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Hydrogen bonding properties and intermediate structure of N-(2-carboxyphenyl)salicylideneimine

Ligtenbarg, Alette G.J.; Hage, Ronald; Meetsma, Auke; Feringa, Ben L.

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_audit_update_record
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Drs. A. Meetsma

;

_publ_contact_author_address

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Hydrogen bonding properties of

N-(2-carboxyphenyl)salicylideneimine

Authors :

Alette G.J. Ligtenbarg, Ronald Hage,

Auke Meetsma, Ben L. Feringa

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_journal_date_from_coeditor        ?
_journal_date_accepted              ?

_journal_date_printers_first       ?
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_journal_techeditor_code            ?
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_journal_issue                      ?
_journal_page_first                 ?
_journal_page_last                  ?

_journal_suppl_publ_number          ?
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# 3. TITLE AND AUTHOR LIST

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;
_publ_section_title_footnote
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?
;

# The loop structure below should contain the names and addresses of all
# authors, in the required order of publication. Repeat as necessary.

loop_
_publ_author_name
_publ_author_address

'Meetsma, Auke'

;
```

Crystal Structure Center,
Chemical Physics,
Materials Science Center,
Groningen University,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.

;

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4. TEXT

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Insert blank lines between paragraphs

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_publ_section_exptl_refinement

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Boer, J.L. de & Duisenberg, A.J.M. (1984). Acta Cryst. A40, C-410.

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University, The Netherlands.

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data_c14h11no

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5. CHEMICAL DATA

_chemical_name_systematic

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_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C14 H11 N O3'

_chemical_formula_structural ?

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)₃, (C6 N6 Cr 3-)₂, 2(H2 O)'

_chemical_formula_sum

'C14 H11 N O3'

_chemical_formula_weight 241.25

_chemical_compound_source 'by syntheses'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

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O O .0106 .0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

N N .0061 .0033

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H H .0000 .0000

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C C .0033 .0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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6. CRYSTAL DATA

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_symmetry_space_group_name_H-M	'I 2/a'

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
1/2-x,y,-z
-x,-y,-z
1/2+x,-y,z
1/2+x,1/2+y,1/2+z
-x,1/2+y,1/2-z
1/2-x,1/2-y,1/2-z
x,1/2-y,1/2+z

_cell_length_a	14.840(1)
_cell_length_b	6.813(1)
_cell_length_c	22.680(1)
_cell_angle_alpha	90
_cell_angle_beta	97.796(6)
_cell_angle_gamma	90
_cell_volume	2271.9(4)
_cell_formula_units_Z	8
_cell_measurement_temperature	295
_cell_measurement_reflns_used	22
_cell_measurement_theta_min	17.14
_cell_measurement_theta_max	20.82
_cell_special_details	

;

Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting. Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

;

_exptl_crystal_description	'block-shaped'
_exptl_crystal_colour	'orange-red'
_exptl_crystal_size_max	0.40
_exptl_crystal_size_mid	0.15
_exptl_crystal_size_min	0.5
_exptl_crystal_size_rad	?
_exptl_crystal_density_meas	'Not Measured'
_exptl_crystal_density_diffrn	1.411
_exptl_crystal_density_method	?
_exptl_crystal_F_000	1008
_exptl_absorpt_coefficient_mu	.10
_exptl_crystal_density_meas_temp	295
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_exptl_absorpt_process_details	?
_exptl_absorpt_correction_T_min	?
_exptl_absorpt_correction_T_max	?

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7. EXPERIMENTAL DATA

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?	
;	
_diffrn_ambient_temperature	295
_diffrn_radiation_wavelength	.71073

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_diffrn_radiation_type          'Mo K\alpha'
_diffrn_radiation_source        'fine focus sealed Philips Mo tube '
_diffrn_radiation_monochromator  'perpendicular mounted graphite'
_diffrn_radiation_detector
;
    scintillation NaI crystal with photomultiplier
;
_diffrn_measurement_device_type
;
    Enraf Nonius CAD-4F diffractometer
;

_diffrn_measurement_method      '\omega/2\theta'

_diffrn_special_details
;
    Enraf-Nonius CAD-4F diffractometer.
    Graphite-monochromated Mo K\alpha radiation,
    \omega/2\theta scan, \Delta\omega = (0.85 + 0.34 tg \theta)\%.
;
_diffrn_detector_area_resol_mean    ?

_diffrn_standards_number           3
_diffrn_standards_interval_count    ?
_diffrn_standards_interval_time     180
_diffrn_standards_decay_%           8.6

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
-4  0  0
-4 -4  0
-2  0  6

# number of measured reflections (redundant set)
_diffrn_reflns_number             2484
_diffrn_reflns_av_R_equivalents   0.0000
_diffrn_reflns_av_sigmaI/netI     0.0120
_diffrn_reflns_limit_h_min        -18
_diffrn_reflns_limit_h_max        18
_diffrn_reflns_limit_k_min        -8
_diffrn_reflns_limit_k_max        0
_diffrn_reflns_limit_l_min        -28
_diffrn_reflns_limit_l_max        28
_diffrn_reflns_theta_min          1.81
_diffrn_reflns_theta_max          26.98

_diffrn_reflns_reduction_process
;
    Intensity data were corrected for Lorentz and polarization effects, scale
    variation, but not for absorption and reduced to  $F_o^2$ 
;

# number of unique reflections
_reflns_number_total              2484
_reflns_number_gt                 1966
_reflns_threshold_expression       >2sigma(I)

_computing_data_collection         'CAD4-UNIX Software Version 5.1, 1994'
_computing_cell_refinement         'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction         'HELENA (Spek, 1993)'
_computing_structure_solution      'SHELXS-86 (Sheldrick, 1990)'
_computing_structure_refinement    'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics
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PLUTO (Meetsma, 1997)
ORTEP (Burnett et al., 1996)
PLATON (Spek, 1994, 1996)
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_computing_publication_material      'PLATON (Spek, 1990)'

#####

# 8. REFINEMENT DATA

_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.
;

_refine_ls_structure_factor_coef      Fsqd
_refine_ls_matrix_type                full
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2^)+(0.0777P)^2^+0.2129P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary          direct
_atom_sites_solution_secondary        difmap
_atom_sites_solution_hydrogens        difmap
_refine_ls_hydrogen_treatment          isotropic
_refine_ls_extinction_method           SHELXL
_refine_ls_extinction_coef             0.0055(9)
_refine_ls_extinction_expression
'Fc^*=kFc[1+0.001xFc^2^/l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns              2484
_refine_ls_number_parameters           208
_refine_ls_number_restraints           0
_refine_ls_R_factor_all                0.0500
_refine_ls_R_factor_gt                 0.0388
_refine_ls_wR_factor_ref               0.1154
_refine_ls_wR_factor_gt               0.1102
_refine_ls_goodness_of_fit_ref         1.032
_refine_ls_restrained_S_all            1.032
_refine_ls_shift/su_max                0.001
_refine_ls_shift/su_mean               0.000

_refine_diff_density_max               .220
_refine_diff_density_min               -.179
_refine_diff_density_rms               .042

#####

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
O1      Uani      .12921(6)  .78696(15)  -.01568(4)  1.000  .0454(3)
O2      Uani      .26694(6)  .80769(17)  .09099(4)  1.000  .0527(3)
O3      Uani      .34029(7)  1.0562(2)  .13964(5)  1.000  .0674(4)
N1      Uani      .08849(7)  .83251(15)  .09386(4)  1.000  .0350(3)
C1      Uani      .04320(8)  .74689(18)  -.03407(5)  1.000  .0356(3)
C2      Uani      .01094(10) .6974(2)   -.09332(6)  1.000  .0443(4)

