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data_co(tza)2 (3)

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_chemical_name_systematic
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;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C6 H6 Co N8 O4'
_chemical_formula_weight          313.12

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 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Co'  'Co'   0.3494   0.9721
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            monoclinic
_symmetry_space_group_name_H-M    P2(1)/n

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x□, y□, -z□'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                    4.871(3)
_cell_length_b                    13.287(7)
_cell_length_c                    7.795(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  103.953(11)
_cell_angle_gamma                 90.00
_cell_volume                      489.7(5)
_cell_formula_units_Z             2
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     1297
_cell_measurement_theta_min       3.0662
_cell_measurement_theta_max       27.4719

_exptl_crystal_description        Prism
_exptl_crystal_colour             Red
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_exptl_crystal_density_diffrn    2.124
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             314
_exptl_absorpt_coefficient_mu    1.785
_exptl_absorpt_correction_type   Multi-scan
_exptl_absorpt_correction_T_min  0.8311
_exptl_absorpt_correction_T_max  1.0000
_exptl_absorpt_process_details   ?

_exptl_special_details
;
????
;

_diffrn_ambient_temperature      293(2)
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_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  Mercury
_diffrn_measurement_method       CCD_Profile_fitting
_diffrn_detector_area_resol_mean 14.6306
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_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?
_diffrn_reflns_number            3737
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_diffrn_reflns_av_sigmaI/netI    0.0232
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_diffrn_reflns_limit_k_min       -17
_diffrn_reflns_limit_k_max       17
_diffrn_reflns_limit_l_min       -10
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_diffrn_reflns_theta_min         3.07
_diffrn_reflns_theta_max         27.48
_reflns_number_total             1124
_reflns_number_gt                997
_reflns_threshold_expression     >2sigma(I)

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_computing_cell_refinement       'CrystalClear (Rigaku/MSC Inc., 2005)'
_computing_data_reduction        'CrystalClear (Rigaku/MSC Inc., 2005)'
_computing_structure_solution    'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics    ?
_computing_publication_material  ?

_refine_special_details
;
 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_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)(0.0397P)^2^.7230P] where P=(Fo^2^▪^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          1124
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_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0319
_refine_ls_wR_factor_ref          0.0997
_refine_ls_wR_factor_gt           0.0969
_refine_ls_goodness_of_fit_ref    1.003
_refine_ls_restrained_S_all       1.003
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 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Co1 Co 0.0000 1.0000 1.0000 0.01470(19) Uani 1 2 d S . .
O1 O -0.2230(5) 1.51215(15) 1.3348(3) 0.0209(5) Uani 1 1 d . . .
O2 O 0.1819(4) 1.45623(17) 1.2811(3) 0.0217(5) Uani 1 1 d . . .
N1 N -0.1076(5) 1.31110(18) 1.0553(3) 0.0178(5) Uani 1 1 d . . .
N2 N 0.0846(6) 1.3147(2) 0.9571(4) 0.0265(6) Uani 1 1 d . . .
N3 N 0.1743(6) 1.2236(2) 0.9481(4) 0.0271(6) Uani 1 1 d . . .
N4 N 0.0436(5) 1.16028(19) 1.0392(4) 0.0205(5) Uani 1 1 d . . .
C1 C -0.1299(7) 1.2162(2) 1.1033(4) 0.0223(6) Uani 1 1 d . . .
H1A H -0.2495 1.1931 1.1714 0.027 Uiso 1 1 calc R . .
C2 C -0.2526(6) 1.4014(2) 1.0944(4) 0.0202(6) Uani 1 1 d . . .
H2B H -0.4324 1.3821 1.1174 0.024 Uiso 1 1 calc R . .
H2A H -0.2915 1.4449 0.9915 0.024 Uiso 1 1 calc R . .
C3 C -0.0814(6) 1.4605(2) 1.2537(4) 0.0157(6) Uani 1 1 d . . .
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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Co1 0.0142(3) 0.0131(3) 0.0185(3) 0.0015(2) 0.0074(2) 0.00088(19)
O1 0.0216(11) 0.0194(10) 0.0258(12) -0.0026(9) 0.0138(9) 0.0011(8)
O2 0.0144(10) 0.0276(11) 0.0235(11) -0.0068(9) 0.0056(8) -0.0011(8)
N1 0.0189(12) 0.0154(12) 0.0200(12) -0.0028(9) 0.0062(10) -0.0007(9)
N2 0.0327(15) 0.0182(13) 0.0349(16) 0.0002(11) 0.0205(13) -0.0010(11)
N3 0.0287(15) 0.0193(13) 0.0389(16) -0.0008(12) 0.0189(13) -0.0015(11)
N4 0.0217(13) 0.0177(12) 0.0252(13) -0.0006(10) 0.0119(11) -0.0009(10)
C1 0.0255(16) 0.0163(13) 0.0296(16) -0.0024(12) 0.0153(13) -0.0017(12)
C2 0.0180(14) 0.0158(13) 0.0267(16) -0.0035(11) 0.0053(12) 0.0021(11)
C3 0.0175(13) 0.0120(12) 0.0194(14) 0.0006(10) 0.0079(11) -0.0006(10)

