C(13) C(14) 1.63(4) . . ?

C(13) H(17) 0.92 . . no

C(13) H(18) 1.04 . . no

C(14) H(19) 0.96 . . no

C(14) H(20) 1.00 . . no

C(15) C(16) 1.36(3) . . ?

C(15) H(21) 0.92 . . no

C(16) C(18) 1.41(3) . . ?

C(17) H(22) 0.94 . . no

C(18) H(24) 1.03 . . no

C(19) C(20) 1.48(4) . . ?

C(19) H(25) 1.00 . . no

C(19) H(26) 0.89 . . no

C(20) H(27) 0.97 . . no

C(20) H(28) 0.95 . . no

C(21) C(22) 1.51(3) . . ?

C(21) H(29) 0.98 . . no

C(22) C(24) 1.32(4) . . ?

C(23) H(30) 0.97 . . no

C(24) H(31) 1.01 . . no

C(25) C(26) 1.58(4) . . ?

C(25) H(32) 0.90 . . no

C(25) H(33) 0.96 . . no

C(26) H(34) 1.05 . . no

C(27) C(28) 1.39(4) . . ?

C(27) H(36) 0.89 . . no

C(28) C(30) 1.44(3) . . ?

C(29) H(37) 0.98 . . no

C(30) H(38) 1.04 . . no

C(31) C(32) 1.38(4) . . ?

C(31) H(39) 0.95 . . no

C(31) H(40) 0.95 . . no

C(32) H(41) 1.06 . . no

C(32) H(42) 0.94 . . no

C(33) C(34) 1.32(3) . . ?

