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 'In'  'In'  -0.7276   1.3100
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 '-x, -y, -z'

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 SIR-92 (Altomare, Cascarano, Giacovazzo, Guagliardi, Burla, Polidori,
        Camalli, 1992)
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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.
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_refine_ls_number_reflns          7130
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N1 N 1.3053(2) 0.5648(2) 0.6752(2) 0.0553(6) Uani 1 1 d . . .
H1 H 1.356(4) 0.613(3) 0.655(3) 0.056(10) Uiso 1 1 d . . .
N2 N 0.9273(3) 0.8487(3) 0.6398(3) 0.0580(7) Uani 1 1 d . . .
H2 H 0.968(4) 0.901(4) 0.608(4) 0.078(14) Uiso 1 1 d . . .
H3 H 0.850(4) 0.862(4) 0.643(3) 0.065(11) Uiso 1 1 d . . .
N3 N 1.1178(2) 0.5114(2) 0.7208(2) 0.0485(5) Uani 1 1 d . . .
C1 C 1.1828(3) 0.6022(3) 0.6815(2) 0.0491(6) Uani 1 1 d . . .
C2 C 1.1211(3) 0.7181(3) 0.6525(2) 0.0477(6) Uani 1 1 d . . .
C21 C 1.1941(3) 0.8150(3) 0.6113(2) 0.0485(6) Uani 1 1 d . . .
C22 C 1.2015(3) 0.8781(3) 0.6686(3) 0.0570(7) Uani 1 1 d . . .
H221 H 1.1582 0.8602 0.7341 0.094(2) Uiso 1 1 calc R . .
C23 C 1.2717(3) 0.9676(3) 0.6313(3) 0.0653(9) Uani 1 1 d . . .
H231 H 1.2759 1.0104 0.6711 0.094(2) Uiso 1 1 calc R . .
C24 C 1.3346(3) 0.9935(3) 0.5364(3) 0.0653(9) Uani 1 1 d . . .
H241 H 1.3832 1.0538 0.5113 0.094(2) Uiso 1 1 calc R . .
C25 C 1.3279(3) 0.9325(3) 0.4775(3) 0.0647(9) Uani 1 1 d . . .
H251 H 1.3711 0.9512 0.4119 0.094(2) Uiso 1 1 calc R . .
C26 C 1.2577(3) 0.8436(3) 0.5146(3) 0.0574(7) Uani 1 1 d . . .
H261 H 1.2529 0.8019 0.4740 0.094(2) Uiso 1 1 calc R . .
C3 C 0.9915(3) 0.7375(3) 0.6661(2) 0.0483(6) Uani 1 1 d . . .
C4 C 0.9255(3) 0.6419(3) 0.7098(2) 0.0486(6) Uani 1 1 d . . .
C41 C 0.7868(3) 0.6626(3) 0.7271(3) 0.0513(7) Uani 1 1 d . . .
C42 C 0.7128(3) 0.7081(3) 0.6448(3) 0.0607(8) Uani 1 1 d . . .
H421 H 0.7500 0.7276 0.5771 0.094(2) Uiso 1 1 calc R . .
C43 C 0.5827(3) 0.7252(3) 0.6616(3) 0.0670(9) Uani 1 1 d . . .
H431 H 0.5325 0.7580 0.6051 0.094(2) Uiso 1 1 calc R . .
C44 C 0.5282(3) 0.6946(3) 0.7597(4) 0.0677(10) Uani 1 1 d . . .
H441 H 0.4405 0.7054 0.7709 0.094(2) Uiso 1 1 calc R . .
C45 C 0.6012(3) 0.6481(3) 0.8415(3) 0.0659(9) Uani 1 1 d . . .
H451 H 0.5637 0.6259 0.9092 0.094(2) Uiso 1 1 calc R . .
C46 C 0.7295(3) 0.6336(3) 0.8253(3) 0.0604(8) Uani 1 1 d . . .
H461 H 0.7788 0.6034 0.8823 0.094(2) Uiso 1 1 calc R . .
C5 C 0.9934(3) 0.5318(3) 0.7364(2) 0.0475(6) Uani 1 1 d . . .
C6 C 0.9354(3) 0.4225(3) 0.7860(3) 0.0516(7) Uani 1 1 d . . .
H61 H 0.9680 0.3761 0.8540 0.094(2) Uiso 1 1 calc R . .
H62 H 0.8448 0.4447 0.7966 0.094(2) Uiso 1 1 calc R . .
C61 C 0.9595(2) 0.3478(3) 0.7244(2) 0.0491(6) Uani 1 1 d . . .
C62 C 0.9381(3) 0.3953(3) 0.6215(3) 0.0564(7) Uani 1 1 d . . .
H621 H 0.9110 0.4764 0.5889 0.094(2) Uiso 1 1 calc R . .
C63 C 0.9553(3) 0.3264(4) 0.5654(3) 0.0649(9) Uani 1 1 d . . .
H631 H 0.9406 0.3604 0.4949 0.094(2) Uiso 1 1 calc R . .
C64 C 0.9943(4) 0.2071(4) 0.6129(3) 0.0703(10) Uani 1 1 d . . .
H641 H 1.0061 0.1594 0.5750 0.094(2) Uiso 1 1 calc R . .
C65 C 1.0155(4) 0.1594(3) 0.7141(3) 0.0683(9) Uani 1 1 d . . .
H651 H 1.0417 0.0780 0.7467 0.094(2) Uiso 1 1 calc R . .
C66 C 0.9988(3) 0.2289(3) 0.7705(3) 0.0591(8) Uani 1 1 d . . .
H661 H 1.0146 0.1947 0.8408 0.094(2) Uiso 1 1 calc R . .
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C7 C 1.3068(3) 0.3159(4) 0.6159(3) 0.0679(9) Uani 1 1 d . . .
H71 H 1.2203 0.3218 0.6038 0.094(2) Uiso 1 1 calc R . .
H72 H 1.3475 0.2347 0.6373 0.094(2) Uiso 1 1 calc R . .
H73 H 1.3499 0.3633 0.5528 0.094(2) Uiso 1 1 calc R . .
C8 C 1.2868(4) 0.2958(4) 0.8980(3) 0.0746(10) Uani 1 1 d . . .
H81 H 1.1996 0.2872 0.9177 0.094(2) Uiso 1 1 calc R . .
H82 H 1.3098 0.3439 0.9288 0.094(2) Uiso 1 1 calc R . .
H83 H 1.3389 0.2191 0.9220 0.094(2) Uiso 1 1 calc R . .
C9 C 1.5878(4) 0.4409(4) 0.6288(4) 0.0825(13) Uani 1 1 d . . .
H91 H 1.6785 0.4311 0.6227 0.094(2) Uiso 1 1 calc R . .
H92 H 1.5534 0.5172 0.6306 0.094(2) Uiso 1 1 calc R . .
H93 H 1.5589 0.4353 0.5700 0.094(2) Uiso 1 1 calc R . .
C10 C 1.5867(4) 0.3601(4) 0.8117(4) 0.0786(11) Uani 1 1 d . . .
H101 H 1.6773 0.3496 0.8075 0.094(2) Uiso 1 1 calc R . .
H102 H 1.5575 0.3006 0.8750 0.094(2) Uiso 1 1 calc R . .
H103 H 1.5520 0.4372 0.8116 0.094(2) Uiso 1 1 calc R . .
N4 N 1.5465(2) 0.3493(2) 0.7239(3) 0.0597(7) Uani 1 1 d . . .
C11 C 1.6031(3) 0.2371(3) 0.7184(3) 0.0624(8) Uani 1 1 d . . .
H111 H 1.6939 0.2269 0.7213 0.094(2) Uiso 1 1 calc R . .
H112 H 1.5878 0.2387 0.6516 0.094(2) Uiso 1 1 calc R . .
C12 C 1.5551(3) 0.1331(3) 0.8031(3) 0.0639(8) Uani 1 1 d . . .
H121 H 1.5814 0.1237 0.8694 0.094(2) Uiso 1 1 calc R . .
H122 H 1.4634 0.1473 0.8069 0.094(2) Uiso 1 1 calc R . .
N5 N 1.6004(4) 0.0284(3) 0.7858(3) 0.0752(9) Uani 1 1 d . . .
C13 C 1.7270(5) -0.0182(4) 0.8132(5) 0.0960(16) Uani 1 1 d . . .
H131 H 1.7800 0.0401 0.7739 0.094(2) Uiso 1 1 calc R . .
H132 H 1.7558 -0.0877 0.7978 0.094(2) Uiso 1 1 calc R . .
H133 H 1.7309 -0.0387 0.8864 0.094(2) Uiso 1 1 calc R . .
C14 C 1.5210(6) -0.0586(4) 0.8433(5) 0.1073(19) Uani 1 1 d . . .
H141 H 1.4355 -0.0267 0.8244 0.094(2) Uiso 1 1 calc R . .
H142 H 1.5243 -0.0796 0.9167 0.094(2) Uiso 1 1 calc R . .
H143 H 1.5499 -0.1277 0.8275 0.094(2) Uiso 1 1 calc R . .
C15 C 0.8431(4) 0.1837(4) 0.0473(3) 0.0679(9) Uani 1 1 d . . .
C16 C 0.7502(4) 0.2744(4) 0.0491(3) 0.0731(10) Uani 1 1 d . . .
H161 H 0.6682 0.2739 0.0372 0.094(2) Uiso 1 1 calc R . .
C17 C 0.7746(4) 0.3653(4) 0.0677(4) 0.0824(12) Uani 1 1 d . . .
H171 H 0.7095 0.4260 0.0700 0.094(2) Uiso 1 1 calc R . .
C18 C 0.8944(5) 0.3678(4) 0.0829(3) 0.0824(12) Uani 1 1 d . . .
H181 H 0.9123 0.4309 0.0943 0.094(2) Uiso 1 1 calc R . .
C19 C 0.9877(4) 0.2781(4) 0.0814(3) 0.0762(11) Uani 1 1 d . . .
H191 H 1.0698 0.2790 0.0927 0.094(2) Uiso 1 1 calc R . .
C20 C 0.9626(4) 0.1878(4) 0.0637(3) 0.0714(10) Uani 1 1 d . . .
H201 H 1.0278 0.1267 0.0625 0.094(2) Uiso 1 1 calc R . .
C201 C 0.8165(5) 0.0851(5) 0.0278(4) 0.0900(13) Uani 1 1 d . . .
H202 H 0.7279 0.0964 0.0189 0.094(2) Uiso 1 1 calc R . .
H203 H 0.8394 0.0122 0.0860 0.094(2) Uiso 1 1 calc R . .
H204 H 0.8647 0.0818 -0.0343 0.094(2) Uiso 1 1 calc R . .

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N2 0.0453(13) 0.0526(15) 0.073(2) -0.0225(14) -0.0012(12) -0.0087(11)
N3 0.0417(11) 0.0502(13) 0.0552(15) -0.0224(11) -0.0015(10) -0.0085(10)
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C2 0.0436(13) 0.0522(15) 0.0476(16) -0.0192(12) -0.0002(11) -0.0112(11)
C21 0.0438(13) 0.0486(14) 0.0499(16) -0.0160(12) -0.0025(11) -0.0078(11)
C22 0.0591(17) 0.0593(17) 0.0565(19) -0.0249(15) 0.0023(14) -0.0172(14)
C23 0.0613(18) 0.0603(18) 0.081(3) -0.0315(18) -0.0011(17) -0.0183(15)
C24 0.0476(15) 0.0530(17) 0.086(3) -0.0143(17) -0.0034(15) -0.0154(13)
C25 0.0506(16) 0.069(2) 0.062(2) -0.0125(16) 0.0030(14) -0.0145(14)
C26 0.0522(15) 0.0636(18) 0.0551(19) -0.0211(15) 0.0015(13) -0.0144(13)
C3 0.0461(14) 0.0526(15) 0.0466(16) -0.0189(13) -0.0020(11) -0.0104(12)
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ef2

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C4 0.0411(13) 0.0549(15) 0.0501(17) -0.0196(13) -0.0018(11) -0.0107(11)
C41 0.0427(13) 0.0516(15) 0.0608(19) -0.0232(14) 0.0010(12) -0.0105(11)
C42 0.0499(16) 0.0625(18) 0.064(2) -0.0161(16) -0.0075(14) -0.0127(13)
C43 0.0500(16) 0.0624(19) 0.084(3) -0.0192(18) -0.0147(16) -0.0108(14)
C44 0.0414(14) 0.0645(19) 0.099(3) -0.036(2) 0.0017(16) -0.0094(13)
C45 0.0537(17) 0.070(2) 0.079(3) -0.0374(19) 0.0115(16) -0.0148(15)
C46 0.0514(16) 0.0675(19) 0.066(2) -0.0300(17) 0.0011(14) -0.0125(14)
C5 0.0438(13) 0.0541(15) 0.0471(16) -0.0208(13) 0.0024(11) -0.0150(11)
C6 0.0471(14) 0.0543(16) 0.0538(18) -0.0215(13) 0.0044(12) -0.0139(12)
C61 0.0396(12) 0.0526(15) 0.0554(17) -0.0207(13) 0.0030(11) -0.0133(11)
C62 0.0529(15) 0.0628(18) 0.0533(18) -0.0188(14) -0.0013(13) -0.0190(13)
C63 0.0678(19) 0.079(2) 0.055(2) -0.0274(17) -0.0032(15) -0.0266(17)
C64 0.070(2) 0.077(2) 0.077(3) -0.042(2) 0.0101(18) -0.0271(18)
C65 0.073(2) 0.0574(18) 0.077(3) -0.0306(18) 0.0044(18) -0.0130(16)
C66 0.0626(17) 0.0578(17) 0.0554(19) -0.0209(15) 0.0004(14) -0.0120(14)
C7 0.0583(18) 0.083(2) 0.071(2) -0.038(2) 0.0028(16) -0.0180(17)
C8 0.066(2) 0.088(3) 0.056(2) -0.0175(19) -0.0013(16) -0.0051(18)
C9 0.0539(18) 0.067(2) 0.105(3) -0.014(2) 0.011(2) -0.0158(16)
C10 0.062(2) 0.085(3) 0.102(3) -0.045(2) -0.016(2) -0.0140(18)
N4 0.0459(12) 0.0567(15) 0.0725(19) -0.0211(13) -0.0007(12) -0.0104(11)
C11 0.0499(15) 0.0620(19) 0.070(2) -0.0239(17) 0.0060(15) -0.0090(14)
C12 0.0609(18) 0.0572(18) 0.067(2) -0.0189(16) -0.0006(16) -0.0093(14)
N5 0.084(2) 0.0641(18) 0.076(2) -0.0282(16) -0.0036(17) -0.0080(16)
C13 0.085(3) 0.076(3) 0.107(4) -0.031(3) 0.007(3) 0.010(2)
C14 0.129(4) 0.067(3) 0.127(5) -0.025(3) -0.027(4) -0.031(3)
C15 0.0649(19) 0.086(2) 0.056(2) -0.0301(18) 0.0044(16) -0.0184(18)
C16 0.0584(18) 0.094(3) 0.062(2) -0.028(2) -0.0026(16) -0.0106(18)
C17 0.086(3) 0.080(3) 0.068(3) -0.024(2) 0.006(2) -0.007(2)
C18 0.106(3) 0.091(3) 0.057(2) -0.030(2) 0.009(2) -0.040(3)
C19 0.070(2) 0.105(3) 0.057(2) -0.030(2) 0.0021(17) -0.030(2)
C20 0.0599(18) 0.099(3) 0.052(2) -0.0280(19) 0.0023(15) -0.0138(19)
C201 0.091(3) 0.099(3) 0.089(3) -0.044(3) 0.007(3) -0.030(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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In1 C7 2.159(4) . ?
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In1 N4 2.523(3) . ?
N1 C1 1.342(4) . ?
N2 C3 1.374(4) . ?
N3 C5 1.348(4) . ?
N3 C1 1.371(4) . ?
C1 C2 1.413(4) . ?
C2 C3 1.401(4) . ?
C2 C21 1.489(4) . ?
C21 C22 1.386(5) . ?
C21 C26 1.400(5) . ?
C22 C23 1.396(5) . ?
C23 C24 1.377(6) . ?
C24 C25 1.381(6) . ?
C25 C26 1.389(5) . ?
C3 C4 1.426(4) . ?
C4 C5 1.378(4) . ?
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C4 C41 1.502(4) . ?
C41 C42 1.391(5) . ?
C41 C46 1.392(5) . ?
C42 C43 1.409(5) . ?
C43 C44 1.377(6) . ?
C44 C45 1.378(6) . ?
C45 C46 1.389(5) . ?
C5 C6 1.517(4) . ?
C6 C61 1.508(4) . ?
C61 C62 1.385(5) . ?
C61 C66 1.389(5) . ?
C62 C63 1.386(5) . ?
C63 C64 1.394(6) . ?
C64 C65 1.363(6) . ?
C65 C66 1.397(5) . ?
C9 N4 1.477(5) . ?
C10 N4 1.463(6) . ?
N4 C11 1.469(5) . ?
C11 C12 1.521(5) . ?
C12 N5 1.434(5) . ?
N5 C13 1.448(6) . ?
N5 C14 1.462(6) . ?
C15 C16 1.385(6) . ?
C15 C20 1.392(6) . ?
C15 C201 1.491(6) . ?
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C17 C18 1.384(7) . ?
C18 C19 1.378(7) . ?
C19 C20 1.367(7) . ?

