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data_ud0534_2

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_chemical_name_systematic
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_chemical_name_common            ?
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_symmetry_space_group_name_Hall   'P 2ac 2ab'
_chemical_formula_moiety         'C15 H9 O2, C5 H10 N3'
_chemical_formula_sum
 'C20 H19 N3 O2'
_chemical_formula_weight         333.38

loop_
 _atom_type_symbol
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 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 '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
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'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'

_symmetry_cell_setting 'ORTHORHOMBIC'

_symmetry_space_group_name_H-M 'P2(1)2(1)2(1)'

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 'x, y, z'

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

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

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

_cell_length_a 10.2623(5)

_cell_length_b 11.3590(6)

_cell_length_c 14.7950(8)

_cell_angle_alpha 90.00

_cell_angle_beta 90.00

_cell_angle_gamma 90.00

_cell_volume 1724.65(16)

_cell_formula_units_Z 4

_cell_measurement_temperature 100(2)

_cell_measurement_reflns_used ?

_cell_measurement_theta_min ?

_cell_measurement_theta_max ?

_exptl_crystal_description 'PLATE'

_exptl_crystal_colour 'BROWN'

_exptl_crystal_size_max 0.546

_exptl_crystal_size_mid 0.283

_exptl_crystal_size_min 0.052

_exptl_crystal_density_meas ?

_exptl_crystal_density_diffrn 1.284

_exptl_crystal_density_method 'not measured'

_exptl_crystal_F_000 704

_exptl_absorpt_coefficient_mu 0.085

_exptl_absorpt_correction_type 'MULTI-SCAN'

_exptl_absorpt_correction_T_min 0.972

_exptl_absorpt_correction_T_max 0.996

_exptl_absorpt_process_details 'SADABS'

_exptl_special_details

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_diffrn_ambient_temperature 100(2)

_diffrn_radiation_wavelength 0.71073

_diffrn_radiation_type MoK\a

_diffrn_radiation_source 'fine-focus sealed tube'

_diffrn_radiation_monochromator graphite

_diffrn_measurement_device_type 'BRUKER CCD AREA'

_diffrn_measurement_method 'OMEGA SCAN'

_diffrn_detector_area_resol_mean 3

_diffrn_standards_number ?

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_diffrn_standards_interval_time ?

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_diffrn_reflns_number 26724

_diffrn_reflns_av_R_equivalents 0.0246

_diffrn_reflns_av_sigmaI/netI 0.0158

_diffrn_reflns_limit_h_min -14

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_diffrn_reflns_limit_k_min -14

_diffrn_reflns_limit_k_max 15

_diffrn_reflns_limit_l_min -21

_diffrn_reflns_limit_l_max 21

_diffrn_reflns_theta_min 2.26

_diffrn_reflns_theta_max 31.23

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_reflns_threshold_expression >2sigma(I)

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_computing_cell_refinement       'SMART APEX II'
_computing_data_reduction        'SMART APEX SAINT'
_computing_structure_solution    'SHELXS-97 (Sheldrick, 1990)'
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_computing_molecular_graphics    'SHELXTL'
_computing_publication_material  'MERCURY 2.2'

_refine_special_details
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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_weighting_scheme      calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0420P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary difmap

_atom_sites_solution_hydrogens geom

_refine_ls_hydrogen_treatment mixed

_refine_ls_extinction_method none

_refine_ls_extinction_coef ?

_refine_ls_abs_structure_details

'Flack H D (1983), Acta Cryst. A39, 876-881'

_refine_ls_number_reflns 3088

_refine_ls_number_parameters 231

_refine_ls_number_restraints 0

_refine_ls_R_factor_all 0.0587

_refine_ls_R_factor_gt 0.0440

_refine_ls_wR_factor_ref 0.1478

_refine_ls_wR_factor_gt 0.1314

_refine_ls_goodness_of_fit_ref 1.076

_refine_ls_restrained_S_all 1.076

_refine_ls_shift/su_max 0.008

_refine_ls_shift/su_mean 0.001

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_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

_atom_site_symmetry_multiplicity

_atom_site_calc_flag

_atom_site_refinement_flags

_atom_site_disorder_assembly

_atom_site_disorder_group

C1 C 0.00890(17) 1.11329(18) 0.06821(11) 0.0421(4) Uani 1 1 d . . .

O2 O -0.11031(15) 1.13469(16) 0.07363(11) 0.0600(4) Uani 1 1 d . . .

O3 O 0.08710(15) 1.17533(15) 0.02543(11) 0.0618(4) Uani 1 1 d . . .