C(33) H(43) 0.96 . . no

```
 C(34) C(36) 1.36(4) . . ?
 C(35) H(44) 0.96 . . no
 C(36) H(45) 1.08 . . no
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loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 N(2) Co(1)  N(3) 83.1(7) . . . ?
 N(2) Co(1)  N(5) 94.5(8) . . . ?
 N(2) Co(1)  N(6) 87.0(7) . . . ?
 N(2) Co(1)  N(8) 97.1(7) . . . ?
 N(2) Co(1)  N(9) 173.5(7) . . . ?
 N(3) Co(1)  N(5) 176.6(9) . . . ?
 N(3) Co(1)  N(6) 93.6(7) . . . ?
 N(3) Co(1)  N(8) 84.9(8) . . . ?
 N(3) Co(1)  N(9) 90.4(8) . . . ?
 N(5) Co(1)  N(6) 83.8(7) . . . ?
 N(5) Co(1)  N(8) 97.9(8) . . . ?
 N(5) Co(1)  N(9) 92.0(8) . . . ?
 N(6) Co(1)  N(8) 175.4(8) . . . ?
 N(6) Co(1)  N(9) 94.2(8) . . . ?
 N(8) Co(1)  N(9) 81.4(8) . . . ?
N(12) Co(2)  N(13) 83.8(8) . . . ?
N(12) Co(2)  N(15) 95.2(9) . . . ?
N(12) Co(2)  N(16) 92.9(8) . . . ?
N(12) Co(2)  N(18) 93.9(8) . . . ?
N(12) Co(2)  N(19) 173.9(9) . . . ?
N(13) Co(2)  N(15) 174.2(9) . . . ?
N(13) Co(2)  N(16) 92.0(8) . . . ?
N(13) Co(2)  N(18) 87.5(9) . . . ?
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N(13) Co(2) N(19) 92.5(8) . . . ?

N(15) Co(2) N(16) 82.3(10) . . . ?

N(15) Co(2) N(18) 98.4(10) . . . ?

N(15) Co(2) N(19) 89.0(9) . . . ?

N(16) Co(2) N(18) 173.1(8) . . . ?

N(16) Co(2) N(19) 92.1(8) . . . ?

N(18) Co(2) N(19) 81.1(8) . . . ?

O(1) Cl(1) O(2) 102.8(11) . . . ?

O(1) Cl(1) O(3) 100.8(13) . . . ?

O(1) Cl(1) O(4) 110.9(12) . . . ?

O(2) Cl(1) O(3) 105.8(12) . . . ?

O(2) Cl(1) O(4) 118.0(12) . . . ?

O(3) Cl(1) O(4) 116.4(13) . . . ?

O(5) Cl(2) O(6) 113.2(21) . . . ?

O(5) Cl(2) O(7) 113.3(22) . . . ?

O(5) Cl(2) O(8) 95.4(20) . . . ?

O(6) Cl(2) O(7) 102.5(24) . . . ?

O(6) Cl(2) O(8) 135.9(23) . . . ?

O(7) Cl(2) O(8) 95.3(20) . . . ?

O(9) Cl(3) O(10) 122.1(27) . . . ?

O(9) Cl(3) O(11) 135.5(43) . . . ?

O(9) Cl(3) O(12) 100.7(38) . . . ?

O(10) Cl(3) O(11) 78.9(35) . . . ?

O(10) Cl(3) O(12) 79.1(30) . . . ?

O(11) Cl(3) O(12) 122.8(45) . . . ?

O(13) Cl(4) O(14) 90.8(32) . . . ?

O(13) Cl(4) O(15) 130.7(35) . . . ?

O(13) Cl(4) O(16) 92.3(31) . . . ?

O(14) Cl(4) O(15) 112.7(22) . . . ?

O(14) Cl(4) O(16) 109.7(21) . . . ?

O(15) Cl(4) O(16) 116.7(25) . . . ?

C(1) N(1) C(7) 115.7(25) . . . ?

C(1) N(1) C(13) 116.5(25) . . . ?

C(7) N(1) C(13) 126.6(29) . . . ?

Co(1) N(2) C(2) 131.8(15) . . . ?

Co(1) N(2) C(3) 116.5(16) . . . ?

C(2) N(2) C(3) 111.6(21) . . . ?

Co(1) N(3) C(4) 113.4(14) . . . ?

Co(1) N(3) C(5) 140.1(18) . . . ?

C(4) N(3) C(5) 104.9(19) . . . ?

C(5) N(4) C(6) 102.9(21) . . . ?

C(5) N(4) H(7) 128.6 . . . no

C(6) N(4) H(7) 128.4 . . . no

Co(1) N(5) C(8) 127.6(16) . . . ?

Co(1) N(5) C(9) 119.0(18) . . . ?

C(8) N(5) C(9) 113.2(20) . . . ?

Co(1) N(6) C(10) 111.1(14) . . . ?

Co(1) N(6) C(11) 141.8(14) . . . ?

C(10) N(6) C(11) 106.9(19) . . . ?

C(11) N(7) C(12) 108.4(20) . . . ?

C(11) N(7) H(15) 117.4 . . . no

C(12) N(7) H(15) 134.0 . . . no

Co(1) N(8) C(14) 121.9(17) . . . ?

Co(1) N(8) C(15) 115.9(16) . . . ?

C(14) N(8) C(15) 122.2(21) . . . ?

Co(1) N(9) C(16) 112.6(14) . . . ?

Co(1) N(9) C(17) 137.4(16) . . . ?

C(16) N(9) C(17) 110.0(18) . . . ?

C(17) N(10) C(18) 105.7(20) . . . ?

C(17) N(10) H(23) 129.1 . . . no

C(18) N(10) H(23) 125.2 . . . no

C(19) N(11) C(25) 123.7(30) . . . ?

C(19) N(11) C(31) 118.0(23) . . . ?

C(25) N(11) C(31) 118.2(28) . . . ?

Co(2) N(12) C(20) 128.1(15) . . . ?

Co(2) N(12) C(21) 112.6(17) . . . ?

C(20) N(12) C(21) 118.9(21) . . . ?

Co(2) N(13) C(22) 114.2(15) . . . ?

Co(2) N(13) C(23) 142.8(17) . . . ?

C(22) N(13) C(23) 102.8(21) . . . ?

C(23) N(14) C(24) 103.2(22) . . . ?

Co(2) N(15) C(26) 117.6(19) . . . ?

Co(2) N(15) C(27) 112.6(17) . . . ?

C(26) N(15) C(27) 129.2(22) . . . ?

Co(2) N(16) C(28) 112.1(17) . . . ?

Co(2) N(16) C(29) 141.1(16) . . . ?

C(28) N(16) C(29) 106.6(17) . . . ?

C(29) N(17) C(30) 109.0(20) . . . ?

Co(2) N(18) C(32) 123.7(18) . . . ?

Co(2) N(18) C(33) 107.9(14) . . . ?

C(32) N(18) C(33) 128.4(22) . . . ?

Co(2) N(19) C(34) 116.5(16) . . . ?

Co(2) N(19) C(35) 139.2(18) . . . ?

C(34) N(19) C(35) 104.2(21) . . . ?

C(35) N(20) C(36) 103.3(20) . . . ?

N(1) C(1) C(2) 113.4(18) . . . ?

N(1) C(1) H(1) 108.8 . . . no

N(1) C(1) H(2) 108.1 . . . no

C(2) C(1) H(1) 109.8 . . . no

C(2) C(1) H(2) 112.9 . . . no

H(1) C(1) H(2) 103.4 . . . no

N(2) C(2) C(1) 112.8(18) . . . ?

N(2) C(2) H(3) 118.9 . . . no

N(2) C(2) H(4) 109.5 . . . no

C(1) C(2) H(3) 101.5 . . . no

C(1) C(2) H(4) 98.0 . . . no

H(3) C(2) H(4) 114.0 . . . no

N(2) C(3) C(4) 116.8(24) . . . ?

N(2) C(3) H(5) 133.8 . . . no

C(4) C(3) H(5) 107.2 . . . no

N(3) C(4) C(3) 109.3(20) . . . ?

N(3) C(4) C(6) 110.9(22) . . . ?

C(3) C(4) C(6) 139.7(23) . . . ?

N(3) C(5) N(4) 114.5(22) . . . ?

N(3) C(5) H(6) 116.2 . . . no

N(4) C(5) H(6) 129.3 . . . no

N(4) C(6) C(4) 106.6(25) . . . ?

N(4) C(6) H(8) 125.7 . . . no

C(4) C(6) H(8) 125.1 . . . no

N(1) C(7) C(8) 111.1(24) . . . ?

N(1) C(7) H(9) 107.7 . . . no

N(1) C(7) H(10) 112.9 . . . no

C(8) C(7) H(9) 104.3 . . . no

C(8) C(7) H(10) 109.0 . . . no

H(9) C(7) H(10) 111.5 . . . no

N(5) C(8) C(7) 106.7(25) . . . ?

N(5) C(8) H(11) 107.5 . . . no

N(5) C(8) H(12) 105.0 . . . no

C(7) C(8) H(11) 109.3 . . . no

C(7) C(8) H(12) 107.0 . . . no

H(11) C(8) H(12) 120.6 . . . no

N(5) C(9) C(10) 112.8(23) . . . ?

N(5) C(9) H(13) 125.8 . . . no

C(10) C(9) H(13) 121.0 . . . no

N(6) C(10) C(9) 113.2(21) . . . ?

N(6) C(10) C(12) 109.9(21) . . . ?

C(9) C(10) C(12) 136.6(25) . . . ?

N(6) C(11) N(7) 111.1(19) . . . ?

N(6) C(11) H(14) 121.6 . . . no

N(7) C(11) H(14) 127.1 . . . no

N(7) C(12) C(10) 103.2(22) . . . ?

N(7) C(12) H(16) 121.5 . . . no

C(10) C(12) H(16) 135.1 . . . no

N(1) C(13) C(14) 106.1(20) . . . ?

N(1) C(13) H(17) 109.9 . . . no

N(1) C(13) H(18) 105.7 . . . no

C(14) C(13) H(17) 118.5 . . . no

C(14) C(13) H(18) 111.8 . . . no

H(17) C(13) H(18) 104.1 . . . no

N(8) C(14) C(13) 115.8(23) . . . ?

N(8) C(14) H(19) 99.3 . . . no

N(8) C(14) H(20) 104.7 . . . no

C(13) C(14) H(19) 93.6 . . . no

C(13) C(14) H(20) 131.9 . . . no

H(19) C(14) H(20) 104.8 . . . no

N(8) C(15) C(16) 115.8(20) . . . ?

N(8) C(15) H(21) 121.0 . . . no

C(16) C(15) H(21) 123.2 . . . no

N(9) C(16) C(15) 114.3(20) . . . ?

N(9) C(16) C(18) 105.2(19) . . . ?

C(15) C(16) C(18) 140.6(21) . . . ?

N(9) C(17) N(10) 110.6(21) . . . ?

N(9) C(17) H(22) 128.6 . . . no

N(10) C(17) H(22) 120.7 . . . no

N(10) C(18) C(16) 108.4(19) . . . ?

N(10) C(18) H(24) 129.8 . . . no

C(16) C(18) H(24) 120.0 . . . no

N(11) C(19) C(20) 118.4(19) . . . ?

N(11) C(19) H(25) 108.6 . . . no

N(11) C(19) H(26) 110.0 . . . no

C(20) C(19) H(25) 101.8 . . . no

C(20) C(19) H(26) 107.3 . . . no

H(25) C(19) H(26) 110.4 . . . no

N(12) C(20) C(19) 110.0(19) . . . ?

N(12) C(20) H(27) 109.7 . . . no

N(12) C(20) H(28) 112.3 . . . no

C(19) C(20) H(27) 106.5 . . . no

C(19) C(20) H(28) 110.5 . . . no

H(27) C(20) H(28) 107.7 . . . no

N(12) C(21) C(22) 118.3(23) . . . ?

N(12) C(21) H(29) 118.4 . . . no

C(22) C(21) H(29) 123.3 . . . no

N(13) C(22) C(21) 111.1(21) . . . ?

N(13) C(22) C(24) 105.1(24) . . . ?

C(21) C(22) C(24) 142.9(27) . . . ?

N(13) C(23) N(14) 115.0(21) . . . ?

N(13) C(23) H(30) 117.9 . . . no

N(14) C(23) H(30) 127.0 . . . no

N(14) C(24) C(22) 113.4(26) . . . ?

N(14) C(24) H(31) 115.8 . . . no

C(22) C(24) H(31) 124.9 . . . no

N(11) C(25) C(26) 116.5(27) . . . ?

N(11) C(25) H(32) 111.1 . . . no

N(11) C(25) H(33) 116.0 . . . no

C(26) C(25) H(32) 98.0 . . . no

C(26) C(25) H(33) 100.0 . . . no

H(32) C(25) H(33) 113.5 . . . no

N(15) C(26) C(25) 108.0(23) . . . ?

N(15) C(26) H(34) 98.1 . . . no

C(25) C(26) H(34) 112.6 . . . no

N(15) C(27) C(28) 114.2(22) . . . ?

N(15) C(27) H(36) 103.1 . . . no

C(28) C(27) H(36) 138.1 . . . no

N(16) C(28) C(27) 117.9(23) . . . ?

N(16) C(28) C(30) 106.1(23) . . . ?

C(27) C(28) C(30) 135.4(29) . . . ?

N(16) C(29) N(17) 110.2(20) . . . ?

N(16) C(29) H(37) 127.3 . . . no

N(17) C(29) H(37) 122.4 . . . no

N(17) C(30) C(28) 107.8(23) . . . ?

N(17) C(30) H(38) 121.9 . . . no

C(28) C(30) H(38) 128.3 . . . no

N(11) C(31) C(32) 115.5(25) . . . ?

N(11) C(31) H(39) 105.7 . . . no

N(11) C(31) H(40) 104.1 . . . no

C(32) C(31) H(39) 110.8 . . . no

C(32) C(31) H(40) 110.6 . . . no

H(39) C(31) H(40) 109.8 . . . no

N(18) C(32) C(31) 114.2(21) . . . ?

N(18) C(32) H(41) 106.7 . . . no

N(18) C(32) H(42) 114.7 . . . no

C(31) C(32) H(41) 104.5 . . . no

C(31) C(32) H(42) 113.1 . . . no

H(41) C(32) H(42) 102.1 . . . no

N(18) C(33) C(34) 123.2(21) . . . ?

N(18) C(33) H(43) 118.0 . . . no

C(34) C(33) H(43) 118.4 . . . no

N(19) C(34) C(33) 111.0(20) . . . ?

N(19) C(34) C(36) 104.5(21) . . . ?

C(33) C(34) C(36) 144.0(22) . . . ?

N(19) C(35) N(20) 113.8(22) . . . ?

N(19) C(35) H(44) 126.5 . . . no

N(20) C(35) H(44) 119.5 . . . no

N(20) C(36) C(34) 113.9(22) . . . ?

N(20) C(36) H(45) 130.7 . . . no

C(34) C(36) H(45) 115.4 . . . no

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Cl(3)	O(23)	2.08(7)	. .	no
Cl(3)	O(13)	2.65(7)	. .	no
O(3)	O(20)	2.88(4)	.	2_565 no
O(5)	O(19)	2.77(4)	.	4_454 no
O(6)	O(22)	2.71(6)	. .	no
O(8)	O(19)	2.97(5)	.	4_454 no
O(9)	O(23)	2.17(6)	. .	no
O(10)	O(23)	2.46(7)	. .	no
O(11)	O(23)	1.94(7)	. .	no
O(11)	O(17)	2.47(7)	.	2_565 no
O(11)	O(13)	2.90(8)	. .	no
O(12)	O(13)	1.94(7)	. .	no
O(17)	O(18)	2.82(6)	. .	no
O(18)	O(20)	2.51(5)	. .	no
O(18)	O(22)	2.54(6)	. .	no
O(19)	O(21)	2.48(4)	.	4 no
O(20)	O(23)	2.84(6)	.	2_564 no
N(4)	N(14)	2.72(3)	.	3_455 no

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  N(7)      N(20)     2.703(13)  . . no
  N(10)     N(17)     2.68(3)    . 3_445 no
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# -- ENTER TORSION ANGLES HERE, ONE PER LINE --
# e.g. C1 C2 C3 C4 52.8(1) . . . . yes
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_geom_contact_distance_DA
_geom_angle_DHA
_geom_contact_site_symmetry_A
'N(4)' 'H(7)' 'N(14)' '0.94' '1.78' '2.72(3)' '177.7' '3_455'
'N(7)' 'H(15)' 'N(20)' '0.96' '1.76' '2.71(2)' '167.1' '.'
'N(10)' 'H(23)' 'N(17)' '0.92' '1.79' '2.68(3)' '160.4' '3_445'
#=========================================================================
# Additional structures and associated data_? identifiers
# should be added at this point if there is more than one
# structure analysis in the CIF.
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#      End of CIF
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#===END


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_computing_cell_refinement          'MSC/AFC Diffractometer Control'
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_computing_structure_solution
;SIR92 (Altomare, et. al. 1993);
_computing_structure_refinement     'teXsan for Windows (MSC, 1997)'
_computing_publication_material     'teXsan for Windows (MSC, 1997)'
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_cell_length_b                      20.4455
_cell_length_c                      20.4455
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                    90
_cell_volume                        8546.6(2)
_cell_formula_units_Z               16
_cell_measurement_temperature        293.2
_cell_measurement_reflns_used       25
_cell_measurement_theta_min          11.7
_cell_measurement_theta_max          14.8
#------------------------------------------------------------------------------
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_symmetry_space_group_name_H-M       'I -4 3 d   '
_symmetry_Int_Tables_number          220
_symmetry_space_group_name_Hall      ?
loop_
_symmetry_equiv_pos_as_xyz
  '   +x,    +y,    +z'
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' +x, +y, +z'

' +z, +x, +y'

' +z, +x, +y'

' +y, +z, +x'

' +y, +z, +x'

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

'1/4+x,1/4+z,1/4+y'

'1/4+x,1/4+z,1/4+y'

'1/4+y,1/4+x,1/4+z'

'1/4+y,1/4+x,1/4+z'

'1/4+z,1/4+y,1/4+x'

'1/4+z,1/4+y,1/4+x'

'3/4+x,1/4-z,3/4-y'

'3/4+x,1/4-z,3/4-y'

'3/4+y,1/4-x,3/4-z'

'3/4+y,1/4-x,3/4-z'

'3/4+z,1/4-y,3/4-x'

'3/4+z,1/4-y,3/4-x'

'3/4-x,3/4+z,1/4-y'

'3/4-x,3/4+z,1/4-y'

'3/4-y,3/4+x,1/4-z'

'3/4-y,3/4+x,1/4-z'

'3/4-z,3/4+y,1/4-x'

'3/4-z,3/4+y,1/4-x'

'1/4-x,3/4-z,3/4+y'

'1/4-x,3/4-z,3/4+y'

'1/4-y,3/4-x,3/4+z'

'1/4-y,3/4-x,3/4+z'

'1/4-z,3/4-y,3/4+x'

'1/4-z,3/4-y,3/4+x'

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

'3/4+x,3/4+z,3/4+y'