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C8 In1 C7 131.48(18) . . ?
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C7 In1 N1 112.57(15) . . ?
C8 In1 N3 93.04(13) . . ?
C7 In1 N3 102.16(13) . . ?
N1 In1 N3 57.75(9) . . ?
C8 In1 N4 96.79(13) . . ?
C7 In1 N4 94.37(12) . . ?
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N3 In1 N4 147.38(9) . . ?
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C5 N3 C1 119.9(3) . . ?
C5 N3 In1 150.8(2) . . ?
C1 N3 In1 89.19(17) . . ?
N1 C1 N3 111.4(3) . . ?
N1 C1 C2 127.6(3) . . ?
N3 C1 C2 120.9(3) . . ?
C3 C2 C1 118.1(3) . . ?
C3 C2 C21 122.0(3) . . ?
C1 C2 C21 119.8(3) . . ?
C22 C21 C26 118.6(3) . . ?
C22 C21 C2 120.5(3) . . ?
C26 C21 C2 120.9(3) . . ?
C21 C22 C23 120.9(3) . . ?
C24 C23 C22 119.6(4) . . ?
C23 C24 C25 120.6(3) . . ?
C24 C25 C26 119.7(3) . . ?
C25 C26 C21 120.6(3) . . ?
N2 C3 C2 120.3(3) . . ?
N2 C3 C4 119.5(3) . . ?
C2 C3 C4 120.2(3) . . ?
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C5 C4 C41 122.0(3) . . ?
C3 C4 C41 120.3(3) . . ?
C42 C41 C46 118.5(3) . . ?
C42 C41 C4 120.4(3) . . ?
C46 C41 C4 121.0(3) . . ?
C41 C42 C43 120.2(4) . . ?
C44 C43 C42 120.1(4) . . ?
C43 C44 C45 119.8(3) . . ?
C44 C45 C46 120.3(4) . . ?
C45 C46 C41 121.0(4) . . ?
N3 C5 C4 123.0(3) . . ?
N3 C5 C6 113.8(3) . . ?
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C61 C6 C5 113.8(2) . . ?
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C10 N4 C9 109.4(3) . . ?
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C11 N4 In1 111.8(2) . . ?
C9 N4 In1 108.1(2) . . ?
N4 C11 C12 114.2(3) . . ?
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C12 N5 C13 111.8(4) . . ?
C12 N5 C14 110.4(4) . . ?
C13 N5 C14 109.8(4) . . ?
C16 C15 C20 118.0(4) . . ?
C16 C15 C201 121.2(4) . . ?
C20 C15 C201 120.8(4) . . ?
C17 C16 C15 121.3(4) . . ?
C16 C17 C18 119.6(4) . . ?
C19 C18 C17 119.7(4) . . ?
C20 C19 C18 120.3(4) . . ?
C19 C20 C15 121.1(4) . . ?

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Bond lengths (Angstr.)

In(1) - N(1)	2.180(3)	In(1) - N(3)	2.439(3)
In(1) - N(4)	2.523(3)	In(1) - C(7)	2.160(5)
In(1) - C(8)	2.148(4)	N(1) - C(1)	1.342(4)
N(2) - C(3)	1.375(4)	N(3) - C(1)	1.370(4)
N(3) - C(5)	1.349(4)	N(4) - C(9)	1.477(6)
N(4) - C(10)	1.463(6)	N(4) - C(11)	1.469(5)
N(5) - C(12)	1.435(5)	N(5) - C(13)	1.448(7)
N(5) - C(14)	1.461(6)	C(1) - C(2)	1.412(5)
C(2) - C(3)	1.401(4)	C(2) - C(21)	1.489(5)
C(3) - C(4)	1.426(4)	C(4) - C(5)	1.378(5)
C(4) - C(41)	1.502(4)	C(5) - C(6)	1.517(5)
C(6) - C(61)	1.509(5)	C(11) - C(12)	1.522(6)
C(21) - C(22)	1.386(5)	C(21) - C(26)	1.400(5)
C(22) - C(23)	1.396(5)	C(23) - C(24)	1.377(5)
C(24) - C(25)	1.382(6)	C(25) - C(26)	1.390(5)
C(41) - C(42)	1.391(5)	C(41) - C(46)	1.390(5)
C(42) - C(43)	1.409(5)	C(43) - C(44)	1.377(6)
C(44) - C(45)	1.378(6)	C(45) - C(46)	1.389(5)
C(61) - C(62)	1.386(5)	C(61) - C(66)	1.389(5)
C(62) - C(63)	1.387(5)	C(63) - C(64)	1.394(7)
C(64) - C(65)	1.363(6)	C(65) - C(66)	1.397(6)
N(1) - H(1)	0.85(4)	N(2) - H(2)	0.82(5)
N(2) - H(3)	0.83(5)	C(6) - H(61)	0.99
C(6) - H(62)	0.99	C(7) - H(71)	0.98
C(7) - H(72)	0.98	C(7) - H(73)	0.98
C(8) - H(81)	0.98	C(8) - H(82)	0.98
C(8) - H(83)	0.98	C(9) - H(91)	0.98
C(9) - H(92)	0.98	C(9) - H(93)	0.98
C(10) - H(101)	0.98	C(10) - H(102)	0.98
C(10) - H(103)	0.98	C(11) - H(111)	0.99
C(11) - H(112)	0.99	C(12) - H(121)	0.99
C(12) - H(122)	0.99	C(13) - H(131)	0.98
C(13) - H(132)	0.98	C(13) - H(133)	0.98
C(14) - H(141)	0.98	C(14) - H(142)	0.98
C(14) - H(143)	0.98	C(22) - H(221)	0.95
C(23) - H(231)	0.95	C(24) - H(241)	0.95
C(25) - H(251)	0.95	C(26) - H(261)	0.95
C(42) - H(421)	0.95	C(43) - H(431)	0.95
C(44) - H(441)	0.95	C(45) - H(451)	0.95
C(46) - H(461)	0.95	C(62) - H(621)	0.95
C(63) - H(631)	0.95	C(64) - H(641)	0.95
C(65) - H(651)	0.95	C(66) - H(661)	0.95
C(15) - C(16)	1.386(6)	C(15) - C(20)	1.392(6)
C(15) - C(201)	1.490(6)	C(16) - C(17)	1.379(7)
C(17) - C(18)	1.384(7)	C(18) - C(19)	1.379(7)
C(19) - C(20)	1.367(7)	C(16) - H(161)	0.95
C(17) - H(171)	0.95	C(18) - H(181)	0.95
C(19) - H(191)	0.95	C(20) - H(201)	0.95
C(201)- H(202)	0.98	C(201)- H(203)	0.98
C(201)- H(204)	0.98		

Bond angles (deg.)

N(1)	In(1)	N(3)	57.72(9)	N(1)	In(1)	N(4)	90.01(9)
N(1)	In(1)	C(7)	112.6(1)	N(1)	In(1)	C(8)	114.5(2)
N(3)	In(1)	N(4)	147.37(9)	N(3)	In(1)	C(7)	102.2(1)
N(3)	In(1)	C(8)	93.1(1)	N(4)	In(1)	C(7)	94.4(1)
N(4)	In(1)	C(8)	96.8(2)	C(7)	In(1)	C(8)	131.5(2)
In(1)	N(1)	C(1)	101.7(2)	In(1)	N(3)	C(1)	89.2(2)
In(1)	N(3)	C(5)	150.7(2)	C(1)	N(3)	C(5)	119.9(3)
In(1)	N(4)	C(9)	108.1(2)	In(1)	N(4)	C(10)	109.5(2)
In(1)	N(4)	C(11)	111.8(2)	C(9)	N(4)	C(10)	109.3(3)
C(9)	N(4)	C(11)	107.2(3)	C(10)	N(4)	C(11)	110.8(3)
C(12)	N(5)	C(13)	111.8(4)	C(12)	N(5)	C(14)	110.4(4)
C(13)	N(5)	C(14)	109.8(4)	N(1)	C(1)	N(3)	111.4(3)
N(1)	C(1)	C(2)	127.6(3)	N(3)	C(1)	C(2)	121.0(3)
C(1)	C(2)	C(3)	118.1(3)	C(1)	C(2)	C(21)	119.9(3)
C(3)	C(2)	C(21)	122.1(3)	N(2)	C(3)	C(2)	120.2(3)
N(2)	C(3)	C(4)	119.5(3)	C(2)	C(3)	C(4)	120.2(3)
C(3)	C(4)	C(5)	117.7(3)	C(3)	C(4)	C(41)	120.2(3)
C(5)	C(4)	C(41)	122.1(3)	N(3)	C(5)	C(4)	123.0(3)
N(3)	C(5)	C(6)	113.8(3)	C(4)	C(5)	C(6)	123.2(3)
C(5)	C(6)	C(61)	113.8(3)	N(4)	C(11)	C(12)	114.2(3)
N(5)	C(12)	C(11)	111.6(3)	C(2)	C(21)	C(22)	120.5(3)
C(2)	C(21)	C(26)	120.9(3)	C(22)	C(21)	C(26)	118.6(3)
C(21)	C(22)	C(23)	120.9(3)	C(22)	C(23)	C(24)	119.6(4)
C(23)	C(24)	C(25)	120.6(4)	C(24)	C(25)	C(26)	119.7(4)
C(21)	C(26)	C(25)	120.6(4)	C(4)	C(41)	C(42)	120.4(3)
C(4)	C(41)	C(46)	121.0(3)	C(42)	C(41)	C(46)	118.5(3)
C(41)	C(42)	C(43)	120.2(4)	C(42)	C(43)	C(44)	120.2(4)
C(43)	C(44)	C(45)	119.8(3)	C(44)	C(45)	C(46)	120.2(4)
C(41)	C(46)	C(45)	121.0(3)	C(6)	C(61)	C(62)	120.9(3)
C(6)	C(61)	C(66)	120.7(3)	C(62)	C(61)	C(66)	118.4(3)
C(61)	C(62)	C(63)	121.2(4)	C(62)	C(63)	C(64)	119.8(4)
C(63)	C(64)	C(65)	119.6(4)	C(64)	C(65)	C(66)	120.7(4)
C(61)	C(66)	C(65)	120.5(3)	In(1)	N(1)	H(1)	138.(3)
C(1)	N(1)	H(1)	120.(3)	C(3)	N(2)	H(2)	116.(4)
C(3)	N(2)	H(3)	121.(4)	H(2)	N(2)	H(3)	121.(5)
C(5)	C(6)	H(61)	108.84(0)	C(5)	C(6)	H(62)	108.83(0)
C(61)	C(6)	H(61)	108.76(0)	C(61)	C(6)	H(62)	108.76(0)
H(61)	C(6)	H(62)	107.68(0)	In(1)	C(7)	H(71)	109.49(0)
In(1)	C(7)	H(72)	109.49(0)	In(1)	C(7)	H(73)	109.42(0)
H(71)	C(7)	H(72)	109.49(0)	H(71)	C(7)	H(73)	109.52(0)
H(72)	C(7)	H(73)	109.42(0)	In(1)	C(8)	H(81)	109.44(0)
In(1)	C(8)	H(82)	109.45(0)	In(1)	C(8)	H(83)	109.45(0)
H(81)	C(8)	H(82)	109.46(0)	H(81)	C(8)	H(83)	109.46(0)
H(82)	C(8)	H(83)	109.56(0)	N(4)	C(9)	H(91)	109.49(0)
N(4)	C(9)	H(92)	109.49(0)	N(4)	C(9)	H(93)	109.48(0)
H(91)	C(9)	H(92)	109.42(0)	H(91)	C(9)	H(93)	109.54(0)
H(92)	C(9)	H(93)	109.40(0)	N(4)	C(10)	H(101)	109.57(0)
N(4)	C(10)	H(102)	109.42(0)	N(4)	C(10)	H(103)	109.46(0)
H(101)	C(10)	H(102)	109.42(0)	H(101)	C(10)	H(103)	109.53(0)
H(102)	C(10)	H(103)	109.43(0)	N(4)	C(11)	H(111)	108.70(0)
N(4)	C(11)	H(112)	108.67(0)	C(12)	C(11)	H(111)	108.67(0)
C(12)	C(11)	H(112)	108.75(0)	H(111)	C(11)	H(112)	107.64(0)
N(5)	C(12)	H(121)	109.32(0)	N(5)	C(12)	H(122)	109.28(0)
C(11)	C(12)	H(121)	109.30(0)	C(11)	C(12)	H(122)	109.29(0)
H(121)	C(12)	H(122)	107.98(0)	N(5)	C(13)	H(131)	109.50(0)
N(5)	C(13)	H(132)	109.47(0)	N(5)	C(13)	H(133)	109.48(0)
H(131)	C(13)	H(132)	109.41(0)	H(131)	C(13)	H(133)	109.55(0)
H(132)	C(13)	H(133)	109.42(0)	N(5)	C(14)	H(141)	109.48(0)
N(5)	C(14)	H(142)	109.43(0)	N(5)	C(14)	H(143)	109.50(0)
H(141)	C(14)	H(142)	109.41(0)	H(141)	C(14)	H(143)	109.52(0)
H(142)	C(14)	H(143)	109.48(0)	C(21)	C(22)	H(221)	119.56(0)

C(23)	-	C(22)	-	H(221)	119.57(0)	C(22)	- C(23) - H(231) 120.15(0)
C(24)	-	C(23)	-	H(231)	120.25(0)	C(23)	- C(24) - H(241) 119.64(0)
C(25)	-	C(24)	-	H(241)	119.72(0)	C(24)	- C(25) - H(251) 120.17(0)
C(26)	-	C(25)	-	H(251)	120.11(0)	C(21)	- C(26) - H(261) 119.72(0)
C(25)	-	C(26)	-	H(261)	119.69(0)	C(41)	- C(42) - H(421) 119.95(0)
C(43)	-	C(42)	-	H(421)	119.90(0)	C(42)	- C(43) - H(431) 119.89(0)
C(44)	-	C(43)	-	H(431)	119.94(0)	C(43)	- C(44) - H(441) 120.04(0)
C(45)	-	C(44)	-	H(441)	120.11(0)	C(44)	- C(45) - H(451) 119.89(0)
C(46)	-	C(45)	-	H(451)	119.87(0)	C(41)	- C(46) - H(461) 119.55(0)
C(45)	-	C(46)	-	H(461)	119.43(0)	C(61)	- C(62) - H(621) 119.41(0)
C(63)	-	C(62)	-	H(621)	119.42(0)	C(62)	- C(63) - H(631) 120.08(0)
C(64)	-	C(63)	-	H(631)	120.16(0)	C(63)	- C(64) - H(641) 120.21(0)
C(65)	-	C(64)	-	H(641)	120.20(0)	C(64)	- C(65) - H(651) 119.70(0)
C(66)	-	C(65)	-	H(651)	119.65(0)	C(61)	- C(66) - H(661) 119.72(0)
C(65)	-	C(66)	-	H(661)	119.83(0)		
C(16)	-	C(15)	-	C(20)	117.9(5)	C(16)	- C(15) - C(201) 121.2(4)
C(20)	-	C(15)	-	C(201)	120.9(5)	C(15)	- C(16) - C(17) 121.3(4)
C(16)	-	C(17)	-	C(18)	119.7(5)	C(17)	- C(18) - C(19) 119.6(5)
C(18)	-	C(19)	-	C(20)	120.3(4)	C(15)	- C(20) - C(19) 121.2(5)
C(15)	-	C(16)	-	H(161)	119.31(0)	C(17)	- C(16) - H(161) 119.43(0)
C(16)	-	C(17)	-	H(171)	120.16(0)	C(18)	- C(17) - H(171) 120.14(0)
C(17)	-	C(18)	-	H(181)	120.23(0)	C(19)	- C(18) - H(181) 120.13(0)
C(18)	-	C(19)	-	H(191)	119.88(0)	C(20)	- C(19) - H(191) 119.81(0)
C(15)	-	C(20)	-	H(201)	119.31(0)	C(19)	- C(20) - H(201) 119.50(0)
C(15)	-	C(201)	-	H(202)	109.47(0)	C(15)	- C(201) - H(203) 109.48(0)
C(15)	-	C(201)	-	H(204)	109.48(0)	H(202)	- C(201) - H(203) 109.47(0)
H(202)	-	C(201)	-	H(204)	109.48(0)	H(203)	- C(201) - H(204) 109.44(0)