```


C3	Uani	-.07955(11)	.6571(2)	-.10989(6)	1.000	.0492(4)
C4	Uani	-.14186(10)	.6656(2)	-.06934(7)	1.000	.0514(4)
C5	Uani	-.11250(9)	.7167(2)	-.01185(6)	1.000	.0453(4)
C6	Uani	-.01997(8)	.75670(18)	.00749(5)	1.000	.0357(3)
C7	Uani	.00554(8)	.80782(18)	.06811(5)	1.000	.0364(3)
C8	Uani	.11521(8)	.88493(18)	.15454(5)	1.000	.0355(3)
C9	Uani	.05234(9)	.8893(2)	.19481(6)	1.000	.0480(4)
C10	Uani	.07955(11)	.9493(3)	.25240(6)	1.000	.0577(5)
C11	Uani	.16761(12)	1.0044(3)	.27080(6)	1.000	.0591(5)
C12	Uani	.22986(11)	1.0010(2)	.23076(6)	1.000	.0502(5)
C13	Uani	.20539(8)	.94030(19)	.17252(5)	1.000	.0381(4)
C14	Uani	.27762(8)	.9385(2)	.13150(5)	1.000	.0415(4)
H1	Uiso	.1731(14)	.803(3)	-.0516(8)	1.000	.086(6)
H1'	Uiso	.1388(12)	.818(2)	.0709(8)	1.000	.061(5)
H2	Uiso	.0558(11)	.692(2)	-.1217(7)	1.000	.054(4)
H3	Uiso	-.1024(13)	.620(3)	-.1514(9)	1.000	.070(5)
H4	Uiso	-.2032(14)	.641(3)	-.0813(9)	1.000	.074(5)
H5	Uiso	-.1544(11)	.725(2)	.0199(8)	1.000	.057(4)
H7	Uiso	-.0442(10)	.826(2)	.0914(7)	1.000	.050(4)
H9	Uiso	-.0072(13)	.851(3)	.1826(8)	1.000	.061(5)
H10	Uiso	.0332(12)	.945(3)	.2810(8)	1.000	.071(5)
H11	Uiso	.1876(13)	1.046(3)	.3090(10)	1.000	.079(6)
H12	Uiso	.2884(13)	1.034(3)	.2420(8)	1.000	.065(5)