```
   '3/4+x,3/4+z,3/4+y'
   '3/4+y,3/4+x,3/4+z'
   '3/4+y,3/4+x,3/4+z'
   '3/4+z,3/4+y,3/4+x'
   '3/4+z,3/4+y,3/4+x'
   '1/4+x,3/4-z,1/4-y'
   '1/4+x,3/4-z,1/4-y'
   '1/4+y,3/4-x,1/4-z'
   '1/4+y,3/4-x,1/4-z'
   '1/4+z,3/4-y,1/4-x'
   '1/4+z,3/4-y,1/4-x'
   '1/4-x,1/4+z,3/4-y'
   '1/4-x,1/4+z,3/4-y'
   '1/4-y,1/4+x,3/4-z'
   '1/4-y,1/4+x,3/4-z'
   '1/4-z,1/4+y,3/4-x'
   '1/4-z,1/4+y,3/4-x'
   '3/4-x,1/4-z,1/4+y'
   '3/4-x,1/4-z,1/4+y'
   '3/4-y,1/4-x,1/4+z'
   '3/4-y,1/4-x,1/4+z'
   '3/4-z,1/4-y,1/4+x'
   '3/4-z,1/4-y,1/4+x'
#--------------------------------------------------------------------------
_publ_section_exptl_prep
;   ENTER EXPERIMENTAL SECTION;
_exptl_crystal_description          'prismatic'
_exptl_crystal_colour               'ruby'
_exptl_crystal_size_max               0.30
_exptl_crystal_size_mid               0.20
_exptl_crystal_size_min               0.20
_exptl_crystal_density_diffrn         1.496
_exptl_crystal_density_meas           'not measured'
_chemical_formula_weight              481.40
_chemical_formula_analytical          ?
_chemical_formula_sum                 'C18 H26 Co N10 O2.50 '
```

```
_chemical_formula_moiety              '?'
_chemical_formula_structural          ?
_chemical_compound_source             ?
_exptl_crystal_F_000                  4016.00
_exptl_absorpt_coefficient_mu         0.845
_exptl_absorpt_correction_type
;¥y scans (North,Phillips & Matthews, 1968);
_exptl_absorpt_correction_T_max       0.990
_exptl_absorpt_correction_T_min       0.971
_exptl_special_details
; ?;
#===============================================================================

# EXPERIMENTAL DATA

_diffrn_special_details
; ?;
_diffrn_ambient_temperature           293.2
_diffrn_radiation_wavelength          0.7107
_diffrn_radiation_type                'Mo K¥a'
_diffrn_radiation_source              'X-ray tube'
_diffrn_radiation_monochromator       graphite
_diffrn_radiation_detector            'scintillation counter'
_diffrn_measurement_device            'AFC7R'
_diffrn_measurement_method            ¥w-2¥q

_diffrn_standards_number              3
_diffrn_standards_interval_count      150
_diffrn_standards_decay_%             0.73
loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
   0     0    -4
  -2    -3    -1
  -2     1    -3
```

```
_diffrn_reflns_number                    2769
_reflns_number_total                     2769
_reflns_number_gt                        1425
_reflns_threshold_expression             I>2.00¥s(I)
_diffrn_reflns_av_R_equivalents          0.00000
_diffrn_reflns_av_sigmaI/netI            0.104
_diffrn_reflns_limit_h_min               0
_diffrn_reflns_limit_h_max               26
_diffrn_reflns_limit_k_min               0
_diffrn_reflns_limit_k_max               18
_diffrn_reflns_limit_l_min               0
_diffrn_reflns_limit_l_max               26
_diffrn_reflns_theta_min                 1.41
_diffrn_reflns_theta_max                 27.50
_diffrn_reflns_reduction_process         'Lp corrections applied'
_diffrn_orient_matrix_UB_11              -0.03044
_diffrn_orient_matrix_UB_12              -0.00470
_diffrn_orient_matrix_UB_13              -0.03800
_diffrn_orient_matrix_UB_21              0.01875
_diffrn_orient_matrix_UB_22              0.04049
_diffrn_orient_matrix_UB_23              -0.02003
_diffrn_orient_matrix_UB_31              0.03338
_diffrn_orient_matrix_UB_32              -0.02703
_diffrn_orient_matrix_UB_33              -0.02340
#---------------------------------------------------------------------------
loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
  Co 0     16 0.299 0.973
;International Tables for Crystallography(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1);
  N  0     160 0.004 0.003
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
```