Atom	x	y	z	Ueq/Uiso	
In(1)	1.31304(2)	0.37734(2)	0.73444(2)	0.0509(1)	
N(1)	1.3053(2)	0.5648(2)	0.6752(2)	0.055(1)	
N(2)	0.9273(3)	0.8487(3)	0.6398(3)	0.058(1)	
N(3)	1.1178(2)	0.5114(2)	0.7208(2)	0.0485(8)	
N(4)	1.5465(2)	0.3493(2)	0.7239(3)	0.060(1)	
N(5)	1.6004(4)	0.0284(3)	0.7858(3)	0.075(1)	
C(1)	1.1828(3)	0.6022(3)	0.6815(2)	0.0491(8)	
C(2)	1.1211(3)	0.7181(3)	0.6525(2)	0.0477(8)	
C(3)	0.9915(3)	0.7375(3)	0.6661(2)	0.048(1)	
C(4)	0.9255(3)	0.6419(3)	0.7098(2)	0.049(1)	
C(5)	0.9934(3)	0.5318(3)	0.7364(2)	0.0475(8)	
C(6)	0.9354(3)	0.4225(3)	0.7860(3)	0.052(1)	
C(7)	1.3068(3)	0.3159(4)	0.6159(3)	0.068(1)	
C(8)	1.2868(4)	0.2958(4)	0.8980(3)	0.075(1)	
C(9)	1.5878(4)	0.4409(4)	0.6288(4)	0.083(1)	
C(10)	1.5867(4)	0.3601(4)	0.8117(4)	0.079(2)	
C(11)	1.6031(3)	0.2371(3)	0.7184(3)	0.062(1)	
C(12)	1.5551(3)	0.1331(3)	0.8031(3)	0.064(1)	
C(13)	1.7270(5)	-0.0182(4)	0.8132(5)	0.096(2)	
C(14)	1.5210(6)	-0.0586(4)	0.8433(5)	0.108(2)	
C(21)	1.1941(3)	0.8150(3)	0.6113(2)	0.0485(8)	
C(22)	1.2015(3)	0.8781(3)	0.6686(3)	0.057(1)	
C(23)	1.2717(3)	0.9676(3)	0.6313(3)	0.065(1)	
C(24)	1.3346(3)	0.9935(3)	0.5364(3)	0.065(1)	
C(25)	1.3279(3)	0.9325(3)	0.4775(3)	0.065(1)	
C(26)	1.2577(3)	0.8436(3)	0.5146(3)	0.057(1)	
C(41)	0.7868(3)	0.6626(3)	0.7271(3)	0.051(1)	
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C(43)	0.5827(3)	0.7252(3)	0.6616(3)	0.067(1)	
C(44)	0.5282(3)	0.6946(3)	0.7597(4)	0.068(1)	
C(45)	0.6012(3)	0.6481(3)	0.8415(3)	0.066(1)	
C(46)	0.7295(3)	0.6336(3)	0.8253(3)	0.060(1)	
C(61)	0.9595(2)	0.3478(3)	0.7244(2)	0.049(1)	
C(62)	0.9381(3)	0.3953(3)	0.6215(3)	0.056(1)	
C(63)	0.9553(3)	0.3264(4)	0.5654(3)	0.065(1)	
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C(66)	0.9988(3)	0.2289(3)	0.7705(3)	0.059(1)	
H(1)	1.356(4)	0.613(3)	0.655(3)	0.06(1)	*
H(2)	0.968(4)	0.901(4)	0.608(4)	0.08(1)	*
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H(61)	0.96800(0)	0.37610(0)	0.85400(0)	0.094(2)	*
H(62)	0.84480(0)	0.44470(0)	0.79660(0)	0.094(2)	*
H(71)	1.22030(0)	0.32180(0)	0.60380(0)	0.094(2)	*
H(72)	1.34750(0)	0.23470(0)	0.63730(0)	0.094(2)	*
H(73)	1.34990(0)	0.36330(0)	0.55280(0)	0.094(2)	*
H(81)	1.19960(0)	0.28720(0)	0.91770(0)	0.094(2)	*
H(82)	1.30980(0)	0.34390(0)	0.92880(0)	0.094(2)	*
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H(91)	1.67850(0)	0.43110(0)	0.62270(0)	0.094(2)	*
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H(122)	1.46340(0)	0.14730(0)	0.80690(0)	0.094(2)	*
H(131)	1.78000(0)	0.04010(0)	0.77390(0)	0.094(2)	*
H(132)	1.75580(0)	-0.08770(0)	0.79780(0)	0.094(2)	*
H(133)	1.73090(0)	-0.03870(0)	0.88640(0)	0.094(2)	*

H(141)	1.43550(0)	-0.02670(0)	0.82440(0)	0.094(2) *
H(142)	1.52430(0)	-0.07960(0)	0.91670(0)	0.094(2) *
H(143)	1.54990(0)	-0.12770(0)	0.82750(0)	0.094(2) *
H(221)	1.15820(0)	0.86020(0)	0.73410(0)	0.094(2) *
H(231)	1.27590(0)	1.01040(0)	0.67110(0)	0.094(2) *
H(241)	1.38320(0)	1.05380(0)	0.51130(0)	0.094(2) *
H(251)	1.37110(0)	0.95120(0)	0.41190(0)	0.094(2) *
H(261)	1.25290(0)	0.80190(0)	0.47400(0)	0.094(2) *
H(421)	0.75000(0)	0.72760(0)	0.57710(0)	0.094(2) *
H(431)	0.53250(0)	0.75800(0)	0.60510(0)	0.094(2) *
H(441)	0.44050(0)	0.70540(0)	0.77090(0)	0.094(2) *
H(451)	0.56370(0)	0.62590(0)	0.90920(0)	0.094(2) *
H(461)	0.77880(0)	0.60340(0)	0.88230(0)	0.094(2) *
H(621)	0.91100(0)	0.47640(0)	0.58890(0)	0.094(2) *
H(631)	0.94060(0)	0.36040(0)	0.49490(0)	0.094(2) *
H(641)	1.00610(0)	0.15940(0)	0.57500(0)	0.094(2) *
H(651)	1.04170(0)	0.07800(0)	0.74670(0)	0.094(2) *
H(661)	1.01460(0)	0.19470(0)	0.84080(0)	0.094(2) *
C(15)	0.8431(4)	0.1837(4)	0.0473(3)	0.068(1)
C(16)	0.7502(4)	0.2744(4)	0.0491(3)	0.073(1)
C(17)	0.7746(4)	0.3653(4)	0.0677(4)	0.082(2)
C(18)	0.8944(5)	0.3678(4)	0.0829(3)	0.082(2)
C(19)	0.9877(4)	0.2781(4)	0.0814(3)	0.076(1)
C(20)	0.9626(4)	0.1878(4)	0.0637(3)	0.071(1)
C(201)	0.8165(5)	0.0851(5)	0.0278(4)	0.090(2)
H(161)	0.66820(0)	0.27390(0)	0.03720(0)	0.094(2) *
H(171)	0.70950(0)	0.42600(0)	0.07000(0)	0.094(2) *
H(181)	0.91230(0)	0.43090(0)	0.09430(0)	0.094(2) *
H(191)	1.06980(0)	0.27900(0)	0.09270(0)	0.094(2) *
H(201)	1.02780(0)	0.12670(0)	0.06250(0)	0.094(2) *
H(202)	0.72790(0)	0.09640(0)	0.01890(0)	0.094(2) *
H(203)	0.83940(0)	0.01220(0)	0.08600(0)	0.094(2) *
H(204)	0.86470(0)	0.08180(0)	-0.03430(0)	0.094(2) *

* refined isotropically

Atom	U11	U22	U33	U23	U13	U12
In(1)	0.0449(1)	0.0508(1)	0.0539(2)	-0.0178(1)	0.0000(1)	-0.0093(1)
N(1)	0.042(1)	0.052(1)	0.070(2)	-0.020(1)	0.000(1)	-0.012(1)
N(2)	0.045(1)	0.053(2)	0.073(2)	-0.023(1)	-0.001(1)	-0.009(1)
N(3)	0.042(1)	0.050(1)	0.055(2)	-0.022(1)	-0.002(1)	-0.009(1)
N(4)	0.046(1)	0.057(2)	0.072(2)	-0.021(1)	-0.001(1)	-0.010(1)
N(5)	0.084(2)	0.064(2)	0.076(2)	-0.028(2)	-0.004(2)	-0.008(2)
C(1)	0.046(1)	0.053(2)	0.048(2)	-0.019(1)	0.000(1)	-0.012(1)
C(2)	0.044(1)	0.052(2)	0.048(2)	-0.019(1)	0.000(1)	-0.011(1)
C(3)	0.046(1)	0.053(2)	0.047(2)	-0.019(1)	-0.002(1)	-0.010(1)
C(4)	0.041(1)	0.055(2)	0.050(2)	-0.020(1)	-0.002(1)	-0.011(1)
C(5)	0.044(1)	0.054(2)	0.047(2)	-0.021(1)	0.002(1)	-0.015(1)
C(6)	0.047(1)	0.054(2)	0.054(2)	-0.022(1)	0.004(1)	-0.014(1)
C(7)	0.058(2)	0.083(2)	0.071(2)	-0.038(2)	0.003(2)	-0.018(2)
C(8)	0.066(2)	0.088(3)	0.056(2)	-0.018(2)	-0.001(2)	-0.005(2)
C(9)	0.054(2)	0.067(2)	0.105(3)	-0.014(2)	0.011(2)	-0.016(2)
C(10)	0.062(2)	0.085(3)	0.102(3)	-0.045(2)	-0.016(2)	-0.014(2)
C(11)	0.050(2)	0.062(2)	0.070(2)	-0.024(2)	0.006(2)	-0.009(1)
C(12)	0.061(2)	0.057(2)	0.067(2)	-0.019(2)	-0.001(2)	-0.009(1)
C(13)	0.085(3)	0.076(3)	0.107(4)	-0.031(3)	0.007(3)	0.010(2)
C(14)	0.129(4)	0.067(3)	0.127(5)	-0.025(3)	-0.027(4)	-0.031(3)
C(21)	0.044(1)	0.049(1)	0.050(2)	-0.016(1)	-0.002(1)	-0.008(1)
C(22)	0.059(2)	0.059(2)	0.056(2)	-0.025(2)	0.002(1)	-0.017(1)
C(23)	0.061(2)	0.060(2)	0.081(3)	-0.032(2)	-0.001(2)	-0.018(2)
C(24)	0.048(2)	0.053(2)	0.086(3)	-0.014(2)	-0.003(2)	-0.015(1)
C(25)	0.051(2)	0.069(2)	0.062(2)	-0.013(2)	0.003(1)	-0.014(1)
C(26)	0.052(2)	0.064(2)	0.055(2)	-0.021(2)	0.002(1)	-0.014(1)
C(41)	0.043(1)	0.052(2)	0.061(2)	-0.023(1)	0.001(1)	-0.010(1)
C(42)	0.050(2)	0.063(2)	0.064(2)	-0.016(2)	-0.007(1)	-0.013(1)
C(43)	0.050(2)	0.062(2)	0.084(3)	-0.019(2)	-0.015(2)	-0.011(1)
C(44)	0.041(1)	0.064(2)	0.099(3)	-0.036(2)	0.002(2)	-0.009(1)
C(45)	0.054(2)	0.070(2)	0.079(3)	-0.037(2)	0.012(2)	-0.015(2)
C(46)	0.051(2)	0.068(2)	0.066(2)	-0.030(2)	0.001(1)	-0.013(1)
C(61)	0.040(1)	0.053(2)	0.055(2)	-0.021(1)	0.003(1)	-0.013(1)
C(62)	0.053(2)	0.063(2)	0.053(2)	-0.019(1)	-0.001(1)	-0.019(1)
C(63)	0.068(2)	0.079(2)	0.055(2)	-0.027(2)	-0.003(2)	-0.027(2)
C(64)	0.070(2)	0.077(2)	0.077(3)	-0.042(2)	0.010(2)	-0.027(2)
C(65)	0.073(2)	0.057(2)	0.077(3)	-0.031(2)	0.004(2)	-0.013(2)
C(66)	0.063(2)	0.058(2)	0.055(2)	-0.021(2)	0.000(1)	-0.012(1)
C(15)	0.065(2)	0.086(2)	0.056(2)	-0.030(2)	0.004(2)	-0.018(2)
C(16)	0.058(2)	0.094(3)	0.062(2)	-0.028(2)	-0.003(2)	-0.011(2)
C(17)	0.086(3)	0.080(3)	0.068(3)	-0.024(2)	0.006(2)	-0.007(2)
C(18)	0.106(3)	0.091(3)	0.057(2)	-0.030(2)	0.009(2)	-0.040(3)
C(19)	0.070(2)	0.105(3)	0.057(2)	-0.030(2)	0.002(2)	-0.030(2)
C(20)	0.060(2)	0.099(3)	0.052(2)	-0.028(2)	0.002(2)	-0.014(2)
C(201)	0.091(3)	0.099(3)	0.089(3)	-0.044(3)	0.007(3)	-0.030(3)