_geom_special_details
;
 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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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Co1 O1 2.084(2) 2_447 ?
Co1 O1 2.084(2) 4_685 ?
Co1 O2 2.092(2) 4_585 ?
Co1 O2 2.092(2) 2_547 ?
Co1 N4 2.155(3) 3_577 ?
Co1 N4 2.155(3) . ?
O1 C3 1.248(4) . ?
O1 Co1 2.084(2) 2_457 ?
O2 C3 1.250(4) . ?
O2 Co1 2.092(2) 2_557 ?
N1 C1 1.327(4) . ?
N1 N2 1.346(4) . ?
N1 C2 1.462(4) . ?
N2 N3 1.295(4) . ?
N3 N4 1.355(4) . ?
N4 C1 1.311(4) . ?
C1 H1A 0.9300 . ?
C2 C3 1.534(4) . ?
C2 H2B 0.9700 . ?
C2 H2A 0.9700 . ?
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 _geom_angle_atom_site_label_3
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O1 Co1 O1 180.000(1) 2_447 4_685 ?
O1 Co1 O2 91.14(10) 2_447 4_585 ?
O1 Co1 O2 88.86(10) 4_685 4_585 ?
O1 Co1 O2 88.86(10) 2_447 2_547 ?
O1 Co1 O2 91.14(10) 4_685 2_547 ?
O2 Co1 O2 180.000(1) 4_585 2_547 ?
O1 Co1 N4 96.19(9) 2_447 3_577 ?
O1 Co1 N4 83.81(9) 4_685 3_577 ?
O2 Co1 N4 97.52(10) 4_585 3_577 ?
O2 Co1 N4 82.48(10) 2_547 3_577 ?
O1 Co1 N4 83.81(9) 2_447 . ?
O1 Co1 N4 96.19(9) 4_685 . ?
O2 Co1 N4 82.48(10) 4_585 . ?
O2 Co1 N4 97.52(10) 2_547 . ?
N4 Co1 N4 180.000(1) 3_577 . ?
C3 O1 Co1 142.15(19) . 2_457 ?
C3 O2 Co1 130.9(2) . 2_557 ?
C1 N1 N2 108.1(2) . . ?
C1 N1 C2 130.2(3) . . ?
N2 N1 C2 121.8(2) . . ?
N3 N2 N1 106.7(2) . . ?
N2 N3 N4 110.2(3) . . ?
C1 N4 N3 106.0(3) . . ?
C1 N4 Co1 124.3(2) . . ?
N3 N4 Co1 125.61(19) . . ?
N4 C1 N1 109.1(3) . . ?
N4 C1 H1A 125.5 . . ?
N1 C1 H1A 125.5 . . ?
N1 C2 C3 113.1(2) . . ?
N1 C2 H2B 108.9 . . ?
C3 C2 H2B 108.9 . . ?
N1 C2 H2A 108.9 . . ?
C3 C2 H2A 108.9 . . ?
H2B C2 H2A 107.8 . . ?
O1 C3 O2 127.4(3) . . ?
O1 C3 C2 115.6(3) . . ?
O2 C3 C2 116.8(3) . . ?

loop_
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 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
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C1 N1 N2 N3 -0.2(4) . . . . ?
C2 N1 N2 N3 179.5(3) . . . . ?
N1 N2 N3 N4 0.0(4) . . . . ?
N2 N3 N4 C1 0.3(4) . . . . ?
N2 N3 N4 Co1 158.1(2) . . . . ?
O1 Co1 N4 C1 -15.5(3) 2_447 . . . ?
O1 Co1 N4 C1 164.5(3) 4_685 . . . ?
O2 Co1 N4 C1 76.5(3) 4_585 . . . ?
O2 Co1 N4 C1 -103.5(3) 2_547 . . . ?
N4 Co1 N4 C1 -160(33) 3_577 . . . ?
O1 Co1 N4 N3 -169.5(3) 2_447 . . . ?
O1 Co1 N4 N3 10.5(3) 4_685 . . . ?
O2 Co1 N4 N3 -77.5(3) 4_585 . . . ?
O2 Co1 N4 N3 102.5(3) 2_547 . . . ?
N4 Co1 N4 N3 46(30) 3_577 . . . ?
N3 N4 C1 N1 -0.4(4) . . . . ?
Co1 N4 C1 N1 -158.6(2) . . . . ?
N2 N1 C1 N4 0.4(4) . . . . ?
C2 N1 C1 N4 -179.3(3) . . . . ?
C1 N1 C2 C3 95.7(4) . . . . ?
N2 N1 C2 C3 -84.0(3) . . . . ?
Co1 O1 C3 O2 -114.4(4) 2_457 . . . ?
Co1 O1 C3 C2 70.2(4) 2_457 . . . ?
Co1 O2 C3 O1 17.2(5) 2_557 . . . ?
Co1 O2 C3 C2 -167.44(19) 2_557 . . . ?
N1 C2 C3 O1 -153.4(3) . . . . ?
N1 C2 C3 O2 30.7(4) . . . . ?

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_diffrn_reflns_theta_full              27.48
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_refine_diff_density_max    0.404
_refine_diff_density_min   -0.421
_refine_diff_density_rms    0.092
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