```
  C  0    288 0.002 0.002
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  H  0    416 0.000 0.000
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  O  0     40 0.008 0.006
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);

#=============================================================================

# ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_refinement_flags
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
Co(1) 0.09542(3) 0.0954 0.0954 0.05475(4) 0.333    S Uani d ?
O(1) -0.0173(2) 0.1940(2) 0.3095(3) 0.224(3) 0.833    S Uani d ?
N(1) 0.1931(1) 0.1931 0.1931 0.0621(3) 0.333    S Uani d ?
N(2) 0.0883(2) 0.0897(2) 0.1906(1) 0.056(1) 1.000    .  Uani d ?
N(3) 0.0023(2) 0.0918(2) 0.1032(2) 0.061(1) 1.000    .  Uani d ?
N(4) -0.1081(2) 0.0886(2) 0.0996(3) 0.090(2) 1.000    .  Uani d ?
C(1) 0.1717(2) 0.1580(2) 0.2503(2) 0.072(2) 1.000    .  Uani d ?
C(2) 0.1445(2) 0.0881(2) 0.2352(2) 0.060(1) 1.000    .  Uani d ?
C(3) 0.0302(2) 0.0850(2) 0.2121(2) 0.060(1) 1.000    .  Uani d ?
C(4) -0.0199(2) 0.0871(2) 0.1657(2) 0.064(2) 1.000    .  Uani d ?
C(5) -0.0878(2) 0.0825(2) 0.1638(2) 0.076(2) 1.000    .  Uani d ?
C(6) -0.0532(2) 0.0943(2) 0.0674(2) 0.084(2) 1.000    .  Uani d ?
H(1) 0.2113 0.1558 0.2820 0.084 1.000    .  Uiso c ?
H(2) 0.1410 0.1834 0.2753 0.084 1.000    .  Uiso c ?
```

H(3) 0.1345 0.0677 0.2787 0.065 1.000 . Uiso c ?

H(4) 0.1818 0.0626 0.2195 0.065 1.000 . Uiso c ?

H(5) 0.0197 0.0816 0.2596 0.066 1.000 . Uiso c ?

H(6) -0.1180 0.0774 0.2047 0.096 1.000 . Uiso c ?

H(7) -0.0527 0.1000 0.0172 0.103 1.000 . Uiso c ?

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

Co(1)	0.0547(3)	0.0547	0.0547	-0.0084(3)	-0.0084	-0.0084
O(1)	0.093(4)	0.166(5)	0.414(9)	-0.023(4)	0.072(5)	-0.108(5)
N(1)	0.062(2)	0.0621	0.0621	-0.012(2)	-0.0119	-0.0119
N(2)	0.064(2)	0.049(2)	0.054(2)	0.014(2)	-0.013(2)	0.001(2)
N(3)	0.058(2)	0.055(2)	0.069(3)	-0.013(2)	-0.009(2)	-0.035(2)
N(4)	0.051(2)	0.090(3)	0.128(4)	-0.008(2)	0.001(3)	-0.015(3)
C(1)	0.080(3)	0.084(3)	0.053(2)	0.001(3)	-0.015(3)	-0.010(3)
C(2)	0.075(3)	0.047(3)	0.059(3)	-0.010(3)	-0.006(3)	-0.005(2)
C(3)	0.062(3)	0.059(3)	0.058(3)	0.003(3)	0.016(3)	0.013(3)
C(4)	0.075(4)	0.041(3)	0.077(3)	-0.017(3)	-0.018(3)	-0.015(3)
C(5)	0.057(3)	0.059(3)	0.110(4)	-0.008(3)	-0.004(3)	-0.001(3)
C(6)	0.069(3)	0.075(3)	0.108(4)	-0.008(3)	-0.038(3)	-0.027(3)

#==========

REFINEMENT DATA

_refine_special_details

; ?;

_refine_ls_structure_factor_coef F

_refine_ls_matrix_type full

_refine_ls_weighting_scheme sigma

_refine_ls_weighting_details 'w = 1/[¥s^2^(Fo) + 0.00000|Fo|^2^]'

```
_refine_ls_hydrogen_treatment          noref
_refine_ls_extinction_method           'Zachariasen (1967)'
_refine_ls_extinction_coef             0.000000050(2)
_refine_ls_extinction_expression       'equ(3) Acta Cryst.(1968) A24, p213.'
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?
_refine_ls_number_reflns               1425
_refine_ls_number_parameters           98
_refine_ls_number_restraints           0
_refine_ls_number_constraints          0
_refine_ls_R_factor_all                0.0652
_refine_ls_R_factor_gt                 0.0650
_refine_ls_wR_factor_all               0.0370
_refine_ls_wR_factor_ref               0.0370
_refine_ls_goodness_of_fit_all         2.615
_refine_ls_goodness_of_fit_ref         2.620
_refine_ls_shift/su_max                0.0000
_refine_ls_shift/su_mean               0.0008
_refine_diff_density_min               -0.58
_refine_diff_density_max               0.93

#===============================================================================
# MOLECULAR GEOMETRY
_geom_special_details
; ?;
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Co(1) N(2) 1.955(5) . . ?
 Co(1) N(2) 1.955(5) . . ?
 Co(1) N(2) 1.955(5) . . ?
 Co(1) N(3) 1.911(5) . . ?
```

```
Co(1) N(3) 1.911(5) . . ?
Co(1) N(3) 1.911(5) . . ?
N(1) C(1) 1.440(7) . . ?
N(1) C(1) 1.440(7) . . ?
N(1) C(1) 1.440(7) . . ?
N(2) C(2) 1.467(8) . . ?
N(2) C(3) 1.270(7) . . ?
N(3) C(4) 1.361(8) . . ?
N(3) C(6) 1.351(8) . . ?
N(4) C(5) 1.38(1) . . ?
N(4) C(6) 1.306(8) . . ?
C(1) C(2) 1.56(1) . . ?
C(1) H(1) 1.04 . . no
C(1) H(2) 0.96 . . no
C(2) H(3) 1.00 . . no
C(2) H(4) 0.98 . . no
C(3) C(4) 1.397(8) . . ?
C(3) H(5) 1.00 . . no
C(4) C(5) 1.391(9) . . ?
C(5) H(6) 1.04 . . no
C(6) H(7) 1.03 . . no
#------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
N(2) Co(1) N(2) 97.4(2) . . . ?
N(2) Co(1) N(2) 97.4(2) . . . ?
N(2) Co(1) N(3) 80.8(2) . . . ?
N(2) Co(1) N(3) 89.1(2) . . . ?
N(2) Co(1) N(3) 173.4(3) . . . ?
```

N(2) Co(1) N(2) 97.4(2) 2 2 2 ?

N(2) Co(1) N(3) 173.4(3) 2 2 2 ?

N(2) Co(1) N(3) 80.8(2) 2 2 2 ?

N(2) Co(1) N(3) 89.1(2) 2 2 2 ?

N(2) Co(1) N(3) 89.1(2) 3 3 3 ?

N(2) Co(1) N(3) 173.4(3) 3 3 3 ?

N(2) Co(1) N(3) 80.8(2) 3 3 3 ?

N(3) Co(1) N(3) 92.7(2) . . . ?

N(3) Co(1) N(3) 92.7(2) . . . ?

N(3) Co(1) N(3) 92.7(2) 2 2 2 ?

C(1) N(1) C(1) 120.00(1) . . . ?

C(1) N(1) C(1) 120.00(1) . . . ?

C(1) N(1) C(1) 120.00(1) 2 2 2 ?

Co(1) N(2) C(2) 124.1(5) . . . ?

Co(1) N(2) C(3) 114.8(5) . . . ?

C(2) N(2) C(3) 121.0(6) . . . ?

Co(1) N(3) C(4) 114.4(5) . . . ?

Co(1) N(3) C(6) 142.2(6) . . . ?

C(4) N(3) C(6) 103.3(7) . . . ?

C(5) N(4) C(6) 103.2(6) . . . ?

N(1) C(1) C(2) 113.7(6) . . . ?

N(1) C(1) H(1) 107.1 . . . no

N(1) C(1) H(2) 111.1 . . . no

C(2) C(1) H(1) 111.1 . . . no

C(2) C(1) H(2) 111.4 . . . no

H(1) C(1) H(2) 101.7 . . . no

N(2) C(2) C(1) 112.4(6) . . . ?

N(2) C(2) H(3) 113.6 . . . no

N(2) C(2) H(4) 114.9 . . . no

C(1) C(2) H(3) 106.1 . . . no

C(1) C(2) H(4) 105.9 . . . no

H(3) C(2) H(4) 103.0 . . . no

N(2) C(3) C(4) 116.7(6) . . . ?

N(2) C(3) H(5) 123.0 . . . no

C(4) C(3) H(5) 120.3 . . . no

N(3) C(4) C(3) 113.2(7) . . . ?