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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.
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C5 C -0.4153(5) 0.5462(3) 0.0891(3) 0.0522(10) Uani 1 1 d . . .
H51 H -0.5013 0.5244 0.0906 0.069(2) Uiso 1 1 calc R . .
C6 C -0.3362(5) 0.6050(3) 0.0060(3) 0.0534(10) Uani 1 1 d . . .
H61 H -0.3676 0.6246 -0.0496 0.069(2) Uiso 1 1 calc R . .
C7 C -0.2102(5) 0.6354(3) 0.0041(3) 0.0511(10) Uani 1 1 d . . .
H71 H -0.1542 0.6748 -0.0535 0.069(2) Uiso 1 1 calc R . .
C8 C -0.1652(4) 0.6086(3) 0.0858(3) 0.0457(9) Uani 1 1 d . . .
H81 H -0.0787 0.6301 0.0836 0.069(2) Uiso 1 1 calc R . .
C9 C -0.0676(4) 0.5224(3) 0.2704(3) 0.0415(8) Uani 1 1 d . . .
C10 C -0.0424(4) 0.5415(3) 0.3521(3) 0.0457(8) Uani 1 1 d . . .
H101 H -0.1160 0.5610 0.3999 0.069(2) Uiso 1 1 calc R . .
C11 C 0.0866(4) 0.5325(3) 0.3636(3) 0.0520(10) Uani 1 1 d . . .
H111 H 0.1003 0.5440 0.4199 0.069(2) Uiso 1 1 calc R . .
C12 C 0.1970(5) 0.5068(3) 0.2938(3) 0.0542(10) Uani 1 1 d . . .
H121 H 0.2864 0.5029 0.3010 0.069(2) Uiso 1 1 calc R . .
C13 C 0.1744(5) 0.4872(3) 0.2145(3) 0.0546(10) Uani 1 1 d . . .
H131 H 0.2491 0.4679 0.1672 0.069(2) Uiso 1 1 calc R . .
C14 C 0.0454(4) 0.4948(3) 0.2017(3) 0.0472(9) Uani 1 1 d . . .
H141 H 0.0332 0.4812 0.1457 0.069(2) Uiso 1 1 calc R . .
C15 C -0.4178(5) 0.6953(4) 0.5678(3) 0.0589(11) Uani 1 1 d . . .
H151 H -0.4065 0.7726 0.5486 0.069(2) Uiso 1 1 calc R . .
H152 H -0.3287 0.6584 0.5629 0.069(2) Uiso 1 1 calc R . .
H153 H -0.4736 0.6760 0.6335 0.069(2) Uiso 1 1 calc R . .
C16 C -0.6910(4) 0.6903(4) 0.4272(3) 0.0557(10) Uani 1 1 d . . .
H161 H -0.7714 0.6669 0.4793 0.069(2) Uiso 1 1 calc R . .
H162 H -0.6850 0.6550 0.3759 0.069(2) Uiso 1 1 calc R . .
H163 H -0.6980 0.7678 0.4032 0.069(2) Uiso 1 1 calc R . .
O1 O -0.3819(3) 0.7723(2) 0.33683(18) 0.0480(6) Uani 1 1 d . . .
C17 C -0.4063(4) 0.7869(3) 0.2444(3) 0.0473(9) Uani 1 1 d . . .
H171 H -0.4922 0.8285 0.2420 0.069(2) Uiso 1 1 calc R . .
H172 H -0.4124 0.7170 0.2310 0.069(2) Uiso 1 1 calc R . .
C18 C -0.2885(5) 0.8460(3) 0.1729(3) 0.0561(11) Uani 1 1 d . . .
H181 H -0.3092 0.9238 0.1587 0.069(2) Uiso 1 1 calc R . .
H182 H -0.2647 0.8215 0.1131 0.069(2) Uiso 1 1 calc R . .
C19 C -0.1743(5) 0.8183(4) 0.2219(3) 0.0576(11) Uani 1 1 d . . .
H191 H -0.1278 0.7494 0.2129 0.069(2) Uiso 1 1 calc R . .
H192 H -0.1070 0.8748 0.1984 0.069(2) Uiso 1 1 calc R . .
C20 C -0.2500(5) 0.8117(4) 0.3238(3) 0.0565(10) Uani 1 1 d . . .
H201 H -0.2011 0.7626 0.3665 0.069(2) Uiso 1 1 calc R . .
H202 H -0.2593 0.8830 0.3381 0.069(2) Uiso 1 1 calc R . .
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N2 N 0.0456(3) -0.0029(2) 0.4005(2) 0.0391(6) Uani 1 1 d . . .
C21 C 0.0628(4) 0.0084(3) 0.3166(3) 0.0386(7) Uani 1 1 d . . .
C22 C 0.0790(4) 0.0227(3) 0.2225(2) 0.0394(8) Uani 1 1 d . . .
C23 C 0.1777(4) -0.0494(3) 0.1715(2) 0.0388(7) Uani 1 1 d . . .
C24 C 0.1908(4) -0.1578(3) 0.2138(3) 0.0449(8) Uani 1 1 d . . .
H241 H 0.1333 -0.1863 0.2748 0.069(2) Uiso 1 1 calc R . .
C25 C 0.2866(5) -0.2242(3) 0.1681(3) 0.0516(10) Uani 1 1 d . . .
H251 H 0.2945 -0.2976 0.1981 0.069(2) Uiso 1 1 calc R . .
C26 C 0.3702(5) -0.1839(3) 0.0792(3) 0.0517(10) Uani 1 1 d . . .
H261 H 0.4357 -0.2295 0.0480 0.069(2) Uiso 1 1 calc R . .
C27 C 0.3586(4) -0.0768(3) 0.0354(3) 0.0514(10) Uani 1 1 d . . .
H271 H 0.4150 -0.0492 -0.0263 0.069(2) Uiso 1 1 calc R . .
C28 C 0.2648(4) -0.0106(3) 0.0818(3) 0.0452(8) Uani 1 1 d . . .
H281 H 0.2593 0.0631 0.0522 0.069(2) Uiso 1 1 calc R . .
C29 C -0.0004(4) 0.1097(3) 0.1749(2) 0.0402(8) Uani 1 1 d . . .
C30 C -0.0576(4) 0.1951(3) 0.2161(3) 0.0458(8) Uani 1 1 d . . .
H301 H -0.0427 0.1982 0.2746 0.069(2) Uiso 1 1 calc R . .
C31 C -0.1354(4) 0.2748(3) 0.1730(3) 0.0508(9) Uani 1 1 d . . .
H311 H -0.1741 0.3313 0.2029 0.069(2) Uiso 1 1 calc R . .
C32 C -0.1579(4) 0.2739(3) 0.0867(3) 0.0530(10) Uani 1 1 d . . .
H321 H -0.2115 0.3288 0.0573 0.069(2) Uiso 1 1 calc R . .
C33 C -0.0996(4) 0.1902(3) 0.0446(3) 0.0494(9) Uani 1 1 d . . .
H331 H -0.1124 0.1884 -0.0148 0.069(2) Uiso 1 1 calc R . .
C34 C -0.0235(4) 0.1097(3) 0.0880(3) 0.0448(8) Uani 1 1 d . . .
H341 H 0.0141 0.0530 0.0583 0.069(2) Uiso 1 1 calc R . .
C35 C 0.0611(5) 0.2380(3) 0.4572(3) 0.0533(10) Uani 1 1 d . . .
H351 H 0.0238 0.2541 0.5197 0.069(2) Uiso 1 1 calc R . .
H352 H -0.0117 0.2436 0.4259 0.069(2) Uiso 1 1 calc R . .
H353 H 0.1307 0.2888 0.4183 0.069(2) Uiso 1 1 calc R . .
C36 C 0.2886(4) -0.0309(3) 0.5349(3) 0.0520(10) Uani 1 1 d . . .
H361 H 0.3763 0.0021 0.5182 0.069(2) Uiso 1 1 calc R . .
H362 H 0.3004 -0.0952 0.5102 0.069(2) Uiso 1 1 calc R . .
H363 H 0.2528 -0.0500 0.6041 0.069(2) Uiso 1 1 calc R . .
O2 O 0.3213(3) 0.1139(2) 0.32029(19) 0.0483(6) Uani 1 1 d . . .
C37 C 0.4365(5) 0.0464(3) 0.2882(3) 0.0559(10) Uani 1 1 d . . .
H371 H 0.4192 0.0083 0.2438 0.069(2) Uiso 1 1 calc R . .
H372 H 0.4585 -0.0065 0.3425 0.069(2) Uiso 1 1 calc R . .
C38 C 0.5488(5) 0.1220(4) 0.2391(3) 0.0573(11) Uani 1 1 d . . .
H381 H 0.6207 0.0918 0.1924 0.069(2) Uiso 1 1 calc R . .
H382 H 0.5893 0.1399 0.2852 0.069(2) Uiso 1 1 calc R . .
C39 C 0.4777(5) 0.2188(4) 0.1903(3) 0.0554(10) Uani 1 1 d . . .
H391 H 0.4903 0.2187 0.1229 0.069(2) Uiso 1 1 calc R . .
H392 H 0.5133 0.2854 0.1933 0.069(2) Uiso 1 1 calc R . .
C40 C 0.3282(4) 0.2092(3) 0.2450(3) 0.0504(9) Uani 1 1 d . . .
H401 H 0.2947 0.2725 0.2715 0.069(2) Uiso 1 1 calc R . .
H402 H 0.2726 0.2031 0.2029 0.069(2) Uiso 1 1 calc R . .

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N1 0.0445(18) 0.0435(16) 0.0373(15) -0.0096(13) -0.0066(13) -0.0043(14)
C1 0.043(2) 0.0355(17) 0.0399(18) -0.0090(14) -0.0106(16) -0.0013(15)
C2 0.046(2) 0.0363(17) 0.0394(18) -0.0072(14) -0.0066(16) -0.0028(15)
C3 0.040(2) 0.0368(17) 0.0371(17) -0.0098(14) -0.0050(15) 0.0014(15)
C4 0.047(2) 0.046(2) 0.046(2) -0.0128(16) -0.0100(17) -0.0028(17)
C5 0.053(2) 0.054(2) 0.053(2) -0.0174(19) -0.0164(19) 0.0022(19)
C6 0.063(3) 0.054(2) 0.046(2) -0.0145(18) -0.0194(19) 0.007(2)
C7 0.061(3) 0.047(2) 0.0387(19) -0.0081(16) -0.0052(18) 0.0005(19)
C8 0.050(2) 0.0422(19) 0.0394(18) -0.0079(15) -0.0032(16) -0.0050(17)
C9 0.046(2) 0.0358(17) 0.0386(18) -0.0036(14) -0.0085(15) -0.0032(15)
C10 0.047(2) 0.045(2) 0.0423(19) -0.0076(15) -0.0083(16) -0.0046(17)
C11 0.054(3) 0.047(2) 0.053(2) -0.0040(17) -0.0167(19) -0.0064(18)
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 C12 0.043(2) 0.046(2) 0.067(3) -0.0024(19) -0.015(2) -0.0025(18)
 C13 0.046(2) 0.045(2) 0.067(3) -0.0132(19) -0.008(2) 0.0011(18)
 C14 0.046(2) 0.043(2) 0.048(2) -0.0135(16) -0.0022(17) -0.0026(17)
 C15 0.081(3) 0.056(2) 0.048(2) -0.0088(18) -0.030(2) -0.015(2)
 C16 0.045(2) 0.066(3) 0.056(2) -0.010(2) -0.0170(19) -0.001(2)
 O1 0.0536(17) 0.0517(15) 0.0388(13) -0.0058(11) -0.0129(12) -0.0126(13)
 C17 0.057(2) 0.043(2) 0.044(2) -0.0100(16) -0.0186(18) 0.0046(18)
 C18 0.075(3) 0.044(2) 0.042(2) -0.0007(17) -0.011(2) -0.004(2)
 C19 0.057(3) 0.049(2) 0.057(2) -0.0043(19) -0.004(2) -0.013(2)
 C20 0.058(3) 0.060(3) 0.053(2) -0.0118(19) -0.015(2) -0.013(2)
 N2 0.0433(17) 0.0410(15) 0.0342(14) -0.0082(12) -0.0114(12) -0.0051(13)
 C21 0.0352(19) 0.0370(17) 0.0435(19) -0.0089(14) -0.0104(15) -0.0020(14)
 C22 0.044(2) 0.0376(17) 0.0366(17) -0.0077(14) -0.0104(15) -0.0041(15)
 C23 0.042(2) 0.0410(18) 0.0348(17) -0.0071(14) -0.0130(15) -0.0031(15)
 C24 0.050(2) 0.044(2) 0.0382(18) -0.0056(15) -0.0105(16) -0.0029(17)
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 C26 0.052(2) 0.057(2) 0.049(2) -0.0192(18) -0.0166(18) 0.0103(19)
 C27 0.055(3) 0.058(2) 0.0392(19) -0.0123(18) -0.0093(18) -0.003(2)
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 C33 0.050(2) 0.053(2) 0.044(2) -0.0003(17) -0.0184(17) -0.0082(18)
 C34 0.047(2) 0.044(2) 0.0431(19) -0.0061(15) -0.0133(16) -0.0046(16)
 C35 0.058(3) 0.041(2) 0.055(2) -0.0087(17) -0.007(2) -0.0042(18)
 C36 0.049(2) 0.055(2) 0.052(2) -0.0084(18) -0.0209(19) 0.0083(19)
 O2 0.0466(16) 0.0414(14) 0.0475(14) -0.0032(11) -0.0040(12) -0.0018(12)
 C37 0.054(3) 0.044(2) 0.062(3) -0.0103(19) -0.009(2) 0.0057(19)
 C38 0.047(2) 0.057(3) 0.059(2) -0.008(2) -0.006(2) 0.001(2)
 C39 0.056(3) 0.054(2) 0.045(2) -0.0038(18) -0.0029(19) 0.001(2)
 C40 0.049(2) 0.046(2) 0.050(2) 0.0012(17) -0.0135(18) -0.0025(18)

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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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C17 O1 In1 121.3(2) . . ?
O1 C17 C18 106.7(3) . . ?
C17 C18 C19 103.5(3) . . ?
C20 C19 C18 101.8(4) . . ?
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C40 O2 In2 126.0(2) . . ?
O2 C37 C38 104.1(3) . . ?
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_refine_diff_density_min   -0.983
_refine_diff_density_rms    0.122
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Bond lengths (Angstr.)

In(1) - O(1)	2.451(3)	In(1) - N(1)	2.252(3)
In(1) - C(15)	2.131(4)	In(1) - C(16)	2.119(4)
In(1) - N(1)a	2.458(3)	O(1) - C(17)	1.450(5)
O(1) - C(20)	1.445(5)	N(1) - C(1)	1.188(5)
C(1) - C(2)	1.358(5)	C(2) - C(3)	1.479(5)
C(2) - C(9)	1.459(6)	C(3) - C(4)	1.395(6)
C(3) - C(8)	1.405(5)	C(4) - C(5)	1.379(6)
C(5) - C(6)	1.374(6)	C(6) - C(7)	1.386(6)
C(7) - C(8)	1.389(6)	C(9) - C(10)	1.415(5)
C(9) - C(14)	1.405(5)	C(10) - C(11)	1.375(6)
C(11) - C(12)	1.390(6)	C(12) - C(13)	1.371(7)
C(13) - C(14)	1.384(6)	C(17) - C(18)	1.504(6)
C(18) - C(19)	1.524(7)	C(19) - C(20)	1.501(6)
C(4) - H(41)	0.95	C(5) - H(51)	0.95
C(6) - H(61)	0.95	C(7) - H(71)	0.95
C(8) - H(81)	0.95	C(10) - H(101)	0.95
C(11) - H(111)	0.95	C(12) - H(121)	0.95
C(13) - H(131)	0.95	C(14) - H(141)	0.95
C(15) - H(151)	0.98	C(15) - H(152)	0.98
C(15) - H(153)	0.98	C(16) - H(161)	0.98
C(16) - H(162)	0.98	C(16) - H(163)	0.98
C(17) - H(171)	0.99	C(17) - H(172)	0.99
C(18) - H(181)	0.99	C(18) - H(182)	0.99
C(19) - H(191)	0.99	C(19) - H(192)	0.99
C(20) - H(201)	0.99	C(20) - H(202)	0.99

In(2) - O(2)	2.456(3)	In(2) - N(2)	2.242(3)
In(2) - C(35)	2.140(4)	In(2) - C(36)	2.143(4)
In(2) - N(2)b	2.435(3)	O(2) - C(37)	1.440(5)
O(2) - C(40)	1.444(5)	N(2) - C(21)	1.201(5)
C(21) - C(22)	1.350(5)	C(22) - C(23)	1.489(5)
C(22) - C(29)	1.477(5)	C(23) - C(24)	1.399(5)
C(23) - C(28)	1.399(5)	C(24) - C(25)	1.387(6)
C(25) - C(26)	1.380(6)	C(26) - C(27)	1.387(6)
C(27) - C(28)	1.380(6)	C(29) - C(30)	1.401(5)
C(29) - C(34)	1.399(5)	C(30) - C(31)	1.382(6)
C(31) - C(32)	1.390(6)	C(32) - C(33)	1.392(6)
C(33) - C(34)	1.379(6)	C(37) - C(38)	1.496(6)
C(38) - C(39)	1.514(6)	C(39) - C(40)	1.528(6)
C(24) - H(241)	0.95	C(25) - H(251)	0.95
C(26) - H(261)	0.95	C(27) - H(271)	0.95
C(28) - H(281)	0.95	C(30) - H(301)	0.95
C(31) - H(311)	0.95	C(32) - H(321)	0.95
C(33) - H(331)	0.95	C(34) - H(341)	0.95
C(35) - H(351)	0.98	C(35) - H(352)	0.98
C(35) - H(353)	0.98	C(36) - H(361)	0.98
C(36) - H(362)	0.98	C(36) - H(363)	0.99
C(37) - H(371)	0.99	C(37) - H(372)	0.99
C(38) - H(381)	0.99	C(38) - H(382)	0.99
C(39) - H(391)	0.99	C(39) - H(392)	0.99
C(40) - H(401)	0.99	C(40) - H(402)	0.99

Bond angles (deg.)