C4 C 0.06184(15) 1.00533(15) 0.11545(11) 0.0366(3) Uani 1 1 d . . .

C5 C 0.10720(15) 1.01519(15) 0.20454(11) 0.0357(3) Uani 1 1 d . . .

C6 C 0.09957(19) 1.12246(19) 0.25396(13) 0.0462(4) Uani 1 1 d . . .

H6 H 0.0640 1.1889 0.2268 0.055 Uiso 1 1 calc R . .

C8 C 0.1968(2) 1.0287(3) 0.38374(14) 0.0622(6) Uani 1 1 d . . .

H8 H 0.2255 1.0339 0.4432 0.075 Uiso 1 1 calc R . .

C7 C 0.1439(2) 1.1288(2) 0.34087(15) 0.0593(5) Uani 1 1 d . . .

H7 H 0.1392 1.1998 0.3721 0.071 Uiso 1 1 calc R . .

C9 C 0.2060(2) 0.9257(2) 0.33913(16) 0.0575(6) Uani 1 1 d . . .

H9 H 0.2408 0.8605 0.3686 0.069 Uiso 1 1 calc R . .

C10 C 0.16375(17) 0.91427(18) 0.24778(13) 0.0450(4) Uani 1 1 d . . .

C11 C 0.1774(2) 0.81130(19) 0.19895(16) 0.0556(5) Uani 1 1 d . . .

H11 H 0.2175 0.7470 0.2262 0.067 Uiso 1 1 calc R . .

C12 C 0.1333(2) 0.80065(19) 0.11063(17) 0.0548(5) Uani 1 1 d . . .

C13 C 0.1481(3) 0.6936(3) 0.0607(2) 0.0813(9) Uani 1 1 d . . .

H13 H 0.1915 0.6297 0.0859 0.098 Uiso 1 1 calc R . .

C14 C 0.0976(4) 0.6864(3) -0.0248(3) 0.1017(13) Uani 1 1 d . . .

H14 H 0.1091 0.6175 -0.0578 0.122 Uiso 1 1 calc R . .

C15 C 0.0295(4) 0.7795(3) -0.0635(2) 0.0881(10) Uani 1 1 d . . .

H15 H -0.0073 0.7704 -0.1206 0.106 Uiso 1 1 calc R . .

C16 C 0.0161(3) 0.8825(3) -0.01951(15) 0.0648(6) Uani 1 1 d . . .

H16 H -0.0283 0.9443 -0.0470 0.078 Uiso 1 1 calc R . .

C17 C 0.06936(19) 0.89809(17) 0.06911(12) 0.0449(4) Uani 1 1 d . . .

N18 N 0.34431(15) 0.21210(14) 0.07622(10) 0.0407(3) Uani 1 1 d . . .

H18A H 0.3378 0.2700 0.1165 0.061 Uiso 1 1 calc R . .

H18B H 0.2650 0.1903 0.0586 0.061 Uiso 1 1 calc R . .

H18C H 0.3895 0.2371 0.0286 0.061 Uiso 1 1 calc R . .

C19 C 0.4120(2) 0.11025(17) 0.11779(17) 0.0530(5) Uani 1 1 d . . .

H19A H 0.4187 0.0475 0.0736 0.064 Uiso 1 1 calc R . .

H19B H 0.3605 0.0813 0.1681 0.064 Uiso 1 1 calc R . .

C20 C 0.5443(2) 0.14092(19) 0.15054(17) 0.0574(5) Uani 1 1 d . . .

H20A H 0.5386 0.2103 0.1886 0.069 Uiso 1 1 calc R . .

H20B H 0.5987 0.1604 0.0991 0.069 Uiso 1 1 calc R . .

C21 C 0.60746(18) 0.04403(16) 0.20275(13) 0.0420(4) Uani 1 1 d . . .

N22 N 0.73611(16) 0.01965(15) 0.19310(12) 0.0467(4) Uani 1 1 d . . .

C23 C 0.7647(2) -0.0694(2) 0.24860(17) 0.0564(5) Uani 1 1 d . . .

H23 H 0.8473 -0.1024 0.2540 0.068 Uiso 1 1 calc R . .

N24 N 0.66347(18) -0.10484(17) 0.29437(13) 0.0566(4) Uani 1 1 d . . .

C25 C 0.56336(19) -0.03402(19) 0.26550(14) 0.0506(5) Uani 1 1 d . . .

H25 H 0.4778 -0.0387 0.2859 0.061 Uiso 1 1 calc R . .