```
  N(3) C(4)  C(5) 108.2(7) . . . ?
  C(3) C(4)  C(5) 138.5(9) . . . ?
  N(4) C(5)  C(4) 108.6(7) . . . ?
  N(4) C(5)  H(6) 126.2 . . . no
  C(4) C(5)  H(6) 125.1 . . . no
  N(3) C(6)  N(4) 116.5(7) . . . ?
  N(3) C(6)  H(7) 122.2 . . . no
  N(4) C(6)  H(7) 121.3 . . . no
#------------------------------------------------------------------------------
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
  O(1)      O(1)      2.39(1)    . 34 no
  O(1)      N(4)      2.766(9)   . 46_455 no
#------------------------------------------------------------------------------
loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag
      ? ? ? ? ? ? ? ? ? ?
# -- ENTER TORSION ANGLES HERE, ONE PER LINE --
# e.g. C1 C2 C3 C4 52.8(1) . . . . yes
#------------------------------------------------------------------------------
#==============================================================================
# Additional structures and associated data_? identifiers
```

```
# should be added at this point if there is more than one
# structure analysis in the CIF.
#=============================================================================
#      End of CIF
#=============================================================================
#===END



#-----------------------------------------------------------------------------
data__[C/TITLE_[CoH1.5HL]Cl1.5
#=============================================================================
_computing_data_collection          'MSC/AFC Diffractometer Control'
_computing_cell_refinement          'MSC/AFC Diffractometer Control'
_computing_data_reduction           'teXsan for Windows (MSC, 1997)'
_computing_structure_solution
;SIR92 (Altomare, et. al. 1993);
_computing_structure_refinement     'teXsan for Windows (MSC, 1997)'
_computing_publication_material     'teXsan for Windows (MSC, 1997)'
#-----------------------------------------------------------------------------
_cell_length_a                      12.277(2)
_cell_length_b                      12.2772
_cell_length_c                      9.321(2)
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   120
_cell_volume                        1216.7(2)
_cell_formula_units_Z               2
_cell_measurement_temperature       296.2
_cell_measurement_reflns_used       0
_cell_measurement_theta_min         0.0
_cell_measurement_theta_max         0.0
#-----------------------------------------------------------------------------
_symmetry_cell_setting              trigonal
_symmetry_space_group_name_H-M      'P 3 '
```

```
_symmetry_Int_Tables_number          143
_symmetry_space_group_name_Hall      ?
loop_
_symmetry_equiv_pos_as_xyz
  '  +x,   +y,   +z'
  '  -y,   +x-y,  +z'
  '  -x+y,  -x,   +z'
#-------------------------------------------------------------------
_publ_section_exptl_prep
;   ENTER EXPERIMENTAL SECTION;
_exptl_crystal_description           'NONE'
_exptl_crystal_colour                'orange'
_exptl_crystal_size_max              0.2
_exptl_crystal_size_mid              0.2
_exptl_crystal_size_min              0.2
_exptl_crystal_density_diffrn        1.537
_exptl_crystal_density_meas          'not measured'
_chemical_formula_weight             563.12
_chemical_formula_analytical         ?
_chemical_formula_sum                'C18 H30.50 Cl1.50 Co N10 O4 '
_chemical_formula_moiety             '?'
_chemical_formula_structural         ?
_chemical_compound_source            ?
_exptl_crystal_F_000                 586.00
_exptl_absorpt_coefficient_mu        0.917
_exptl_absorpt_correction_type       ?
_exptl_absorpt_correction_T_max      0.860
_exptl_absorpt_correction_T_min      0.789
_exptl_special_details
; ?;
#===================================================================
# EXPERIMENTAL DATA
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; ?;
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_diffrn_radiation_source	'X-ray tube'
_diffrn_radiation_monochromator	graphite
_diffrn_radiation_detector	'scintillation counter'
_diffrn_measurement_device	'AFC7'
_diffrn_measurement_method	¥w-2¥q
_diffrn_standards_number	0
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_diffrn_standard_refln_index_k	
_diffrn_standard_refln_index_l	
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_reflns_number_total	1655
_reflns_number_gt	1407
_reflns_threshold_expression	I>2.00¥s(I)
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_diffrn_reflns_av_sigmaI/netI	0.073
_diffrn_reflns_limit_h_min	-12
_diffrn_reflns_limit_h_max	12
_diffrn_reflns_limit_k_min	0
_diffrn_reflns_limit_k_max	14
_diffrn_reflns_limit_l_min	0
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_diffrn_reflns_theta_min	13.53
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_diffrn_reflns_reduction_process	'Lp corrections applied'
_diffrn_orient_matrix_UB_11	0.00000
_diffrn_orient_matrix_UB_12	0.00000
_diffrn_orient_matrix_UB_13	0.00000
_diffrn_orient_matrix_UB_21	0.00000
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_diffrn_orient_matrix_UB_31	0.00000

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_atom_type_number_in_cell
_atom_type_scat_dispersion_real
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;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  H  0     61 0.000 0.000
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  N  0     20 0.004 0.003
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  Cl 0      3 0.132 0.159
;International Tables for Crystallography(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1);
  Co 0      2 0.299 0.973
;International Tables for Crystallography(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1);
  O  0      8 0.008 0.006
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# ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_occupancy
_atom_site_refinement_flags
_atom_site_adp_type
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_atom_site_calc_flag

_atom_site_calc_attached_atom

Co(1) -0.3333 0.3333 0.8112 0.0221(3) 0.333 S Uani d ?

Co(2) 0.3333 0.6667 0.6284(3) 0.0212(3) 0.333 S Uani d ?

Cl(1) 0.2709(9) 0.2705(8) 0.2195(13) 0.192(4) 1.000 . Uani d ?

O(1) 0.0000 0.0000 1.203(5) 0.180(7) 0.333 S Uani d ?

O(2) 0.079(2) 0.080(2) 0.724(4) 0.054(7) 0.333 S Uani d ?

O(3) 0.1794(12) 0.1440(12) 0.514(2) 0.131(6) 1.000 . Uani d ?

O(4) -0.1790(13) -0.0342(11) 0.923(2) 0.137(6) 1.000 . Uani d ?

N(1) -0.3333 0.3333 0.447(2) 0.041(3) 0.333 S Uani d ?

N(2) -0.2917(8) 0.2203(7) 0.7067(9) 0.028(2) 1.000 . Uani d ?

N(3) -0.1944(7) 0.3582(7) 0.9260(8) 0.024(2) 1.000 . Uani d ?

N(4) -0.0582(8) 0.3762(8) 1.0917(9) 0.039(2) 1.000 . Uani d ?

N(5) 0.3333 0.6667 0.995(2) 0.036(3) 0.333 S Uani d ?

N(6) 0.2913(8) 0.5118(8) 0.7365(8) 0.027(2) 1.000 . Uani d ?

N(7) 0.1953(7) 0.5529(7) 0.5139(8) 0.025(2) 1.000 . Uani d ?

N(8) 0.0577(8) 0.4332(8) 0.3496(9) 0.038(2) 1.000 . Uani d ?

C(1) -0.3185(10) 0.2248(11) 0.4432(10) 0.037(3) 1.000 . Uani d ?

C(2) -0.3586(9) 0.1460(9) 0.5779(10) 0.033(3) 1.000 . Uani d ?

C(3) -0.2035(10) 0.2083(11) 0.7645(13) 0.029(3) 1.000 . Uani d ?