O(1)	In(1)	N(1)	86.1(1)	O(1)	In(1)	C(15)	91.9(1)
O(1)	In(1)	C(16)	90.8(1)	O(1)	In(1)	N(1)a	160.05(9)
N(1)	In(1)	C(15)	112.2(2)	N(1)	In(1)	C(16)	108.2(2)
N(1)	In(1)	N(1)a	73.9(1)	C(15)	In(1)	C(16)	139.6(2)
C(15)	In(1)	N(1)a	96.1(2)	C(16)	In(1)	N(1)a	94.9(2)
In(1)	O(1)	C(17)	121.3(2)	In(1)	O(1)	C(20)	127.4(2)
C(17)	O(1)	C(20)	108.6(3)	In(1)	N(1)	C(1)	129.2(3)
In(1)	N(1)	In(1)a	106.1(1)	C(1)	N(1)	In(1)a	124.6(3)
N(1)	C(1)	C(2)	179.4(4)	C(1)	C(2)	C(3)	115.9(4)
C(1)	C(2)	C(9)	117.6(4)	C(3)	C(2)	C(9)	126.3(4)
C(2)	C(3)	C(4)	120.9(3)	C(2)	C(3)	C(8)	121.7(4)
C(4)	C(3)	C(8)	117.3(3)	C(3)	C(4)	C(5)	121.5(4)
C(4)	C(5)	C(6)	120.6(5)	C(5)	C(6)	C(7)	119.4(4)
C(6)	C(7)	C(8)	120.4(4)	C(3)	C(8)	C(7)	120.7(4)
C(2)	C(9)	C(10)	120.3(4)	C(2)	C(9)	C(14)	122.9(4)
C(10)	C(9)	C(14)	116.8(4)	C(9)	C(10)	C(11)	121.3(4)
C(10)	C(11)	C(12)	120.8(4)	C(11)	C(12)	C(13)	118.7(5)
C(12)	C(13)	C(14)	121.6(4)	C(9)	C(14)	C(13)	120.8(4)
O(1)	C(17)	C(18)	106.7(3)	C(17)	C(18)	C(19)	103.5(3)
C(18)	C(19)	C(20)	101.8(4)	O(1)	C(20)	C(19)	106.6(4)
C(3)	C(4)	H(41)	119.25(0)	C(5)	C(4)	H(41)	119.24(0)
C(4)	C(5)	H(51)	119.67(0)	C(6)	C(5)	H(51)	119.73(0)
C(5)	C(6)	H(61)	120.31(0)	C(7)	C(6)	H(61)	120.30(0)
C(6)	C(7)	H(71)	119.79(0)	C(8)	C(7)	H(71)	119.82(0)
C(3)	C(8)	H(81)	119.69(0)	C(7)	C(8)	H(81)	119.57(0)
C(9)	C(10)	H(101)	119.32(0)	C(11)	C(10)	H(101)	119.34(0)
C(10)	C(11)	H(111)	119.57(0)	C(12)	C(11)	H(111)	119.68(0)
C(11)	C(12)	H(121)	120.59(0)	C(13)	C(12)	H(121)	120.72(0)
C(12)	C(13)	H(131)	119.18(0)	C(14)	C(13)	H(131)	119.22(0)
C(9)	C(14)	H(141)	119.62(0)	C(13)	C(14)	H(141)	119.55(0)
In(1)	C(15)	H(151)	109.42(0)	In(1)	C(15)	H(152)	109.48(0)
In(1)	C(15)	H(153)	109.43(0)	H(151)	C(15)	H(152)	109.47(0)
H(151)	C(15)	H(153)	109.46(0)	H(152)	C(15)	H(153)	109.56(0)
In(1)	C(16)	H(161)	109.52(0)	In(1)	C(16)	H(162)	109.47(0)
In(1)	C(16)	H(163)	109.47(0)	H(161)	C(16)	H(162)	109.44(0)
H(161)	C(16)	H(163)	109.49(0)	H(162)	C(16)	H(163)	109.43(0)
O(1)	C(17)	H(171)	110.44(0)	O(1)	C(17)	H(172)	110.41(0)
C(18)	C(17)	H(171)	110.37(0)	C(18)	C(17)	H(172)	110.33(0)
H(171)	C(17)	H(172)	108.58(0)	C(17)	C(18)	H(181)	111.05(0)
C(17)	C(18)	H(182)	111.01(0)	C(19)	C(18)	H(181)	111.08(0)
C(19)	C(18)	H(182)	111.07(0)	H(181)	C(18)	H(182)	109.04(0)
C(18)	C(19)	H(191)	111.41(0)	C(18)	C(19)	H(192)	111.38(0)
C(20)	C(19)	H(191)	111.43(0)	C(20)	C(19)	H(192)	111.40(0)
H(191)	C(19)	H(192)	109.31(0)	O(1)	C(20)	H(201)	110.44(0)
O(1)	C(20)	H(202)	110.45(0)	C(19)	C(20)	H(201)	110.41(0)
C(19)	C(20)	H(202)	110.40(0)	H(201)	C(20)	H(202)	108.51(0)

O(2)	In(2)	N(2)	83.7(1)	O(2)	In(2)	C(35)	95.7(1)
O(2)	In(2)	C(36)	89.8(1)	O(2)	In(2)	N(2)b	159.81(9)
N(2)	In(2)	C(35)	104.9(2)	N(2)	In(2)	C(36)	109.4(1)
N(2)	In(2)	N(2)b	76.6(1)	C(35)	In(2)	C(36)	145.7(2)
C(35)	In(2)	N(2)b	93.7(1)	C(36)	In(2)	N(2)b	92.4(1)
In(2)	O(2)	C(37)	127.7(2)	In(2)	O(2)	C(40)	125.9(2)
C(37)	O(2)	C(40)	106.4(3)	In(2)	N(2)	C(21)	127.8(3)
In(2)	N(2)	In(2)b	103.4(1)	C(21)	N(2)	In(2)b	126.8(3)
N(2)	C(21)	C(22)	178.5(4)	C(21)	C(22)	C(23)	118.2(3)
C(21)	C(22)	C(29)	118.6(3)	C(23)	C(22)	C(29)	123.2(3)
C(22)	C(23)	C(24)	120.9(3)	C(22)	C(23)	C(28)	121.4(3)
C(24)	C(23)	C(28)	117.6(4)	C(23)	C(24)	C(25)	121.0(4)
C(24)	C(25)	C(26)	120.1(4)	C(25)	C(26)	C(27)	120.0(4)
C(26)	C(27)	C(28)	119.7(4)	C(23)	C(28)	C(27)	121.5(4)

C(22)	C(29)	C(30)	121.0(3)	C(22)	C(29)	C(34)	121.7(3)
C(30)	C(29)	C(34)	117.3(4)	C(29)	C(30)	C(31)	121.0(4)
C(30)	C(31)	C(32)	121.2(4)	C(31)	C(32)	C(33)	118.1(4)
C(32)	C(33)	C(34)	120.9(4)	C(29)	C(34)	C(33)	121.5(4)
O(2)	C(37)	C(38)	104.1(3)	C(37)	C(38)	C(39)	102.9(4)
C(38)	C(39)	C(40)	105.0(4)	O(2)	C(40)	C(39)	105.8(3)
C(23)	C(24)	H(241)	119.44(0)	C(25)	C(24)	H(241)	119.53(0)
C(24)	C(25)	H(251)	119.90(0)	C(26)	C(25)	H(251)	120.01(0)
C(25)	C(26)	H(261)	119.97(0)	C(27)	C(26)	H(261)	120.02(0)
C(26)	C(27)	H(271)	120.10(0)	C(28)	C(27)	H(271)	120.17(0)
C(23)	C(28)	H(281)	119.18(0)	C(27)	C(28)	H(281)	119.28(0)
C(29)	C(30)	H(301)	119.47(0)	C(31)	C(30)	H(301)	119.49(0)
C(30)	C(31)	H(311)	119.35(0)	C(32)	C(31)	H(311)	119.45(0)
C(31)	C(32)	H(321)	120.97(0)	C(33)	C(32)	H(321)	120.95(0)
C(32)	C(33)	H(331)	119.63(0)	C(34)	C(33)	H(331)	119.45(0)
C(29)	C(34)	H(341)	119.20(0)	C(33)	C(34)	H(341)	119.32(0)
In(2)	C(35)	H(351)	109.47(0)	In(2)	C(35)	H(352)	109.45(0)
In(2)	C(35)	H(353)	109.47(0)	H(351)	C(35)	H(352)	109.46(0)
H(351)	C(35)	H(353)	109.55(0)	H(352)	C(35)	H(353)	109.42(0)
In(2)	C(36)	H(361)	109.44(0)	In(2)	C(36)	H(362)	109.42(0)
In(2)	C(36)	H(363)	109.46(0)	H(361)	C(36)	H(362)	109.46(0)
H(361)	C(36)	H(363)	109.50(0)	H(362)	C(36)	H(363)	109.54(0)
O(2)	C(37)	H(371)	110.96(0)	O(2)	C(37)	H(372)	110.91(0)
C(38)	C(37)	H(371)	110.93(0)	C(38)	C(37)	H(372)	110.86(0)
H(371)	C(37)	H(372)	109.07(0)	C(37)	C(38)	H(381)	111.18(0)
C(37)	C(38)	H(382)	111.21(0)	C(39)	C(38)	H(381)	111.19(0)
C(39)	C(38)	H(382)	111.16(0)	H(381)	C(38)	H(382)	109.13(0)
C(38)	C(39)	H(391)	110.76(0)	C(38)	C(39)	H(392)	110.79(0)
C(40)	C(39)	H(391)	110.79(0)	C(40)	C(39)	H(392)	110.75(0)
H(391)	C(39)	H(392)	108.75(0)	O(2)	C(40)	H(401)	110.61(0)
O(2)	C(40)	H(402)	110.59(0)	C(39)	C(40)	H(401)	110.58(0)
C(39)	C(40)	H(402)	110.59(0)	H(401)	C(40)	H(402)	108.65(0)

Atom	x	y	z	Ueq/Uiso	
In(1)	-0.51500(3)	0.64978(2)	0.47708(2)	0.0399(1)	
O(1)	-0.3819(3)	0.7723(2)	0.3368(2)	0.048(1)	
N(1)	-0.3985(3)	0.5178(2)	0.4123(2)	0.042(1)	
C(1)	-0.3090(4)	0.5234(3)	0.3416(2)	0.040(1)	
C(2)	-0.2059(4)	0.5290(3)	0.2613(3)	0.042(1)	
C(3)	-0.2462(4)	0.5502(3)	0.1716(2)	0.039(1)	
C(4)	-0.3710(4)	0.5186(3)	0.1704(3)	0.046(1)	
C(5)	-0.4153(5)	0.5462(3)	0.0891(3)	0.052(1)	
C(6)	-0.3362(5)	0.6050(3)	0.0060(3)	0.054(1)	
C(7)	-0.2102(5)	0.6354(3)	0.0041(3)	0.051(1)	
C(8)	-0.1652(4)	0.6086(3)	0.0858(3)	0.046(1)	
C(9)	-0.0676(4)	0.5224(3)	0.2704(3)	0.041(1)	
C(10)	-0.0424(4)	0.5415(3)	0.3521(3)	0.046(1)	
C(11)	0.0866(4)	0.5325(3)	0.3636(3)	0.052(1)	
C(12)	0.1970(5)	0.5068(3)	0.2938(3)	0.054(1)	
C(13)	0.1744(5)	0.4872(3)	0.2145(3)	0.054(1)	
C(14)	0.0454(4)	0.4948(3)	0.2017(3)	0.047(1)	
C(15)	-0.4178(5)	0.6953(4)	0.5678(3)	0.059(1)	
C(16)	-0.6910(4)	0.6903(4)	0.4272(3)	0.056(1)	
C(17)	-0.4063(4)	0.7869(3)	0.2444(3)	0.047(1)	
C(18)	-0.2885(5)	0.8460(3)	0.1729(3)	0.056(1)	
C(19)	-0.1743(5)	0.8183(4)	0.2219(3)	0.057(1)	
C(20)	-0.2500(5)	0.8117(4)	0.3238(3)	0.056(2)	
H(41)	-0.42680(0)	0.47720(0)	0.22690(0)	0.069(2)	*
H(51)	-0.50130(0)	0.52440(0)	0.09060(0)	0.069(2)	*
H(61)	-0.36760(0)	0.62460(0)	-0.04960(0)	0.069(2)	*
H(71)	-0.15420(0)	0.67480(0)	-0.05350(0)	0.069(2)	*
H(81)	-0.07870(0)	0.63010(0)	0.08360(0)	0.069(2)	*
H(101)	-0.11600(0)	0.56100(0)	0.39990(0)	0.069(2)	*
H(111)	0.10030(0)	0.54400(0)	0.41990(0)	0.069(2)	*
H(121)	0.28640(0)	0.50290(0)	0.30100(0)	0.069(2)	*
H(131)	0.24910(0)	0.46790(0)	0.16720(0)	0.069(2)	*
H(141)	0.03320(0)	0.48120(0)	0.14570(0)	0.069(2)	*
H(151)	-0.40650(0)	0.77260(0)	0.54860(0)	0.069(2)	*
H(152)	-0.32870(0)	0.65840(0)	0.56290(0)	0.069(2)	*
H(153)	-0.47360(0)	0.67600(0)	0.63350(0)	0.069(2)	*
H(161)	-0.77140(0)	0.66690(0)	0.47930(0)	0.069(2)	*
H(162)	-0.68500(0)	0.65500(0)	0.37590(0)	0.069(2)	*
H(163)	-0.69800(0)	0.76780(0)	0.40320(0)	0.069(2)	*
H(171)	-0.49220(0)	0.82850(0)	0.24200(0)	0.069(2)	*
H(172)	-0.41240(0)	0.71700(0)	0.23100(0)	0.069(2)	*
H(181)	-0.30920(0)	0.92380(0)	0.15870(0)	0.069(2)	*
H(182)	-0.26470(0)	0.82150(0)	0.11310(0)	0.069(2)	*
H(191)	-0.12780(0)	0.74940(0)	0.21290(0)	0.069(2)	*
H(192)	-0.10700(0)	0.87480(0)	0.19840(0)	0.069(2)	*
H(201)	-0.20110(0)	0.76260(0)	0.36650(0)	0.069(2)	*
H(202)	-0.25930(0)	0.88300(0)	0.33810(0)	0.069(2)	*
In(2)	0.14931(3)	0.07951(2)	0.47386(2)	0.0384(1)	
O(2)	0.3213(3)	0.1139(2)	0.3203(2)	0.0483(8)	
N(2)	0.0456(3)	-0.0029(2)	0.4005(2)	0.039(1)	
C(21)	0.0628(4)	0.0084(3)	0.3166(3)	0.039(1)	
C(22)	0.0790(4)	0.0227(3)	0.2225(2)	0.040(1)	
C(23)	0.1777(4)	-0.0494(3)	0.1715(2)	0.039(1)	
C(24)	0.1908(4)	-0.1578(3)	0.2138(3)	0.045(1)	
C(25)	0.2866(5)	-0.2242(3)	0.1681(3)	0.052(1)	
C(26)	0.3702(5)	-0.1839(3)	0.0792(3)	0.052(1)	
C(27)	0.3586(4)	-0.0768(3)	0.0354(3)	0.051(1)	
C(28)	0.2648(4)	-0.0106(3)	0.0818(3)	0.045(1)	
C(29)	-0.0004(4)	0.1097(3)	0.1749(2)	0.040(1)	
C(30)	-0.0576(4)	0.1951(3)	0.2161(3)	0.046(1)	
C(31)	-0.1354(4)	0.2748(3)	0.1730(3)	0.051(1)	
C(32)	-0.1579(4)	0.2739(3)	0.0867(3)	0.053(1)	

C(33)	-0.0996(4)	0.1902(3)	0.0446(3)	0.049(1)
C(34)	-0.0235(4)	0.1097(3)	0.0880(3)	0.045(1)
C(35)	0.0611(5)	0.2380(3)	0.4572(3)	0.053(1)
C(36)	0.2886(4)	-0.0309(3)	0.5349(3)	0.052(1)
C(37)	0.4365(5)	0.0464(3)	0.2882(3)	0.056(2)
C(38)	0.5488(5)	0.1220(4)	0.2391(3)	0.057(1)
C(39)	0.4777(5)	0.2188(4)	0.1903(3)	0.056(1)
C(40)	0.3282(4)	0.2092(3)	0.2450(3)	0.051(1)
H(241)	0.13330(0)	-0.18630(0)	0.27480(0)	0.069(2) *
H(251)	0.29450(0)	-0.29760(0)	0.19810(0)	0.069(2) *
H(261)	0.43570(0)	-0.22950(0)	0.04800(0)	0.069(2) *
H(271)	0.41500(0)	-0.04920(0)	-0.02630(0)	0.069(2) *
H(281)	0.25930(0)	0.06310(0)	0.05220(0)	0.069(2) *
H(301)	-0.04270(0)	0.19820(0)	0.27460(0)	0.069(2) *
H(311)	-0.17410(0)	0.33130(0)	0.20290(0)	0.069(2) *
H(321)	-0.21150(0)	0.32880(0)	0.05730(0)	0.069(2) *
H(331)	-0.11240(0)	0.18840(0)	-0.01480(0)	0.069(2) *
H(341)	0.01410(0)	0.05300(0)	0.05830(0)	0.069(2) *
H(351)	0.02380(0)	0.25410(0)	0.51970(0)	0.069(2) *
H(352)	-0.01170(0)	0.24360(0)	0.42590(0)	0.069(2) *
H(353)	0.13070(0)	0.28880(0)	0.41830(0)	0.069(2) *
H(361)	0.37630(0)	0.00210(0)	0.51820(0)	0.069(2) *
H(362)	0.30040(0)	-0.09520(0)	0.51020(0)	0.069(2) *
H(363)	0.25280(0)	-0.05000(0)	0.60410(0)	0.069(2) *
H(371)	0.41920(0)	0.00830(0)	0.24380(0)	0.069(2) *
H(372)	0.45850(0)	-0.00650(0)	0.34250(0)	0.069(2) *
H(381)	0.62070(0)	0.09180(0)	0.19240(0)	0.069(2) *
H(382)	0.58930(0)	0.13990(0)	0.28520(0)	0.069(2) *
H(391)	0.49030(0)	0.21870(0)	0.12290(0)	0.069(2) *
H(392)	0.51330(0)	0.28540(0)	0.19330(0)	0.069(2) *
H(401)	0.29470(0)	0.27250(0)	0.27150(0)	0.069(2) *
H(402)	0.27260(0)	0.20310(0)	0.20290(0)	0.069(2) *