H22 H 0.787(3) 0.048(3) 0.150(2) 0.068(8) Uiso 1 1 d . . .

loop_

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_atom_site_aniso_U_11

_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

C1 0.0405(8) 0.0481(10) 0.0377(7) 0.0105(7) -0.0041(7) -0.0033(7)

O2 0.0447(7) 0.0679(10) 0.0676(9) 0.0286(8) 0.0044(7) 0.0110(7)

O3 0.0485(8) 0.0710(10) 0.0659(9) 0.0352(8) -0.0061(7) -0.0125(8)

C4 0.0302(7) 0.0397(8) 0.0400(7) 0.0071(6) 0.0020(6) -0.0032(6)

C5 0.0287(7) 0.0396(8) 0.0389(7) 0.0083(6) 0.0023(6) -0.0011(6)

C6 0.0447(9) 0.0477(9) 0.0461(9) 0.0000(8) -0.0021(7) -0.0008(8)

C8 0.0522(11) 0.0935(18) 0.0409(9) 0.0120(11) -0.0087(8) -0.0132(11)

C7 0.0570(12) 0.0714(14) 0.0496(10) -0.0090(10) -0.0014(9) -0.0088(11)

C9 0.0421(10) 0.0764(15) 0.0540(10) 0.0266(11) -0.0073(8) -0.0013(10)

C10 0.0347(8) 0.0488(10) 0.0516(9) 0.0198(8) 0.0022(7) 0.0003(7)

C11 0.0514(10) 0.0414(10) 0.0740(13) 0.0162(9) 0.0056(10) 0.0067(8)

C12 0.0505(10) 0.0417(10) 0.0722(12) -0.0014(9) 0.0168(10) -0.0025(8)

C13 0.0841(18) 0.0471(13) 0.113(2) -0.0182(14) 0.0300(18) -0.0030(13)

C14 0.115(3) 0.0755(19) 0.115(3) -0.049(2) 0.046(2) -0.029(2)

C15 0.096(2) 0.098(2) 0.0701(15) -0.0358(16) 0.0210(16) -0.0322(19)

C16 0.0673(13) 0.0772(15) 0.0500(10) -0.0116(11) 0.0070(10) -0.0212(13)

C17 0.0424(9) 0.0463(10) 0.0460(8) -0.0013(8) 0.0082(7) -0.0094(7)

N18 0.0408(7) 0.0394(8) 0.0419(7) 0.0022(6) 0.0007(6) -0.0042(6)

C19 0.0468(10) 0.0371(9) 0.0750(13) 0.0048(9) -0.0109(9) -0.0028(8)

C20 0.0500(10) 0.0478(11) 0.0744(13) 0.0173(10) -0.0121(10) -0.0098(9)

C21 0.0416(8) 0.0363(8) 0.0480(8) -0.0002(7) -0.0018(7) -0.0039(7)

N22 0.0443(8) 0.0394(8) 0.0563(9) 0.0042(7) 0.0092(7) -0.0026(6)

C23 0.0478(10) 0.0432(10) 0.0781(14) 0.0120(10) 0.0060(10) 0.0058(8)

N24 0.0520(9) 0.0519(10) 0.0659(10) 0.0169(8) 0.0035(8) -0.0010(8)

C25 0.0416(9) 0.0516(11) 0.0585(10) 0.0076(9) 0.0077(8) -0.0018(8)

_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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C1 O3 1.241(2) . ?

C1 O2 1.250(2) . ?

C1 C4 1.513(2) . ?

C4 C17 1.400(3) . ?

C4 C5 1.402(2) . ?

C5 C6 1.423(3) . ?

C5 C10 1.435(2) . ?

C6 C7 1.366(3) . ?

C6 H6 0.9300 . ?

C8 C9 1.347(4) . ?

C8 C7 1.410(4) . ?

C8 H8 0.9300 . ?

C7 H7 0.9300 . ?

C9 C10 1.425(3) . ?

C9 H9 0.9300 . ?

C10 C11 1.382(3) . ?

C11 C12 1.388(3) . ?

C11 H11 0.9300 . ?

C12 C17 1.426(3) . ?

C12 C13 1.432(3) . ?

C13 C14 1.368(5) . ?

C13 H13 0.9300 . ?

C14 C15 1.391(6) . ?

C14 H14 0.9300 . ?

C15 C16 1.347(4) . ?

C15 H15 0.9300 . ?

C16 C17 1.431(3) . ?

C16 H16 0.9300 . ?

N18 C19 1.483(2) . ?

N18 H18A 0.8900 . ?

N18 H18B 0.8900 . ?

N18 H18C 0.8900 . ?

C19 C20 1.484(3) . ?

C19 H19A 0.9700 . ?

C19 H19B 0.9700 . ?

C20 C21 1.493(3) . ?