C(4) -0.1469(8) 0.2805(9) 0.8876(9) 0.028(2) 1.000 . Uani d ?

C(5) -0.0619(10) 0.2933(10) 0.9914(12) 0.041(3) 1.000 . Uani d ?

C(6) -0.1389(11) 0.4138(10) 1.0503(12) 0.030(3) 1.000 . Uani d ?

C(7) 0.3203(10) 0.5438(10) 0.9982(11) 0.039(3) 1.000 . Uani d ?

C(8) 0.3586(10) 0.5043(9) 0.8624(10) 0.034(3) 1.000 . Uani d ?

C(9) 0.2027(12) 0.4110(12) 0.680(1) 0.035(4) 1.000 . Uani d ?

C(10) 0.1469(9) 0.4275(8) 0.5523(10) 0.030(2) 1.000 . Uani d ?

C(11) 0.0624(10) 0.3564(10) 0.4487(12) 0.041(3) 1.000 . Uani d ?

C(12) 0.1391(11) 0.5514(12) 0.392(1) 0.037(3) 1.000 . Uani d ?

H(1) -0.3665 0.1740 0.3656 0.043 1.000 . Uiso c ?

H(2) -0.2316 0.2538 0.4269 0.043 1.000 . Uiso c ?

H(3) -0.4459 0.1121 0.5915 0.041 1.000 . Uiso c ?

H(4) -0.3403 0.0798 0.5672 0.041 1.000 . Uiso c ?

H(5) -0.1767 0.1532 0.7251 0.035 1.000 . Uiso c ?

H(6) -0.0134 0.2508 0.9915 0.047 1.000 . Uiso c ?

H(7) -0.1557 0.4708 1.1008 0.034 1.000 . Uiso c ?

H(8) -0.0078 0.4025 1.1755 0.047 1.000 . Uiso c ?

H(9) 0.3700 0.5418 1.0743 0.047 1.000 . Uiso c ?

H(10) 0.2340 0.4846 1.0157 0.047 1.000 . Uiso c ?

H(11) 0.3416 0.4207 0.8728 0.041 1.000 . Uiso c ?

H(12) 0.4463 0.5590 0.8476 0.041 1.000 . Uiso c ?

H(13) 0.1761 0.3294 0.7191 0.041 1.000 . Uiso c ?

H(14) 0.0136 0.2650 0.4471 0.049 1.000 . Uiso c ?

H(15) 0.1534 0.6238 0.3425 0.044 1.000 . Uiso c ?

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_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

Co(1)	0.0248(8)	0.0248	0.0168(12)	0.0124	0.0000	0.0000
Co(2)	0.0247(8)	0.0247	0.0144(12)	0.0123	0.0000	0.0000
Cl(1)	0.226(9)	0.218(9)	0.178(7)	0.145(7)	0.002(8)	-0.006(7)
O(1)	0.21(2)	0.2107	0.12(2)	0.1054	0.0000	0.0000
O(2)	0.019(13)	0.019(13)	0.10(2)	-0.007(7)	-0.001(12)	0.010(12)
O(3)	0.093(9)	0.099(10)	0.22(2)	0.064(8)	-0.038(10)	-0.025(11)
O(4)	0.114(11)	0.064(7)	0.23(2)	0.045(8)	-0.050(11)	-0.022(10)
N(1)	0.041(7)	0.0410	0.040(12)	0.0205	0.0000	0.0000
N(2)	0.033(5)	0.024(4)	0.026(4)	0.013(4)	-0.000(4)	-0.003(4)
N(3)	0.029(4)	0.028(4)	0.017(4)	0.015(4)	-0.003(3)	-0.003(3)
N(4)	0.034(5)	0.041(5)	0.036(5)	0.015(4)	-0.021(4)	-0.007(4)
N(5)	0.038(6)	0.0376	0.032(11)	0.0188	0.0000	0.0000
N(6)	0.034(5)	0.035(4)	0.016(4)	0.020(4)	-0.006(4)	0.000(3)
N(7)	0.024(4)	0.031(4)	0.022(4)	0.015(3)	-0.006(3)	0.002(3)
N(8)	0.039(5)	0.048(5)	0.031(5)	0.024(4)	-0.014(4)	-0.015(4)
C(1)	0.047(6)	0.058(7)	0.014(5)	0.032(6)	-0.010(4)	-0.010(4)
C(2)	0.039(6)	0.036(5)	0.027(5)	0.020(5)	-0.014(4)	-0.014(4)
C(3)	0.031(6)	0.032(6)	0.028(7)	0.018(6)	-0.006(5)	-0.003(5)
C(4)	0.033(5)	0.038(5)	0.017(4)	0.020(4)	-0.001(4)	0.001(4)

C(5)	0.037(6)	0.048(6)	0.045(6)	0.026(5)	-0.009(5)	0.006(5)
C(6)	0.039(6)	0.034(6)	0.013(5)	0.016(5)	-0.006(4)	-0.007(4)
C(7)	0.047(7)	0.047(6)	0.025(5)	0.025(5)	-0.010(5)	0.004(5)
C(8)	0.045(6)	0.035(5)	0.026(5)	0.024(5)	-0.007(4)	0.001(4)
C(9)	0.040(7)	0.033(7)	0.027(7)	0.014(6)	-0.001(5)	0.007(5)
C(10)	0.032(5)	0.027(5)	0.026(5)	0.013(4)	-0.005(4)	-0.001(4)
C(11)	0.041(6)	0.034(6)	0.042(6)	0.015(5)	-0.012(5)	-0.013(5)
C(12)	0.033(6)	0.044(7)	0.038(7)	0.022(5)	-0.006(5)	0.001(5)

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 Co(1) N(2) 1.961(9) . . ?
 Co(1) N(2) 1.961(9) . . ?
 Co(1) N(3) 1.905(8) . . ?
 Co(1) N(3) 1.905(8) . . ?
 Co(1) N(3) 1.905(8) . . ?
 Co(2) N(6) 1.980(9) . . ?
 Co(2) N(6) 1.980(9) . . ?
 Co(2) N(6) 1.980(9) . . ?
 Co(2) N(7) 1.896(8) . . ?
 Co(2) N(7) 1.896(8) . . ?
 Co(2) N(7) 1.896(8) . . ?
 O(2) O(2) 1.70(3) . . ?
 O(2) O(2) 1.70(3) . . ?
 N(1) C(1) 1.433(12) . . ?
 N(1) C(1) 1.433(12) . . ?
 N(1) C(1) 1.433(12) . . ?
 N(2) C(2) 1.483(12) . . ?
 N(2) C(3) 1.28(1) . . ?
 N(3) C(4) 1.391(12) . . ?
 N(3) C(6) 1.344(13) . . ?
 N(4) C(5) 1.37(2) . . ?
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N(4) C(6) 1.34(2) . . ?

N(4) H(8) 0.95 . . no

N(5) C(7) 1.435(12) . . ?

N(5) C(7) 1.435(12) . . ?

N(5) C(7) 1.435(12) . . ?

N(6) C(8) 1.463(12) . . ?

N(6) C(9) 1.28(2) . . ?

N(7) C(10) 1.391(13) . . ?

N(7) C(12) 1.32(2) . . ?

N(8) C(11) 1.34(2) . . ?

N(8) C(12) 1.35(2) . . ?

C(1) C(2) 1.51(2) . . ?

C(1) H(1) 0.95 . . no

C(1) H(2) 0.95 . . no

C(2) H(3) 0.94 . . no

C(2) H(4) 0.95 . . no

C(3) C(4) 1.40(2) . . ?

C(3) H(5) 0.96 . . no

C(4) C(5) 1.37(1) . . ?

C(5) H(6) 0.97 . . no

C(6) H(7) 0.95 . . no

C(7) C(8) 1.51(2) . . ?

C(7) H(9) 0.94 . . no

C(7) H(10) 0.95 . . no

C(8) H(11) 0.94 . . no

C(8) H(12) 0.95 . . no

C(9) C(10) 1.44(2) . . ?

C(9) H(13) 0.96 . . no

C(10) C(11) 1.37(1) . . ?

C(11) H(14) 0.97 . . no

C(12) H(15) 0.94 . . no

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N(2) Co(1) N(2) 97.5(3) . . . ?

N(2) Co(1) N(2) 97.5(3) . . . ?

N(2) Co(1) N(3) 82.1(3) . . . ?