* refined isotropically

Atom	U11	U22	U33	U23	U13	U12
In(1)	0.0420(2)	0.0406(2)	0.0370(2)	-0.0097(1)	-0.0093(1)	-0.0031(1)
O(1)	0.054(2)	0.052(2)	0.039(1)	-0.006(1)	-0.013(1)	-0.013(1)
N(1)	0.045(2)	0.043(2)	0.037(2)	-0.010(1)	-0.007(1)	-0.004(1)
C(1)	0.043(2)	0.036(2)	0.040(2)	-0.009(1)	-0.011(2)	-0.001(2)
C(2)	0.046(2)	0.036(2)	0.039(2)	-0.007(1)	-0.007(2)	-0.003(2)
C(3)	0.040(2)	0.037(2)	0.037(2)	-0.010(1)	-0.005(2)	0.001(2)
C(4)	0.047(2)	0.046(2)	0.046(2)	-0.013(2)	-0.010(2)	-0.003(2)
C(5)	0.053(2)	0.054(2)	0.053(2)	-0.017(2)	-0.016(2)	0.002(2)
C(6)	0.063(3)	0.054(2)	0.046(2)	-0.014(2)	-0.019(2)	0.007(2)
C(7)	0.061(3)	0.047(2)	0.039(2)	-0.008(2)	-0.005(2)	0.001(2)
C(8)	0.050(2)	0.042(2)	0.039(2)	-0.008(2)	-0.003(2)	-0.005(2)
C(9)	0.046(2)	0.036(2)	0.039(2)	-0.004(1)	-0.009(2)	-0.003(2)
C(10)	0.047(2)	0.045(2)	0.042(2)	-0.008(2)	-0.008(2)	-0.005(2)
C(11)	0.054(3)	0.047(2)	0.053(2)	-0.004(2)	-0.017(2)	-0.006(2)
C(12)	0.043(2)	0.046(2)	0.067(3)	-0.002(2)	-0.015(2)	-0.002(2)
C(13)	0.046(2)	0.045(2)	0.067(3)	-0.013(2)	-0.008(2)	0.001(2)
C(14)	0.046(2)	0.043(2)	0.048(2)	-0.014(2)	-0.002(2)	-0.003(2)
C(15)	0.081(3)	0.056(2)	0.048(2)	-0.009(2)	-0.030(2)	-0.015(2)
C(16)	0.045(2)	0.066(3)	0.056(2)	-0.010(2)	-0.017(2)	-0.001(2)
C(17)	0.057(2)	0.043(2)	0.044(2)	-0.010(2)	-0.019(2)	0.005(2)
C(18)	0.075(3)	0.044(2)	0.042(2)	-0.001(2)	-0.011(2)	-0.004(2)
C(19)	0.057(3)	0.049(2)	0.057(2)	-0.004(2)	-0.004(2)	-0.013(2)
C(20)	0.058(3)	0.060(3)	0.053(2)	-0.012(2)	-0.015(2)	-0.013(2)
In(2)	0.0389(2)	0.0382(2)	0.0381(2)	-0.0081(1)	-0.0103(1)	-0.0034(1)
O(2)	0.047(2)	0.041(1)	0.047(1)	-0.003(1)	-0.004(1)	-0.002(1)
N(2)	0.043(2)	0.041(2)	0.034(1)	-0.008(1)	-0.011(1)	-0.005(1)
C(21)	0.035(2)	0.037(2)	0.043(2)	-0.009(1)	-0.010(2)	-0.002(1)
C(22)	0.044(2)	0.038(2)	0.037(2)	-0.008(1)	-0.010(2)	-0.004(2)
C(23)	0.042(2)	0.041(2)	0.035(2)	-0.007(1)	-0.013(2)	-0.003(2)
C(24)	0.050(2)	0.044(2)	0.038(2)	-0.006(2)	-0.010(2)	-0.003(2)
C(25)	0.059(3)	0.046(2)	0.049(2)	-0.008(2)	-0.019(2)	0.007(2)
C(26)	0.052(2)	0.057(2)	0.049(2)	-0.019(2)	-0.017(2)	0.010(2)
C(27)	0.055(3)	0.058(2)	0.039(2)	-0.012(2)	-0.009(2)	-0.003(2)
C(28)	0.050(2)	0.043(2)	0.041(2)	-0.008(2)	-0.010(2)	-0.003(2)
C(29)	0.042(2)	0.040(2)	0.037(2)	-0.004(1)	-0.010(2)	-0.009(2)
C(30)	0.050(2)	0.043(2)	0.044(2)	-0.009(2)	-0.013(2)	-0.003(2)
C(31)	0.047(2)	0.040(2)	0.060(2)	-0.006(2)	-0.012(2)	-0.002(2)
C(32)	0.044(2)	0.047(2)	0.060(2)	0.004(2)	-0.015(2)	-0.003(2)
C(33)	0.050(2)	0.053(2)	0.044(2)	0.000(2)	-0.018(2)	-0.008(2)
C(34)	0.047(2)	0.044(2)	0.043(2)	-0.006(2)	-0.013(2)	-0.005(2)
C(35)	0.058(3)	0.041(2)	0.055(2)	-0.009(2)	-0.007(2)	-0.004(2)
C(36)	0.049(2)	0.055(2)	0.052(2)	-0.008(2)	-0.021(2)	0.008(2)
C(37)	0.054(3)	0.044(2)	0.062(3)	-0.010(2)	-0.009(2)	0.006(2)
C(38)	0.047(2)	0.057(3)	0.059(2)	-0.008(2)	-0.006(2)	0.001(2)
C(39)	0.056(3)	0.054(2)	0.045(2)	-0.004(2)	-0.003(2)	0.001(2)
C(40)	0.049(2)	0.046(2)	0.050(2)	0.001(2)	-0.014(2)	-0.002(2)

