
C8' 0.149(9) 0.079(6) 0.071(5) -0.005(4) 0.019(5) 0.008(5)
C9 0.201(7) 0.201(7) 0.070(4) -0.005(3) 0.005(3) 0.094(9)
C10 0.161(14) 0.123(11) 0.058(6) 0.000 0.000 0.031(11)
C11 0.221(19) 0.101(11) 0.107(9) 0.000 0.000 0.025(12)
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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 O3 2.154(4) . ?
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O1 C1 1.267(4) . ?
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C6 C7 1.439(12) . ?
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