N(2) Co(1) N(3) 88.9(4) . . . ?

N(2) Co(1) N(3) 173.6(4) . . . ?

N(2) Co(1) N(2) 97.5(3) 3_455 3_455 3_455 ?

N(2) Co(1) N(3) 173.6(4) 3_455 3_455 3_455 ?

N(2) Co(1) N(3) 82.1(3) 3_455 3_455 3_455 ?

N(2) Co(1) N(3) 88.9(4) 3_455 3_455 3_455 ?

N(2) Co(1) N(3) 88.9(4) 2_565 2_565 2_565 ?

N(2) Co(1) N(3) 173.6(4) 2_565 2_565 2_565 ?

N(2) Co(1) N(3) 82.1(3) 2_565 2_565 2_565 ?

N(3) Co(1) N(3) 91.5(3) . . . ?

N(3) Co(1) N(3) 91.5(3) . . . ?

N(3) Co(1) N(3) 91.5(3) 3_455 3_455 3_455 ?

N(6) Co(2) N(6) 96.4(3) . . . ?

N(6) Co(2) N(6) 96.4(3) . . . ?

N(6) Co(2) N(7) 82.6(3) . . . ?

N(6) Co(2) N(7) 173.9(4) . . . ?

N(6) Co(2) N(7) 89.7(4) . . . ?

N(6) Co(2) N(6) 96.4(3) 3_565 3_565 3_565 ?

N(6) Co(2) N(7) 89.7(4) 3_565 3_565 3_565 ?

N(6) Co(2) N(7) 82.6(3) 3_565 3_565 3_565 ?

N(6) Co(2) N(7) 173.9(4) 3_565 3_565 3_565 ?

N(6) Co(2) N(7) 173.9(4) 2_665 2_665 2_665 ?

N(6) Co(2) N(7) 89.7(4) 2_665 2_665 2_665 ?

N(6) Co(2) N(7) 82.6(3) 2_665 2_665 2_665 ?

N(7) Co(2) N(7) 91.4(3) . . . ?

N(7) Co(2) N(7) 91.4(3) . . . ?

N(7) Co(2) N(7) 91.4(3) 3_565 3_565 3_565 ?

O(2) O(2) O(2) 60.00 2 2 2 ?

C(1) N(1) C(1) 119.95(7) . . . ?

C(1) N(1) C(1) 119.95(7) . . . ?

C(1) N(1) C(1) 119.95(7) 3_455 3_455 3_455 ?

Co(1) N(2) C(2) 125.2(7) . . . ?

Co(1) N(2) C(3) 114.0(8) . . . ?

C(2) N(2) C(3) 120.7(9) . . . ?

Co(1) N(3) C(4) 113.2(6) . . . ?

Co(1) N(3) C(6) 138.7(8) . . . ?

C(4) N(3) C(6) 106.9(9) . . . ?

C(5) N(4) C(6) 107.7(9) . . . ?

C(5) N(4) H(8) 126.3 . . . no

C(6) N(4) H(8) 126.0 . . . no

C(7) N(5) C(7) 119.95(7) . . . ?

C(7) N(5) C(7) 119.95(7) . . . ?

C(7) N(5) C(7) 119.95(7) 3_565 3_565 3_565 ?

Co(2) N(6) C(8) 125.7(7) . . . ?

Co(2) N(6) C(9) 113.9(8) . . . ?

C(8) N(6) C(9) 120.1(10) . . . ?

Co(2) N(7) C(10) 113.6(6) . . . ?

Co(2) N(7) C(12) 139.5(8) . . . ?

C(10) N(7) C(12) 105.9(9) . . . ?

C(11) N(8) C(12) 106.5(9) . . . ?

N(1) C(1) C(2) 115.2(11) . . . ?

N(1) C(1) H(1) 107.7 . . . no

N(1) C(1) H(2) 107.2 . . . no

C(2) C(1) H(1) 108.5 . . . no

C(2) C(1) H(2) 108.5 . . . no

H(1) C(1) H(2) 109.6 . . . no

N(2) C(2) C(1) 112.1(8) . . . ?

N(2) C(2) H(3) 108.7 . . . no

N(2) C(2) H(4) 108.4 . . . no

C(1) C(2) H(3) 109.2 . . . no

C(1) C(2) H(4) 108.6 . . . no

H(3) C(2) H(4) 109.8 . . . no

N(2) C(3) C(4) 116.8(11) . . . ?

N(2) C(3) H(5) 121.8 . . . no

C(4) C(3) H(5) 121.4 . . . no

N(3) C(4) C(3) 113.6(9) . . . ?

N(3) C(4) C(5) 107.2(9) . . . ?

C(3) C(4) C(5) 139.1(11) . . . ?

N(4) C(5) C(4) 107.9(9) . . . ?

N(4) C(5) H(6) 126.9 . . . no

C(4) C(5) H(6) 125.2 . . . no

N(3) C(6) N(4) 110.3(10) . . . ?

N(3) C(6) H(7) 124.2 . . . no

N(4) C(6) H(7) 125.5 . . . no

N(5) C(7) C(8) 115.4(11) . . . ?

N(5) C(7) H(9) 108.1 . . . no

N(5) C(7) H(10) 107.6 . . . no

C(8) C(7) H(9) 108.2 . . . no

C(8) C(7) H(10) 107.7 . . . no

H(9) C(7) H(10) 109.8 . . . no

N(6) C(8) C(7) 112.1(8) . . . ?

N(6) C(8) H(11) 109.0 . . . no

N(6) C(8) H(12) 108.3 . . . no

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C(7) C(8) H(12) 108.6 . . . no

H(11) C(8) H(12) 109.7 . . . no

N(6) C(9) C(10) 116.0(11) . . . ?

N(6) C(9) H(13) 122.3 . . . no

C(10) C(9) H(13) 121.7 . . . no

N(7) C(10) C(9) 113.5(9) . . . ?

N(7) C(10) C(11) 107.0(9) . . . ?

C(9) C(10) C(11) 139.4(11) . . . ?

N(8) C(11) C(10) 108.9(9) . . . ?

N(8) C(11) H(14) 125.6 . . . no

C(10) C(11) H(14) 125.5 . . . no

N(7) C(12) N(8) 111.7(11) . . . ?

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N(8) C(12) H(15) 124.1 . . . no

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 _geom_contact_site_symmetry_1
 _geom_contact_site_symmetry_2
 _geom_contact_publ_flag
  O(2)    O(4)    2.14(4)   . 3 no
  O(2)    O(3)    2.23(4)   . . no
  N(4)    N(8)    2.701(11) . 1_556 no
#------------------------------------------------------------------------------
loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion
 _geom_torsion_publ_flag
      ? ? ? ? ? ???? ?
# -- ENTER TORSION ANGLES HERE, ONE PER LINE --
# e.g. C1 C2 C3 C4 52.8(1) . . . . yes
#------------------------------------------------------------------------------
loop_
 _geom_bond_atom_site_label_D
 _geom_bond_atom_site_label_H
 _geom_contact_atom_site_label_A
 _geom_bond_distance_DH
 _geom_contact_distance_HA
 _geom_contact_distance_DA
 _geom_angle_DHA
 _geom_contact_site_symmetry_A
'N(4)' 'H(8)' 'N(8)' '0.95' '1.77' '2.701(11)' '168.7' '1_556'
```

```
#=============================================================================
# Additional structures and associated data_? identifiers
# should be added at this point if there is more than one
# structure analysis in the CIF.
#=============================================================================
#       End of CIF
#=============================================================================
#===END


#-----------------------------------------------------------------------------
data__[CoH3L2](ClO4)30.5H2O


#=============================================================================
_computing_data_collection              'MSC/AFC Diffractometer Control'
_computing_cell_refinement              'MSC/AFC Diffractometer Control'
_computing_data_reduction               'teXsan for Windows (MSC, 1997)'
_computing_structure_solution
;'DIRDIF92 PATTY (Beurskens, 1992);
_computing_structure_refinement         'teXsan for Windows (MSC, 1997)'
_computing_publication_material         'teXsan for Windows (MSC, 1997)'
#-----------------------------------------------------------------------------
_cell_length_a                          13.195(4)
_cell_length_b                          13.873(5)
_cell_length_c                          33.930(4)
_cell_angle_alpha                       90
_cell_angle_beta                        96.39(2)
_cell_angle_gamma                       90
_cell_volume                            6172(3)
_cell_formula_units_Z                   8
_cell_measurement_temperature           293.2
_cell_measurement_reflns_used           25
_cell_measurement_theta_min             13.8
_cell_measurement_theta_max             16.5
#-----------------------------------------------------------------------------
_symmetry_cell_setting                  monoclinic
```