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ef17

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Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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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.
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Li1 Li 0.0946(7) 0.3374(7) -0.6316(4) 0.082(3) Uani 1 1 d . M .
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C1 C 0.1029(4) 0.3028(4) -0.5004(3) 0.0709(15) Uani 1 1 d . . .
C2 C 0.11853(18) 0.32817(15) -0.43585(11) 0.0715(15) Uani 1 1 d . A .
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C7 C 0.35424(18) 0.48166(15) -0.29272(11) 0.133(3) Uani 1 1 d R N .
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C131 C -0.06353(18) 0.30546(15) -0.33692(11) 0.114(3) Uani 0.70 1 d PR A 1
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C141 C 0.02309(18) 0.33732(15) -0.35451(11) 0.099(3) Uani 0.70 1 d PR A 1
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C92 C 0.04301(18) 0.28860(15) -0.41662(11) 0.050(7) Uani 0.30 1 d PR A 2
C102 C -0.06512(18) 0.25944(15) -0.46177(11) 0.069(6) Uani 0.30 1 d PR A 2
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C112 C -0.16047(18) 0.21840(15) -0.44797(11) 0.085(7) Uani 0.30 1 d PR A 2
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C122 C -0.14493(18) 0.19921(15) -0.38293(11) 0.105(10) Uani 0.30 1 d PR A 2
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C132 C -0.03551(18) 0.22681(15) -0.33783(11) 0.076(5) Uani 0.30 1 d PR A 2
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C142 C 0.05376(18) 0.26721(15) -0.35381(11) 0.081(6) Uani 0.30 1 d PR A 2
H142 H 0.1230 0.2809 -0.3227 0.207(4) Uiso 0.30 1 d PR K 2
C15 C 0.0864(4) 0.1887(4) -0.7444(3) 0.0764(15) Uani 1 1 d . . .
C16 C 0.08607(13) 0.15256(12) -0.80604(8) 0.0711(15) Uani 1 1 d . N .
C17 C -0.00497(13) 0.07337(12) -0.84732(8) 0.0671(14) Uani 1 1 d R . .
C18 C -0.02745(13) 0.04999(12) -0.91322(8) 0.0799(16) Uani 1 1 d R N .
H181 H 0.0161 0.0849 -0.9319 0.207(4) Uiso 1 1 d R N .
C19 C -0.11295(13) -0.02398(12) -0.95208(8) 0.0878(17) Uani 1 1 d R N .
H191 H -0.1285 -0.0401 -0.9976 0.207(4) Uiso 1 1 d R N .
C20 C -0.17598(13) -0.07458(12) -0.92505(8) 0.0937(18) Uani 1 1 d R N .
H201 H -0.2350 -0.1257 -0.9519 0.207(4) Uiso 1 1 d R N .
C21 C -0.15351(13) -0.05121(12) -0.85915(8) 0.0902(18) Uani 1 1 d R N .
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C22 C -0.06800(13) 0.02277(12) -0.82029(8) 0.0787(16) Uani 1 1 d R N .
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C23 C 0.17606(13) 0.19903(12) -0.82335(8) 0.0678(14) Uani 1 1 d R N .
C24 C 0.21267(13) 0.14761(12) -0.86499(8) 0.0771(15) Uani 1 1 d R N .
H241 H 0.1806 0.0823 -0.8821 0.207(4) Uiso 1 1 d R N .
C25 C 0.29575(13) 0.19072(12) -0.88193(8) 0.0868(17) Uani 1 1 d R N .
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C26 C 0.34222(13) 0.28525(12) -0.85722(8) 0.0928(18) Uani 1 1 d R N .
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C28 C 0.22253(13) 0.29357(12) -0.79864(8) 0.0897(18) Uani 1 1 d R N .
H281 H 0.1973 0.3291 -0.7699 0.207(4) Uiso 1 1 d R N .
O1 O -0.0269(3) 0.3859(3) -0.6586(2) 0.1115(14) Uani 1 1 d . . .
C29 C -0.0744(7) 0.4191(6) -0.6082(4) 0.146(3) Uiso 1 1 d . L .
H291 H -0.0846 0.4787 -0.6110 0.207(4) Uiso 0.60 1 d PR . .
H292 H -0.0247 0.4264 -0.5665 0.207(4) Uiso 0.60 1 d PR . .
H293 H -0.0740 0.4829 -0.6027 0.207(4) Uiso 0.40 1 d PR . .
H294 H -0.0420 0.4074 -0.5676 0.207(4) Uiso 0.40 1 d PR . .
C301 C -0.1721(12) 0.3600(11) -0.6166(8) 0.136(5) Uiso 0.60 1 d P L 3
H301 H -0.1968 0.3851 -0.5835 0.207(4) Uiso 0.60 1 d PR L 3
H302 H -0.2229 0.3535 -0.6577 0.207(4) Uiso 0.60 1 d PR L 3
H303 H -0.1624 0.3006 -0.6127 0.207(4) Uiso 0.60 1 d PR L 3
C302 C -0.171(3) 0.360(2) -0.6479(16) 0.233(17) Uiso 0.40 1 d P L 4
H304 H -0.2176 0.3687 -0.6242 0.207(4) Uiso 0.40 1 d PR L 4
H305 H -0.1983 0.3728 -0.6888 0.207(4) Uiso 0.40 1 d PR L 4
H306 H -0.1664 0.2977 -0.6539 0.207(4) Uiso 0.40 1 d PR L 4
C31 C -0.0722(7) 0.3944(8) -0.7221(4) 0.176(4) Uani 1 1 d . . .
H311 H -0.1366 0.3424 -0.7445 0.207(4) Uiso 1 1 calc R . .
H312 H -0.0945 0.4522 -0.7191 0.207(4) Uiso 1 1 calc R . .
C32 C -0.0077(6) 0.3955(6) -0.7605(4) 0.137(3) Uani 1 1 d . . .
H321 H 0.0604 0.4414 -0.7369 0.207(4) Uiso 1 1 calc R N .
H322 H -0.0422 0.4117 -0.8000 0.207(4) Uiso 1 1 calc R . .
H323 H 0.0036 0.3342 -0.7712 0.207(4) Uiso 1 1 calc R . .
O2 O 0.2321(4) 0.4277(4) -0.6087(2) 0.1295(17) Uani 1 1 d D . .
C33 C 0.2152(10) 0.5387(8) -0.5944(6) 0.209(4) Uiso 1 1 d . M 5
H331 H 0.2729 0.5812 -0.6014 0.207(4) Uiso 1 1 calc R M 5
H332 H 0.1482 0.5382 -0.6265 0.207(4) Uiso 1 1 calc R M 5
C34 C 0.2136(10) 0.5687(9) -0.5432(6) 0.270(6) Uiso 1 1 d . M 5
H341 H 0.2795 0.5697 -0.5108 0.207(4) Uiso 1 1 calc R M 5
H342 H 0.1539 0.5296 -0.5366 0.207(4) Uiso 1 1 calc R M 5
H343 H 0.2062 0.6317 -0.5394 0.207(4) Uiso 1 1 calc R M 5
C351 C 0.3289(13) 0.3998(19) -0.6079(14) 0.204(17) Uani 0.50 1 d PD M 5
H351 H 0.3111 0.3599 -0.6514 0.207(4) Uiso 0.50 1 calc PR M 5
H352 H 0.3804 0.4572 -0.6053 0.207(4) Uiso 0.50 1 calc PR M 5
C361 C 0.3834(17) 0.3591(13) -0.5697(10) 0.123(8) Uani 0.50 1 d P M 5
H361 H 0.4137 0.3190 -0.5936 0.207(4) Uiso 0.50 1 calc PR M 5
H362 H 0.3372 0.3219 -0.5524 0.207(4) Uiso 0.50 1 calc PR M 5
H363 H 0.4402 0.4059 -0.5345 0.207(4) Uiso 0.50 1 calc PR M 5
C352 C 0.3050(17) 0.4922(15) -0.5855(10) 0.201(10) Uiso 0.50 1 d P M 6
H353 H 0.3208 0.5221 -0.5398 0.207(4) Uiso 0.50 1 d PR M 6
H354 H 0.3277 0.5356 -0.6096 0.207(4) Uiso 0.50 1 d PR M 6
C362 C 0.3342(17) 0.3573(15) -0.6061(10) 0.21(3) Uani 0.50 1 d PR M 6
H364 H 0.3646 0.3413 -0.5658 0.207(4) Uiso 0.50 1 d PR M 6
H365 H 0.3835 0.3590 -0.6297 0.207(4) Uiso 0.50 1 d PR M 6
H366 H 0.2676 0.3107 -0.6319 0.207(4) Uiso 0.50 1 d PR M 6
O3 O 0.2053(5) 0.1173(4) -0.5752(3) 0.167(2) Uani 1 1 d D N .
C371 C 0.2676(14) 0.0700(13) -0.5877(9) 0.167(7) Uiso 0.60 1 d P N 7
H371 H 0.2437 0.0051 -0.5861 0.207(4) Uiso 0.60 1 calc PR N 7
H372 H 0.3408 0.0978 -0.5576 0.207(4) Uiso 0.60 1 calc PR N 7
C381 C 0.2586(13) 0.0765(13) -0.6546(9) 0.144(6) Uiso 0.60 1 d P N 7
H381 H 0.2817 0.0266 -0.6753 0.207(4) Uiso 0.60 1 calc PR N 7
H382 H 0.3030 0.1364 -0.6530 0.207(4) Uiso 0.60 1 calc PR N 7
H383 H 0.1850 0.0708 -0.6791 0.207(4) Uiso 0.60 1 calc PR N 7
C391 C 0.2533(14) 0.1495(12) -0.5046(3) 0.178(6) Uiso 0.60 1 d PD N 7
H391 H 0.3289 0.1737 -0.4982 0.207(4) Uiso 0.60 1 calc PR N 7
H392 H 0.2288 0.2053 -0.4950 0.207(4) Uiso 0.60 1 calc PR N 7
C401 C 0.2564(17) 0.1223(13) -0.4617(9) 0.211(8) Uiso 0.60 1 d P N 7
H401 H 0.3143 0.1640 -0.4243 0.207(4) Uiso 0.60 1 calc PR N 7
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H402 H 0.2681 0.0607 -0.4692 0.207(4) Uiso 0.60 1 calc PR N 7
H403 H 0.1896 0.1181 -0.4539 0.207(4) Uiso 0.60 1 calc PR N 7
C372 C 0.267(2) 0.104(3) -0.6179(15) 0.207(16) Uiso 0.40 1 d PD N 8
H373 H 0.3374 0.0996 -0.5923 0.207(4) Uiso 0.40 1 calc PR N 8
H374 H 0.2789 0.1586 -0.6353 0.207(4) Uiso 0.40 1 calc PR N 8
C382 C 0.2162(12) 0.0194(11) -0.6724(10) 0.116(7) Uani 0.40 1 d P N 8
H384 H 0.2238 0.0339 -0.7116 0.207(4) Uiso 0.40 1 calc PR N 8
H385 H 0.1412 -0.0017 -0.6782 0.207(4) Uiso 0.40 1 calc PR N 8
H386 H 0.2499 -0.0296 -0.6631 0.207(4) Uiso 0.40 1 calc PR N 8
C392 C 0.2658(18) 0.074(2) -0.5285(13) 0.260(16) Uiso 0.40 1 d PD N 8
H393 H 0.3386 0.1118 -0.5025 0.207(4) Uiso 0.40 1 calc PR N 8
H394 H 0.2619 0.0089 -0.5454 0.207(4) Uiso 0.40 1 calc PR N 8
C402 C 0.180(2) 0.0904(19) -0.4993(13) 0.185(10) Uiso 0.40 1 d PD N 8
H404 H 0.1564 0.0360 -0.4846 0.207(4) Uiso 0.40 1 d PR N 8
H405 H 0.1204 0.0986 -0.5321 0.207(4) Uiso 0.40 1 d PR N 8
H406 H 0.2091 0.1454 -0.4631 0.207(4) Uiso 0.40 1 d PR N 8
O4 O -0.0445(4) 0.0673(3) -0.6394(2) 0.1170(14) Uani 1 1 d . N .
C41 C -0.1383(7) 0.1048(8) -0.6480(6) 0.200(5) Uani 1 1 d . . .
H411 H -0.1634 0.0985 -0.6117 0.207(4) Uiso 1 1 calc R N .
H412 H -0.1144 0.1717 -0.6445 0.207(4) Uiso 1 1 calc R . .
C42 C -0.2221(9) 0.0666(8) -0.7031(5) 0.191(4) Uani 1 1 d . N .
H421 H -0.1992 0.0712 -0.7399 0.207(4) Uiso 1 1 calc R . .
H422 H -0.2761 0.0997 -0.7034 0.207(4) Uiso 1 1 calc R . .
H423 H -0.2515 0.0014 -0.7057 0.207(4) Uiso 1 1 calc R . .
C43 C -0.0497(10) -0.0230(9) -0.6192(6) 0.238(5) Uiso 1 1 d . N 9
H431 H 0.0121 -0.0157 -0.5809 0.207(4) Uiso 1 1 calc R N 9
H432 H -0.1146 -0.0423 -0.6088 0.207(4) Uiso 1 1 calc R N 9
C44 C -0.0502(12) -0.0831(10) -0.6669(7) 0.322(8) Uiso 1 1 d . N 9
H441 H -0.0749 -0.1454 -0.6620 0.207(4) Uiso 1 1 calc R N 9
H442 H 0.0213 -0.0737 -0.6685 0.207(4) Uiso 1 1 calc R N 9
H443 H -0.0974 -0.0763 -0.7067 0.207(4) Uiso 1 1 calc R N 9
N3 N -0.3777(4) 0.1881(4) -0.1858(3) 0.0942(16) Uani 1 1 d . O 9
N4 N -0.2840(4) 0.3115(3) -0.0487(2) 0.0857(14) Uani 1 1 d . O 9
Li3 Li -0.2325(7) 0.2660(7) -0.1206(5) 0.086(3) Uani 1 1 d . O 9
Li4 Li -0.4313(7) 0.2440(7) -0.1160(5) 0.090(3) Uani 1 1 d . O 9
C45 C -0.4125(5) 0.1416(4) -0.2390(4) 0.0844(18) Uani 1 1 d . O 9
C46 C -0.45348(13) 0.08772(16) -0.30105(10) 0.0856(17) Uani 1 1 d . O 9
C47 C -0.45853(13) 0.13648(16) -0.35375(10) 0.0839(17) Uani 1 1 d R O 9
C48 C -0.44425(13) 0.09555(16) -0.40956(10) 0.0864(17) Uani 1 1 d R O 9
H481 H -0.4354 0.0342 -0.4158 0.207(4) Uiso 1 1 d R O 9
C49 C -0.44276(13) 0.14339(16) -0.45631(10) 0.113(2) Uani 1 1 d R O 9
H491 H -0.4329 0.1151 -0.4949 0.207(4) Uiso 1 1 d R O 9
C50 C -0.45555(13) 0.23216(16) -0.44724(10) 0.131(3) Uani 1 1 d R O 9
H501 H -0.4545 0.2652 -0.4795 0.207(4) Uiso 1 1 d R O 9
C51 C -0.46982(13) 0.27310(16) -0.39142(10) 0.128(3) Uani 1 1 d R O 9
H511 H -0.4787 0.3344 -0.3852 0.207(4) Uiso 1 1 d R O 9
C52 C -0.47131(13) 0.22526(16) -0.34467(10) 0.109(2) Uani 1 1 d R O 9
H521 H -0.4812 0.2535 -0.3061 0.207(4) Uiso 1 1 d R O 9
C53 C -0.48911(13) -0.01517(16) -0.31235(10) 0.0782(16) Uani 1 1 d R O 9
C54 C -0.44506(13) -0.05623(16) -0.26475(10) 0.0950(18) Uani 1 1 d R O 9
H541 H -0.3931 -0.0187 -0.2249 0.207(4) Uiso 1 1 d R O 9
C55 C -0.47631(13) -0.15169(16) -0.27481(10) 0.109(2) Uani 1 1 d R O 9
H551 H -0.4459 -0.1800 -0.2419 0.207(4) Uiso 1 1 d R O 9
C56 C -0.55162(13) -0.20609(16) -0.33248(10) 0.106(2) Uani 1 1 d R O 9
H561 H -0.5732 -0.2720 -0.3394 0.207(4) Uiso 1 1 d R O 9
C57 C -0.59566(13) -0.16504(16) -0.38008(10) 0.101(2) Uani 1 1 d R O 9
H571 H -0.6477 -0.2026 -0.4199 0.207(4) Uiso 1 1 d R O 9
C58 C -0.56441(13) -0.06958(16) -0.37001(10) 0.0898(18) Uani 1 1 d R O 9
H581 H -0.5948 -0.0412 -0.4029 0.207(4) Uiso 1 1 d R O 9
C59 C -0.2699(4) 0.3475(4) 0.0056(3) 0.0785(16) Uani 1 1 d . O 9
C60 C -0.25848(12) 0.38949(15) 0.06786(9) 0.0790(16) Uani 1 1 d . O 9
C61 C -0.27943(12) 0.32364(15) 0.10823(9) 0.0782(16) Uani 1 1 d R O 9
C62 C -0.24735(12) 0.24291(15) 0.10330(9) 0.1010(19) Uani 1 1 d R O 9
H621 H -0.2068 0.2304 0.0763 0.207(4) Uiso 1 1 d R O 9
C63 C -0.27397(12) 0.18025(15) 0.13743(9) 0.118(2) Uani 1 1 d R O 9
H631 H -0.2518 0.1245 0.1340 0.207(4) Uiso 1 1 d R O 9
C64 C -0.33267(12) 0.19833(15) 0.17648(9) 0.116(2) Uani 1 1 d R O 9
H641 H -0.3511 0.1550 0.2000 0.207(4) Uiso 1 1 d R O 9
C65 C -0.36475(12) 0.27905(15) 0.18141(9) 0.1009(19) Uani 1 1 d R O 9
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H651 H -0.4053 0.2915 0.2084 0.207(4) Uiso 1 1 d R O 9
C66 C -0.33814(12) 0.34172(15) 0.14729(9) 0.0893(17) Uani 1 1 d R O 9
H661 H -0.3603 0.3975 0.1507 0.207(4) Uiso 1 1 d R O 9
C67 C -0.22965(12) 0.49192(15) 0.08859(9) 0.0778(16) Uani 1 1 d R O 9
C68 C -0.19614(12) 0.53669(15) 0.15326(9) 0.0803(16) Uani 1 1 d R O 9
H681 H -0.1923 0.5013 0.1846 0.207(4) Uiso 1 1 d R O 9
C69 C -0.16821(12) 0.63270(15) 0.17261(9) 0.0905(18) Uani 1 1 d R O 9
H691 H -0.1451 0.6636 0.2173 0.207(4) Uiso 1 1 d R O 9
C70 C -0.17380(12) 0.68393(15) 0.12727(9) 0.099(2) Uani 1 1 d R O 9
H701 H -0.1545 0.7502 0.1406 0.207(4) Uiso 1 1 d R O 9
C71 C -0.20731(12) 0.63915(15) 0.06259(9) 0.0948(18) Uani 1 1 d R O 9
H711 H -0.2112 0.6745 0.0313 0.207(4) Uiso 1 1 d R O 9
C72 C -0.23524(12) 0.54315(15) 0.04325(9) 0.0878(17) Uani 1 1 d R O 9
H721 H -0.2584 0.5122 -0.0014 0.207(4) Uiso 1 1 d R O 9
O5 O -0.1806(4) 0.3703(3) -0.1520(2) 0.1104(14) Uani 1 1 d D O 9
C731 C -0.2149(18) 0.3763(16) -0.2183(13) 0.177(8) Uiso 0.60 1 d P P 11
H731 H -0.1496 0.3893 -0.2289 0.207(4) Uiso 0.60 1 d PR P 11
H732 H -0.2557 0.3126 -0.2437 0.207(4) Uiso 0.60 1 d PR P 11
C741 C -0.2694(11) 0.4297(10) -0.2442(7) 0.160(5) Uiso 0.60 1 d P P 11
H741 H -0.2939 0.4091 -0.2911 0.207(4) Uiso 0.60 1 d PR P 11
H742 H -0.2245 0.4934 -0.2301 0.207(4) Uiso 0.60 1 d PR P 11
H743 H -0.3302 0.4268 -0.2299 0.207(4) Uiso 0.60 1 d PR P 11
C732 C -0.2583(11) 0.4071(12) -0.1936(7) 0.122(6) Uiso 0.40 1 d PD Q 12
H733 H -0.2427 0.4754 -0.1823 0.207(4) Uiso 0.40 1 d PR Q 12
H734 H -0.3327 0.3774 -0.2001 0.207(4) Uiso 0.40 1 d PR Q 12
C742 C -0.217(4) 0.367(3) -0.2465(18) 0.29(3) Uiso 0.40 1 d PD Q 12
H744 H -0.2764 0.3432 -0.2871 0.207(4) Uiso 0.40 1 d PR Q 12
H745 H -0.1872 0.3166 -0.2357 0.207(4) Uiso 0.40 1 d PR Q 12
H746 H -0.1629 0.4156 -0.2507 0.207(4) Uiso 0.40 1 d PR Q 12
C75 C -0.0652(7) 0.4264(7) -0.1218(5) 0.152(3) Uani 1 1 d . . .
H751 H -0.0250 0.3940 -0.0935 0.207(4) Uiso 1 1 calc R O 9
H752 H -0.0343 0.4328 -0.1558 0.207(4) Uiso 1 1 calc R O 9
C76 C -0.0587(9) 0.5085(8) -0.0886(5) 0.209(5) Uani 1 1 d . O .
H761 H -0.0772 0.5477 -0.1177 0.207(4) Uiso 1 1 calc R . .
H762 H 0.0135 0.5368 -0.0586 0.207(4) Uiso 1 1 calc R . .
H763 H -0.1074 0.5025 -0.0646 0.207(4) Uiso 1 1 calc R . .
O6 O -0.1298(4) 0.1973(4) -0.0971(3) 0.1355(18) Uani 1 1 d D . .
C771 C -0.086(3) 0.215(3) -0.0265(4) 0.254(19) Uiso 0.50 1 d PD O 13
H771 H -0.0898 0.1528 -0.0238 0.207(4) Uiso 0.50 1 d PR O 13
H772 H -0.1358 0.2351 -0.0091 0.207(4) Uiso 0.50 1 d PR O 13
C772 C -0.1030(11) 0.1736(11) -0.0392(7) 0.114(6) Uiso 0.50 1 d PD O 14
H773 H -0.0840 0.1166 -0.0465 0.207(4) Uiso 0.50 1 d PR O 14
H774 H -0.1593 0.1650 -0.0221 0.207(4) Uiso 0.50 1 d PR O 14
C78 C -0.0026(10) 0.2477(7) 0.0082(5) 0.231(7) Uani 1 1 d D . .
H781 H 0.0105 0.2423 0.0513 0.207(4) Uiso 0.50 1 d PR O .
H782 H 0.0489 0.2276 -0.0076 0.207(4) Uiso 0.50 1 d PR . .
H783 H 0.0023 0.3110 0.0073 0.207(4) Uiso 0.50 1 d PR . .
H784 H 0.0217 0.2322 0.0483 0.207(4) Uiso 0.50 1 d PR . .
H785 H 0.0530 0.2556 -0.0096 0.207(4) Uiso 0.50 1 d PR . .
H786 H -0.0228 0.3042 0.0149 0.207(4) Uiso 0.50 1 d PR . .
C79 C -0.0970(8) 0.1400(7) -0.1377(6) 0.185(5) Uani 1 1 d . O .
H791 H -0.1365 0.0749 -0.1452 0.207(4) Uiso 1 1 calc R . .
H792 H -0.0210 0.1458 -0.1174 0.207(4) Uiso 1 1 calc R . .
C80 C -0.1146(8) 0.1647(8) -0.1986(6) 0.209(5) Uani 1 1 d . . .
H801 H -0.1904 0.1526 -0.2208 0.207(4) Uiso 1 1 calc R O .
H802 H -0.0851 0.1276 -0.2252 0.207(4) Uiso 1 1 calc R . .
H803 H -0.0800 0.2304 -0.1908 0.207(4) Uiso 1 1 calc R . .
O7 O -0.5041(3) 0.1449(3) -0.0873(2) 0.0955(12) Uani 1 1 d . . .
C81 C -0.5243(5) 0.1560(5) -0.0277(3) 0.105(2) Uani 1 1 d . O .
H811 H -0.4619 0.1537 0.0070 0.207(4) Uiso 1 1 calc R . .
H812 H -0.5850 0.1052 -0.0314 0.207(4) Uiso 1 1 calc R . .
C82 C -0.5477(5) 0.2476(4) -0.0121(3) 0.111(2) Uani 1 1 d . . .
H821 H -0.4865 0.2976 -0.0074 0.207(4) Uiso 1 1 calc R O .
H822 H -0.5626 0.2554 0.0281 0.207(4) Uiso 1 1 calc R . .
H823 H -0.6090 0.2496 -0.0468 0.207(4) Uiso 1 1 calc R . .
C83 C -0.5058(7) 0.0515(5) -0.1133(4) 0.136(3) Uani 1 1 d . O .
H831 H -0.5180 0.0417 -0.1598 0.207(4) Uiso 1 1 calc R . .
H832 H -0.5654 0.0086 -0.1082 0.207(4) Uiso 1 1 calc R . .
C84 C -0.4066(9) 0.0290(6) -0.0821(5) 0.178(4) Uani 1 1 d . . .
                                Seite 6
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H841 H -0.3474 0.0705 -0.0877 0.207(4) Uiso 1 1 calc R 0 .
H842 H -0.4118 -0.0352 -0.1017 0.207(4) Uiso 1 1 calc R . .
H843 H -0.3950 0.0370 -0.0363 0.207(4) Uiso 1 1 calc R . .
O8 O -0.5092(4) 0.3313(4) -0.1437(3) 0.1360(18) Uani 1 1 d . . .
C85 C -0.5966(7) 0.3136(6) -0.1996(5) 0.133(3) Uani 1 1 d . . 0 .
H851 H -0.5734 0.3380 -0.2324 0.207(4) Uiso 1 1 calc R . .
H852 H -0.6477 0.3459 -0.1899 0.207(4) Uiso 1 1 calc R . .
C86 C -0.6482(5) 0.2138(6) -0.2249(4) 0.142(3) Uani 1 1 d . . .
H861 H -0.5977 0.1819 -0.2345 0.207(4) Uiso 1 1 calc R 0 .
H862 H -0.7083 0.2031 -0.2640 0.207(4) Uiso 1 1 calc R . .
H863 H -0.6729 0.1899 -0.1928 0.207(4) Uiso 1 1 calc R . .
C871 C -0.4946(15) 0.4201(13) -0.0872(11) 0.112(7) Uani 0.50 1 d P 0 15
H871 H -0.5632 0.4246 -0.0832 0.207(4) Uiso 0.50 1 calc PR 0 15
H872 H -0.4466 0.4183 -0.0455 0.207(4) Uiso 0.50 1 calc PR 0 15
C881 C -0.449(2) 0.4957(18) -0.1102(11) 0.146(9) Uani 0.50 1 d P 0 15
H881 H -0.4351 0.5546 -0.0794 0.207(4) Uiso 0.50 1 calc PR 0 15
H882 H -0.4976 0.4953 -0.1517 0.207(4) Uiso 0.50 1 calc PR 0 15
H883 H -0.3822 0.4882 -0.1150 0.207(4) Uiso 0.50 1 calc PR 0 15
C872 C -0.4495(14) 0.4324(13) -0.1335(9) 0.107(5) Uani 0.50 1 d P 0 16
H873 H -0.4671 0.4529 -0.1735 0.207(4) Uiso 0.50 1 calc PR 0 16
H874 H -0.3722 0.4435 -0.1147 0.207(4) Uiso 0.50 1 calc PR 0 16
C882 C -0.496(2) 0.478(2) -0.0850(12) 0.134(9) Uani 0.50 1 d P 0 16
H884 H -0.4613 0.5448 -0.0701 0.207(4) Uiso 0.50 1 calc PR 0 16
H885 H -0.4840 0.4507 -0.0484 0.207(4) Uiso 0.50 1 calc PR 0 16
H886 H -0.5719 0.4680 -0.1060 0.207(4) Uiso 0.50 1 calc PR 0 16