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

O1	.0334(5)	.0687(6)	.0352(5)	-.0002(4)	.0081(3)	-.0067(4)
O2	.0361(5)	.0801(7)	.0439(5)	-.0143(5)	.0130(4)	-.0059(5)
O3	.0428(6)	.0910(9)	.0713(7)	-.0196(6)	.0184(5)	-.0223(6)
N1	.0309(5)	.0411(6)	.0339(5)	.0019(4)	.0077(4)	-.0003(4)
C1	.0352(6)	.0364(6)	.0348(6)	.0034(5)	.0037(5)	-.0016(5)
C2	.0482(8)	.0457(7)	.0385(7)	-.0004(5)	.0044(6)	-.0017(6)
C3	.0542(8)	.0474(8)	.0426(7)	-.0019(6)	-.0055(6)	-.0035(6)
C4	.0390(7)	.0545(8)	.0573(8)	.0014(7)	-.0062(6)	-.0066(6)
C5	.0347(7)	.0511(8)	.0499(7)	.0039(6)	.0047(6)	-.0038(6)
C6	.0330(6)	.0362(6)	.0379(6)	.0037(5)	.0048(5)	-.0020(5)
C7	.0321(6)	.0396(6)	.0388(6)	.0043(5)	.0091(5)	-.0006(5)
C8	.0349(6)	.0400(6)	.0321(6)	.0040(5)	.0065(5)	.0023(5)
C9	.0389(7)	.0680(9)	.0389(7)	.0074(6)	.0117(6)	.0016(6)
C10	.0540(8)	.0843(11)	.0381(7)	.0034(7)	.0178(6)	.0073(8)
C11	.0648(10)	.0800(11)	.0330(7)	-.0078(7)	.0086(6)	.0028(9)
C12	.0452(8)	.0640(9)	.0406(7)	-.0042(6)	.0024(6)	-.0023(7)
C13	.0366(6)	.0419(7)	.0364(6)	.0011(5)	.0071(5)	.0019(5)
C14	.0296(6)	.0573(8)	.0374(6)	-.0002(6)	.0036(5)	-.0013(5)

#=====

10. MOLECULAR GEOMETRY

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;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

;

loop_

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_geom_bond_atom_site_label_2

_geom_bond_distance							
_geom_bond_site_symmetry_1							
_geom_bond_site_symmetry_2							
_geom_bond_publ_flag							
O1	C1	1.3165(15)	.	.	.	yes	
O2	C14	1.2744(16)	.	.	.	yes	
O3	C14	1.2229(18)	.	.	.	yes	
O1	H1	1.115(19)	.	.	.	no	
N1	C7	1.2999(16)	.	.	.	yes	
N1	C8	1.4250(15)	.	.	.	yes	
N1	H1'	.972(18)	.	.	.	no	
C1	C2	1.4050(18)	.	.	.	no	
C1	C6	1.4183(17)	.	.	.	no	
C2	C3	1.372(2)	.	.	.	no	
C3	C4	1.391(2)	.	.	.	no	
C4	C5	1.363(2)	.	.	.	no	
C5	C6	1.4102(18)	.	.	.	no	
C6	C7	1.4190(16)	.	.	.	no	
C8	C13	1.3970(17)	.	.	.	no	
C8	C9	1.3917(18)	.	.	.	no	
C9	C10	1.376(2)	.	.	.	no	
C10	C11	1.369(2)	.	.	.	no	
C11	C12	1.381(2)	.	.	.	no	
C12	C13	1.3847(18)	.	.	.	no	
C13	C14	1.5117(17)	.	.	.	no	
C2	H2	.987(16)	.	.	.	no	
C3	H3	.99(2)	.	.	.	no	
C4	H4	.93(2)	.	.	.	no	
C5	H5	1.015(17)	.	.	.	no	
C7	H7	.972(15)	.	.	.	no	
C9	H9	.927(19)	.	.	.	no	
C10	H10	1.008(18)	.	.	.	no	
C11	H11	.92(2)	.	.	.	no	
C12	H12	.900(19)	.	.	.	no	
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_geom_angle_atom_site_label_2							
_geom_angle_atom_site_label_3							
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_geom_angle_site_symmetry_3							
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C1	O1	H1	115.2(10)	.	.	.	no
C7	N1	C8	126.07(10)	.	.	.	yes
C7	N1	H1'	119.7(11)	.	.	.	no
C8	N1	H1'	114.2(11)	.	.	.	no
O1	C1	C2	122.87(11)	.	.	.	yes
O1	C1	C6	118.65(10)	.	.	.	yes
C2	C1	C6	118.47(11)	.	.	.	no
C1	C2	C3	120.25(13)	.	.	.	no
C2	C3	C4	121.61(13)	.	.	.	no
C3	C4	C5	119.23(14)	.	.	.	no
C4	C5	C6	121.23(12)	.	.	.	no
C1	C6	C5	119.19(11)	.	.	.	no
C1	C6	C7	122.82(11)	.	.	.	no
C5	C6	C7	117.99(11)	.	.	.	no
N1	C7	C6	125.38(11)	.	.	.	yes
C9	C8	C13	120.24(11)	.	.	.	no
N1	C8	C13	118.66(10)	.	.	.	yes
N1	C8	C9	121.04(11)	.	.	.	yes
C8	C9	C10	119.53(13)	.	.	.	no
C9	C10	C11	121.05(14)	.	.	.	no
C10	C11	C12	119.41(13)	.	.	.	no
C11	C12	C13	121.34(14)	.	.	.	no
C12	C13	C14	118.25(11)	.	.	.	no