C20 H20A 0.9700 . ?

C20 H20B 0.9700 . ?

C21 N22 1.357(3) . ?

C21 C25 1.361(3) . ?

N22 C23 1.336(3) . ?

N22 H22 0.88(3) . ?

C23 N24 1.304(3) . ?

C23 H23 0.9300 . ?

N24 C25 1.373(3) . ?

C25 H25 0.9300 . ?

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O3 C1 O2 123.72(18) . . ?

O3 C1 C4 117.62(16) . . ?

O2 C1 C4 118.66(16) . . ?

C17 C4 C5 120.76(16) . . ?

C17 C4 C1 119.94(15) . . ?

C5 C4 C1 119.26(15) . . ?

C4 C5 C6 122.21(15) . . ?

C4 C5 C10 119.30(17) . . ?

C6 C5 C10 118.49(16) . . ?

C7 C6 C5 120.7(2) . . ?

C7 C6 H6 119.7 . . ?

C5 C6 H6 119.7 . . ?

C9 C8 C7 120.46(18) . . ?

C9 C8 H8 119.8 . . ?

C7 C8 H8 119.8 . . ?

C6 C7 C8 120.6(2) . . ?

C6 C7 H7 119.7 . . ?

C8 C7 H7 119.7 . . ?

C8 C9 C10 121.5(2) . . ?

C8 C9 H9 119.3 . . ?

C10 C9 H9 119.3 . . ?

C11 C10 C9 122.81(19) . . ?

C11 C10 C5 118.94(18) . . ?

C9 C10 C5 118.2(2) . . ?

C10 C11 C12 122.20(19) . . ?

C10 C11 H11 118.9 . . ?

C12 C11 H11 118.9 . . ?

C11 C12 C17 119.2(2) . . ?

C11 C12 C13 121.7(2) . . ?

C17 C12 C13 119.1(2) . . ?

C14 C13 C12 119.2(3) . . ?

C14 C13 H13 120.4 . . ?

C12 C13 H13 120.4 . . ?

C13 C14 C15 121.7(3) . . ?

C13 C14 H14 119.1 . . ?

C15 C14 H14 119.1 . . ?

C16 C15 C14 120.8(3) . . ?

C16 C15 H15 119.6 . . ?

C14 C15 H15 119.6 . . ?

C15 C16 C17 120.8(3) . . ?

C15 C16 H16 119.6 . . ?

C17 C16 H16 119.6 . . ?

C4 C17 C12 119.33(17) . . ?

C4 C17 C16 122.3(2) . . ?

C12 C17 C16 118.3(2) . . ?

C19 N18 H18A 109.5 . . ?

C19 N18 H18B 109.5 . . ?

H18A N18 H18B 109.5 . . ?

C19 N18 H18C 109.5 . . ?

H18A N18 H18C 109.5 . . ?

H18B N18 H18C 109.5 . . ?

N18 C19 C20 112.39(16) . . ?

N18 C19 H19A 109.1 . . ?

C20 C19 H19A 109.1 . . ?

N18 C19 H19B 109.1 . . ?

C20 C19 H19B 109.1 . . ?

H19A C19 H19B 107.9 . . ?

C19 C20 C21 113.16(17) . . ?

C19 C20 H20A 108.9 . . ?

C21 C20 H20A 108.9 . . ?

C19 C20 H20B 108.9 . . ?

C21 C20 H20B 108.9 . . ?

H20A C20 H20B 107.8 . . ?

N22 C21 C25 105.21(18) . . ?

N22 C21 C20 121.24(18) . . ?

C25 C21 C20 133.54(18) . . ?

C23 N22 C21 107.70(17) . . ?

C23 N22 H22 126(2) . . ?

C21 N22 H22 125.6(19) . . ?

N24 C23 N22 112.19(19) . . ?

N24 C23 H23 123.9 . . ?

N22 C23 H23 123.9 . . ?

C23 N24 C25 104.72(17) . . ?

C21 C25 N24 110.19(18) . . ?

C21 C25 H25 124.9 . . ?

N24 C25 H25 124.9 . . ?

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_geom_hbond_atom_site_label_H

_geom_hbond_atom_site_label_A

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_geom_hbond_site_symmetry_A

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N18 H18B O3 0.89 1.90 2.776(2) 168.7 1_545

N18 H18C O2 0.89 2.10 2.857(2) 142.4 4_565

N18 H18C O3 0.89 2.40 3.179(2) 146.9 4_565

N22 H22 O2 0.88(3) 1.83(3) 2.705(2) 168(3) 1_645

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_diffrn_reflns_theta_full 31.23

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