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N2 0.086(3) 0.084(3) 0.077(3) 0.000(3) 0.037(3) 0.014(3)
Li1 0.086(6) 0.084(7) 0.077(6) 0.016(5) 0.032(5) 0.024(5)
Li2 0.091(7) 0.102(8) 0.081(7) 0.017(6) 0.031(6) 0.034(6)
C1 0.069(4) 0.073(4) 0.085(4) 0.026(3) 0.037(3) 0.028(3)
C2 0.091(4) 0.073(4) 0.061(4) 0.014(3) 0.042(3) 0.025(3)
C3 0.075(4) 0.065(4) 0.085(4) 0.012(3) 0.031(3) 0.021(3)
C4 0.135(6) 0.187(8) 0.115(6) -0.029(6) 0.073(6) -0.063(6)
C5 0.129(7) 0.179(8) 0.119(7) -0.011(6) 0.054(6) -0.037(6)
C6 0.091(5) 0.105(5) 0.119(6) 0.019(5) 0.012(5) 0.022(4)
C7 0.120(6) 0.153(7) 0.094(6) 0.025(5) 0.015(5) 0.005(5)
C8 0.103(5) 0.165(7) 0.057(4) 0.011(4) 0.016(4) 0.007(5)
C91 0.074(7) 0.072(9) 0.096(11) 0.013(8) 0.040(8) 0.026(7)
C101 0.096(8) 0.076(6) 0.088(7) 0.023(5) 0.038(7) 0.015(5)
C111 0.081(8) 0.098(8) 0.110(10) 0.035(8) 0.033(8) 0.037(7)
C121 0.099(10) 0.111(8) 0.109(10) 0.044(7) 0.054(9) 0.021(6)
C131 0.124(8) 0.123(9) 0.108(8) 0.026(7) 0.064(7) 0.028(7)
C141 0.111(7) 0.101(7) 0.093(7) 0.013(6) 0.055(6) 0.026(6)
C92 0.077(15) 0.060(17) 0.030(13) 0.010(12) 0.034(13) 0.030(14)
C102 0.057(13) 0.051(12) 0.119(19) 0.039(12) 0.050(14) 0.015(10)
C112 0.085(18) 0.092(17) 0.078(17) 0.032(15) 0.027(15) 0.018(15)
C122 0.12(3) 0.073(16) 0.10(2) -0.003(14) 0.02(2) 0.025(14)
C132 0.103(15) 0.069(13) 0.074(13) 0.029(11) 0.054(12) 0.016(12)
C142 0.134(17) 0.062(13) 0.049(11) 0.013(9) 0.041(12) 0.023(12)
C15 0.069(4) 0.070(4) 0.086(4) 0.011(3) 0.030(3) 0.013(3)
C16 0.081(4) 0.071(4) 0.066(4) 0.011(3) 0.037(3) 0.022(3)
C17 0.072(4) 0.066(4) 0.073(4) 0.016(3) 0.034(3) 0.029(3)
C18 0.087(4) 0.073(4) 0.076(4) 0.011(3) 0.029(3) 0.018(3)
C19 0.082(4) 0.087(5) 0.083(4) 0.004(3) 0.028(4) 0.015(3)
C20 0.074(4) 0.090(5) 0.107(5) 0.011(4) 0.029(4) 0.015(3)
C21 0.088(4) 0.083(4) 0.107(5) 0.024(4) 0.046(4) 0.019(4)
C22 0.076(4) 0.073(4) 0.095(4) 0.017(3) 0.044(4) 0.020(3)
C23 0.070(3) 0.071(4) 0.059(3) 0.008(3) 0.024(3) 0.019(3)
C24 0.081(4) 0.088(4) 0.064(3) 0.014(3) 0.030(3) 0.025(3)
C25 0.088(4) 0.095(5) 0.078(4) 0.014(4) 0.037(4) 0.022(4)
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C26 0.086(4) 0.108(5) 0.087(4) 0.027(4) 0.038(4) 0.019(4)
C27 0.088(4) 0.092(5) 0.104(5) 0.017(4) 0.044(4) 0.007(3)
C28 0.092(4) 0.068(4) 0.103(5) 0.003(3) 0.044(4) 0.010(3)
O1 0.111(3) 0.137(4) 0.111(4) 0.051(3) 0.050(3) 0.051(3)
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O2 0.114(4) 0.130(4) 0.113(4) 0.022(3) 0.026(3) -0.006(3)
C351 0.040(10) 0.35(4) 0.28(3) 0.19(3) 0.078(16) 0.051(15)
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C362 0.10(2) 0.20(3) 0.23(5) -0.12(3) 0.07(3) -0.008(17)
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C382 0.058(9) 0.058(11) 0.21(2) -0.005(12) 0.042(12) 0.014(9)
O4 0.115(4) 0.110(4) 0.123(4) 0.025(3) 0.047(3) 0.020(3)
C41 0.080(6) 0.223(11) 0.233(13) -0.045(10) 0.045(7) 0.007(7)
C42 0.198(11) 0.228(12) 0.197(11) 0.074(10) 0.100(10) 0.100(10)
N3 0.115(4) 0.077(4) 0.092(4) 0.018(3) 0.046(4) 0.017(3)
N4 0.085(3) 0.079(3) 0.090(4) 0.014(3) 0.033(3) 0.020(3)
Li3 0.082(6) 0.080(7) 0.112(8) 0.036(6) 0.052(6) 0.020(5)
Li4 0.088(7) 0.082(7) 0.106(8) 0.014(6) 0.052(6) 0.018(6)
C45 0.090(5) 0.075(4) 0.104(5) 0.039(4) 0.047(5) 0.022(4)
C46 0.084(4) 0.090(5) 0.078(4) 0.009(4) 0.031(4) 0.020(4)
C47 0.075(4) 0.085(5) 0.086(4) 0.023(4) 0.023(3) 0.014(3)
C48 0.074(4) 0.114(5) 0.077(4) 0.037(4) 0.031(3) 0.018(3)
C49 0.075(4) 0.129(6) 0.116(6) 0.043(5) 0.020(4) -0.004(4)
C50 0.100(5) 0.155(8) 0.102(6) 0.056(6) 0.004(5) -0.015(5)
C51 0.132(6) 0.109(6) 0.131(6) 0.065(5) 0.015(5) 0.023(5)
C52 0.114(5) 0.090(5) 0.115(6) 0.033(4) 0.024(4) 0.028(4)
C53 0.087(4) 0.074(4) 0.075(4) 0.013(3) 0.036(4) 0.018(3)
C54 0.111(5) 0.090(5) 0.088(5) 0.027(4) 0.039(4) 0.024(4)
C55 0.130(6) 0.099(6) 0.096(5) 0.032(4) 0.037(5) 0.023(5)
C56 0.143(6) 0.077(5) 0.102(5) 0.022(4) 0.053(5) 0.026(4)
C57 0.110(5) 0.102(5) 0.083(5) 0.019(4) 0.038(4) 0.011(4)
C58 0.096(4) 0.086(5) 0.087(5) 0.024(4) 0.039(4) 0.009(4)
C59 0.069(4) 0.068(4) 0.103(5) 0.025(4) 0.033(4) 0.021(3)
C60 0.069(4) 0.093(5) 0.077(4) 0.015(4) 0.032(3) 0.022(3)
C61 0.076(4) 0.076(4) 0.080(4) 0.016(3) 0.033(3) 0.010(3)
C62 0.113(5) 0.089(5) 0.104(5) 0.027(4) 0.042(4) 0.025(4)
C63 0.143(6) 0.097(5) 0.114(6) 0.034(5) 0.046(5) 0.022(5)
C64 0.116(6) 0.103(6) 0.122(6) 0.041(5) 0.039(5) 0.004(4)
C65 0.097(5) 0.103(5) 0.093(5) 0.028(4) 0.026(4) 0.015(4)
C66 0.075(4) 0.104(5) 0.089(4) 0.035(4) 0.027(3) 0.016(3)
C67 0.070(4) 0.078(4) 0.086(4) 0.012(4) 0.034(3) 0.019(3)
C68 0.069(4) 0.085(4) 0.084(4) 0.010(3) 0.028(3) 0.024(3)
C69 0.084(4) 0.097(5) 0.096(5) 0.016(4) 0.042(4) 0.027(4)
C70 0.091(4) 0.092(5) 0.126(6) 0.024(4) 0.054(4) 0.029(4)
C71 0.090(4) 0.097(5) 0.107(5) 0.030(4) 0.043(4) 0.029(4)
C72 0.091(4) 0.082(4) 0.095(5) 0.025(4) 0.039(4) 0.020(4)
O5 0.101(3) 0.107(4) 0.125(4) 0.042(3) 0.044(3) 0.012(3)
C75 0.150(8) 0.149(8) 0.208(10) 0.068(8) 0.103(8) 0.068(7)
C76 0.265(13) 0.183(11) 0.186(10) 0.010(9) 0.099(9) 0.074(10)
O6 0.142(4) 0.156(5) 0.164(5) 0.073(4) 0.087(4) 0.080(4)
C78 0.41(3) 0.144(10) 0.183(10) 0.092(9) 0.128(15) 0.099(14)
C79 0.200(10) 0.147(8) 0.323(15) 0.098(10) 0.191(11) 0.108(7)
C80 0.189(10) 0.189(11) 0.275(15) 0.001(10) 0.148(11) 0.056(8)
O7 0.098(3) 0.079(3) 0.113(3) 0.021(2) 0.051(3) 0.014(2)
C81 0.095(5) 0.117(6) 0.114(5) 0.027(4) 0.055(4) 0.027(4)
C82 0.090(4) 0.098(5) 0.136(6) 0.004(4) 0.056(4) 0.008(4)
C83 0.187(8) 0.070(5) 0.168(8) 0.019(5) 0.107(7) 0.015(5)
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C86 0.090(5) 0.128(7) 0.184(8) 0.019(6) 0.038(5) 0.013(5)
C871 0.085(10) 0.112(17) 0.168(18) 0.051(16) 0.063(11) 0.049(12)
C881 0.23(3) 0.113(18) 0.088(15) 0.041(14) 0.045(14) 0.041(19)
C872 0.099(10) 0.094(14) 0.135(15) 0.028(11) 0.048(11) 0.034(11)
C882 0.18(2) 0.15(2) 0.108(16) 0.048(17) 0.048(13) 0.10(2)

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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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Li1 O1 1.949(10) . ?
Li1 O2 1.967(11) . ?
Li1 Li2 2.756(14) . ?
Li2 O3 1.897(11) . ?
Li2 O4 1.981(11) . ?
Li2 C372 2.77(3) . ?
C1 C2 1.379(6) . ?
C2 C92 1.3195 . ?
C2 C3 1.5100 . ?
C2 C91 1.5251 . ?
C3 C4 1.3900 . ?
C3 C8 1.3901 . ?
C4 C5 1.3900 . ?
C5 C6 1.3900 . ?
C6 C7 1.3899 . ?
C7 C8 1.3900 . ?
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C121 C131 1.3900 . ?
C131 C141 1.3899 . ?
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C92 C142 1.4843 . ?
C102 C112 1.4809 . ?
C112 C122 1.5114 . ?
C122 C132 1.4755 . ?
C132 C142 1.4342 . ?
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O2 C352 1.165(18) . ?
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O2 C33 1.745(12) . ?
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O3 C392 1.4803(10) . ?
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O3 C372 1.4803(10) . ?
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C46 C47 1.5055 . ?
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C47 C52 1.3900 . ?
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C49 C50 1.3899 . ?
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C53 C54 1.3900 . ?
C54 C55 1.3900 . ?
C55 C56 1.3901 . ?
C56 C57 1.3899 . ?
C57 C58 1.3900 . ?
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C60 C61 1.5137 . ?
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C61 C66 1.3902 . ?
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C71 C72 1.3899 . ?
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O6 C79 1.390(9) . ?
O6 C771 1.4801(11) . ?
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O7 C81 1.440(6) . ?
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Li1 Li2 C372 115.9(9) . . ?
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C92 C2 C1 117.1(2) . . ?
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C41 O4 Li2 114.3(6) . . ?
C43 O4 Li2 121.3(7) . . ?
C42 C41 O4 118.0(9) . . ?
C44 C43 O4 106.3(12) . . ?
C45 N3 Li4 138.7(6) . . ?
C45 N3 Li3 138.0(5) . . ?
Li4 N3 Li3 83.0(4) . . ?
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C59 N4 Li3 152.5(5) . . ?
C59 N4 Li4 123.6(5) . . ?
Li3 N4 Li4 83.6(4) . . ?
O6 Li3 O5 112.5(4) . . ?
O6 Li3 N4 113.2(5) . . ?
O5 Li3 N4 109.1(5) . . ?
O6 Li3 N3 115.0(5) . . ?
O5 Li3 N3 108.9(5) . . ?
N4 Li3 N3 97.0(4) . . ?
O6 Li3 Li4 131.9(5) . . ?
O5 Li3 Li4 115.6(5) . . ?
N4 Li3 Li4 48.9(3) . . ?
N3 Li3 Li4 48.3(3) . . ?
O8 Li4 O7 116.5(5) . . ?
O8 Li4 N3 110.7(5) . . ?
O7 Li4 N3 109.6(5) . . ?
O8 Li4 N4 111.5(5) . . ?
O7 Li4 N4 110.6(5) . . ?
N3 Li4 N4 96.0(4) . . ?
O8 Li4 Li3 118.9(5) . . ?
O7 Li4 Li3 124.6(5) . . ?
N3 Li4 Li3 48.7(3) . . ?
N4 Li4 Li3 47.5(3) . . ?
N3 C45 C46 179.6(7) . . ?
C45 C46 C53 118.7(3) . . ?
C45 C46 C47 117.4(3) . . ?
C53 C46 C47 123.9 . . ?
C48 C47 C52 120.0 . . ?
C48 C47 C46 120.4 . . ?
C52 C47 C46 119.5 . . ?
C47 C48 C49 120.0 . . ?
C50 C49 C48 120.0 . . ?
C49 C50 C51 120.0 . . ?
C50 C51 C52 120.0 . . ?
C47 C52 C51 120.0 . . ?
C58 C53 C54 120.0 . . ?
C58 C53 C46 120.7 . . ?
C54 C53 C46 119.3 . . ?
C55 C54 C53 120.0 . . ?
C54 C55 C56 120.0 . . ?
C57 C56 C55 120.0 . . ?
C56 C57 C58 120.0 . . ?
C53 C58 C57 120.0 . . ?
N4 C59 C60 177.3(6) . . ?
C59 C60 C67 118.8(2) . . ?
C59 C60 C61 115.0(2) . . ?
C67 C60 C61 126.2 . . ?
C62 C61 C66 120.0 . . ?
C62 C61 C60 121.0 . . ?
C66 C61 C60 118.8 . . ?
C61 C62 C63 120.0 . . ?
C64 C63 C62 120.0 . . ?
C65 C64 C63 120.0 . . ?
C64 C65 C66 120.0 . . ?
C65 C66 C61 120.0 . . ?
C68 C67 C72 120.0 . . ?
C68 C67 C60 120.1 . . ?
C72 C67 C60 119.9 . . ?
C67 C68 C69 120.0 . . ?
C68 C69 C70 120.0 . . ?
C71 C70 C69 120.0 . . ?
C72 C71 C70 120.0 . . ?
C71 C72 C67 120.0 . . ?
C75 O5 Li3 119.9(5) . . ?
C76 C75 O5 109.5(8) . . ?
C772 O6 C79 106.5(10) . . ?
C772 O6 C771 24.5(19) . . ?
C79 O6 C771 122.3(19) . . ?
C772 O6 Li3 123.0(9) . . ?
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C79 O6 Li3 127.6(7) . . ?
C771 O6 Li3 110.1(18) . . ?
C78 C771 O6 131(3) . . ?
O6 C772 C78 108.3(10) . . ?
C771 C78 C772 20(3) . . ?
O6 C79 C80 110.5(8) . . ?
C83 O7 C81 112.3(5) . . ?
C83 O7 Li4 118.5(4) . . ?
C81 O7 Li4 125.6(5) . . ?
O7 C81 C82 108.8(5) . . ?
O7 C83 C84 112.8(7) . . ?
C85 O8 C872 104.2(8) . . ?
C85 O8 C871 115.4(8) . . ?
C872 O8 C871 51.9(8) . . ?
C85 O8 Li4 126.9(6) . . ?
C872 O8 Li4 119.8(7) . . ?
C871 O8 Li4 114.8(9) . . ?
O8 C85 C86 110.9(7) . . ?
C881 C871 O8 101.4(18) . . ?
O8 C872 C882 98.2(17) . . ?

_diffrn_measured_fraction_theta_max    0.984
_diffrn_reflns_theta_full              26.41
_diffrn_measured_fraction_theta_full   0.984
_refine_diff_density_max    0.262
_refine_diff_density_min   -0.260
_refine_diff_density_rms    0.039
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