```
_symmetry_space_group_name_H-M          'P 21/c        '
_symmetry_Int_Tables_number             14
_symmetry_space_group_name_Hall         ?
loop_
_symmetry_equiv_pos_as_xyz
   '    +x,     +y,     +z'
   '    -x,1/2+y,1/2-z'
   '    -x,     -y,     -z'
   '    +x,1/2-y,1/2+z'
#---------------------------------------------------------------------------
_publ_section_exptl_prep
;      ENTER EXPERIMENTAL SECTION;
_exptl_crystal_description              'prismatic'
_exptl_crystal_colour                   'darkred'
_exptl_crystal_size_max                 0.40
_exptl_crystal_size_mid                 0.30
_exptl_crystal_size_min                 0.20
_exptl_crystal_density_diffrn           1.698
_exptl_crystal_density_meas             'not measured'
_chemical_formula_weight                788.83
_chemical_formula_analytical            ?
_chemical_formula_sum                   'C21 H31 Cl3 Co N10 O12.50 '
_chemical_formula_moiety                '?'
_chemical_formula_structural            ?
_chemical_compound_source               ?
_exptl_crystal_F_000                    3240.00
_exptl_absorpt_coefficient_mu           0.895
_exptl_absorpt_correction_type
;¥y scans (North,Phillips & Matthews, 1968);
_exptl_absorpt_correction_T_max         1.000
_exptl_absorpt_correction_T_min         0.804
_exptl_special_details
; ?;
#===========================================================================
# EXPERIMENTAL DATA
_diffrn_special_details
```

; ?;

_diffrn_ambient_temperature 293.2

_diffrn_radiation_wavelength 0.7107

_diffrn_radiation_type 'Mo K¥a'

_diffrn_radiation_source 'X-ray tube'

_diffrn_radiation_monochromator graphite

_diffrn_radiation_detector 'scintillation counter'

_diffrn_measurement_device 'AFC7R'

_diffrn_measurement_method ¥w-2¥q

_diffrn_standards_number 3

_diffrn_standards_interval_count 150

_diffrn_standards_decay_% -0.66

loop_

_diffrn_standard_refln_index_h

_diffrn_standard_refln_index_k

_diffrn_standard_refln_index_l

0 2 3

0 2 4

-1 2 -3

_diffrn_reflns_number 11361

_reflns_number_total 10851

_reflns_number_gt 7021

_reflns_threshold_expression I>2.00¥s(I)

_diffrn_reflns_av_R_equivalents 0.02081

_diffrn_reflns_av_sigmaI/netI ?

_diffrn_reflns_limit_h_min 0

_diffrn_reflns_limit_h_max 15

_diffrn_reflns_limit_k_min 0

_diffrn_reflns_limit_k_max 16

_diffrn_reflns_limit_l_min -40

_diffrn_reflns_limit_l_max 40

_diffrn_reflns_theta_min 1.47

_diffrn_reflns_theta_max 25.00

_diffrn_reflns_reduction_process 'Lp corrections applied'

_diffrn_orient_matrix_UB_11 -0.06392

_diffrn_orient_matrix_UB_12 0.03452

```
_diffrn_orient_matrix_UB_13          0.00493
_diffrn_orient_matrix_UB_21          0.02023
_diffrn_orient_matrix_UB_22         -0.00435
_diffrn_orient_matrix_UB_23          0.02924
_diffrn_orient_matrix_UB_31          0.03634
_diffrn_orient_matrix_UB_32          0.06313
_diffrn_orient_matrix_UB_33         -0.00068
#---------------------------------------------------------------------------
loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
  C  0    168 0.002 0.002
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  H  0    248 0.000 0.000
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  N  0     80 0.004 0.003
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  O  0    100 0.008 0.006
;International Tables for Crystallography(1992, Vol. C, Table 6.1.1.2);
  Cl 0     24 0.132 0.159
;International Tables for Crystallography(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1);
  Co 0      8 0.299 0.973
;International Tables for Crystallography(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1);
#===========================================================================
# ATOMIC COORDINATES AND THERMAL PARAMETERS
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
```

_atom_site_refinement_flags

_atom_site_adp_type

_atom_site_calc_flag

_atom_site_calc_attached_atom

Co(1) 0.00719(4) 0.02994(4) 0.13236(2) 0.0322(2) 1.000 . Uani d ?

Co(2) -0.52491(4) 0.56839(4) 0.11300(2) 0.0317(2) 1.000 . Uani d ?

Cl(1) 0.2991(1) 0.36578(9) 0.27912(4) 0.0533(4) 1.000 . Uani d ?

Cl(2) -0.1463(1) 0.52940(9) 0.02524(4) 0.0553(4) 1.000 . Uani d ?

Cl(3) -1.0510(1) 0.4756(1) 0.17621(4) 0.0574(4) 1.000 . Uani d ?

Cl(4) -0.29833(9) 0.28188(8) 0.26772(4) 0.0515(4) 1.000 . Uani d ?

Cl(5) -0.58266(9) 0.09131(8) 0.15200(4) 0.0465(4) 1.000 . Uani d ?

Cl(6) -0.2841(1) 0.1091(1) 0.00346(5) 0.0890(6) 1.000 . Uani d ?

O(1) 0.3302(3) 0.3063(3) 0.2498(1) 0.128(2) 1.000 . Uani d ?

O(2) 0.2110(3) 0.4156(3) 0.2661(1) 0.147(2) 1.000 . Uani d ?

O(3) 0.3794(3) 0.4221(3) 0.2914(2) 0.175(2) 1.000 . Uani d ?

O(4) 0.2769(4) 0.3114(4) 0.3093(2) 0.192(3) 1.000 . Uani d ?

O(5) -0.1228(3) 0.4311(2) 0.0205(1) 0.093(1) 1.000 . Uani d ?

O(6) -0.2535(3) 0.5406(3) 0.0205(1) 0.109(2) 1.000 . Uani d ?

O(7) -0.1082(3) 0.5822(3) -0.0054(1) 0.099(2) 1.000 . Uani d ?

O(8) -0.1055(3) 0.5627(3) 0.0633(1) 0.106(2) 1.000 . Uani d ?

O(9) -1.0038(3) 0.4549(3) 0.1416(1) 0.085(1) 1.000 . Uani d ?

O(10) -1.1561(3) 0.4719(3) 0.1677(1) 0.115(2) 1.000 . Uani d ?

O(11) -1.0224(3) 0.4091(3) 0.2062(1) 0.119(2) 1.000 . Uani d ?

O(12) -1.0203(4) 0.5664(3) 0.1899(1) 0.165(2) 1.000 . Uani d ?

O(13) -0.3803(3) 0.3371(2) 0.2799(1) 0.084(1) 1.000 . Uani d ?

O(14) -0.2313(3) 0.2565(3) 0.3011(1) 0.109(2) 1.000 . Uani d ?

O(15) -0.3372(2) 0.1962(2) 0.24830(9) 0.062(1) 1.000 . Uani d ?

O(16) -0.2469(3) 0.3386(2) 0.2406(1) 0.086(1) 1.000 . Uani d ?

O(17) -0.6485(3) 0.1626(3) 0.1330(1) 0.093(1) 1.000 . Uani d ?

O(18) -0.5546(2) 0.0265(2) 0.12226(9) 0.070(1) 1.000 . Uani d ?

O(19) -0.6354(3) 0.0409(3) 0.1799(1) 0.094(2) 1.000 . Uani d ?

O(20) -0.4941(2) 0.1347(2) 0.1718(1) 0.081(1) 1.000 . Uani d ?

O(21) -0.3089(8) 0.1297(8) 0.0379(2) 0.176(5) 0.660 S Uani d ?

O(22) -0.2816(9) 0.2095(6) 0.0074(3) 0.220(5) 0.660 S Uani d ?

O(23) -0.3275(3) 0.1126(5) -0.0337(1) 0.168(3) 1.000 . Uani d ?

O(24) -0.3419(8) 0.0258(7) 0.0184(3) 0.194(5) 0.660 S Uani d ?