C8	C13	C12	118.42(12)	.	.	.	no
C8	C13	C14	123.32(10)	.	.	.	no
O2	C14	O3	125.81(12)	.	.	.	yes
O2	C14	C13	114.84(11)	.	.	.	yes
O3	C14	C13	119.34(11)	.	.	.	yes
C1	C2	H2	117.4(9)	.	.	.	no
C3	C2	H2	122.4(9)	.	.	.	no
C2	C3	H3	120.5(11)	.	.	.	no
C4	C3	H3	117.8(11)	.	.	.	no
C3	C4	H4	120.8(13)	.	.	.	no
C5	C4	H4	119.9(13)	.	.	.	no
C4	C5	H5	123.1(10)	.	.	.	no
C6	C5	H5	115.7(10)	.	.	.	no
N1	C7	H7	118.8(9)	.	.	.	no
C6	C7	H7	115.8(9)	.	.	.	no
C8	C9	H9	119.6(11)	.	.	.	no
C10	C9	H9	120.8(11)	.	.	.	no
C9	C10	H10	117.7(11)	.	.	.	no
C11	C10	H10	121.2(10)	.	.	.	no
C10	C11	H11	122.9(12)	.	.	.	no
C12	C11	H11	117.7(12)	.	.	.	no
C11	C12	H12	121.0(12)	.	.	.	no
C13	C12	H12	117.6(12)	.	.	.	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
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag

C7	N1	C8	C13	-168.51(12)	.	.	.	.	no
C7	N1	C8	C9	8.80(19)	.	.	.	.	no
C8	N1	C7	C6	179.61(11)	.	.	.	.	no
C2	C1	C6	C5	.00(18)	.	.	.	.	no
C2	C1	C6	C7	-179.16(12)	.	.	.	.	no
O1	C1	C2	C3	-179.98(12)	.	.	.	.	no
C6	C1	C2	C3	-.90(19)	.	.	.	.	no
O1	C1	C6	C5	179.15(12)	.	.	.	.	no
O1	C1	C6	C7	-.03(18)	.	.	.	.	no
C1	C2	C3	C4	.6(2)	.	.	.	.	no
C2	C3	C4	C5	.5(2)	.	.	.	.	no
C3	C4	C5	C6	-1.4(2)	.	.	.	.	no
C4	C5	C6	C1	1.2(2)	.	.	.	.	no
C4	C5	C6	C7	-179.62(12)	.	.	.	.	no
C1	C6	C7	N1	-7.0(2)	.	.	.	.	no
C5	C6	C7	N1	173.85(12)	.	.	.	.	no
N1	C8	C13	C12	176.65(11)	.	.	.	.	no
N1	C8	C9	C10	-177.01(14)	.	.	.	.	no
C13	C8	C9	C10	.3(2)	.	.	.	.	no
C9	C8	C13	C14	179.69(12)	.	.	.	.	no
N1	C8	C13	C14	-2.97(18)	.	.	.	.	no
C9	C8	C13	C12	-.68(19)	.	.	.	.	no
C8	C9	C10	C11	-.2(3)	.	.	.	.	no
C9	C10	C11	C12	.5(3)	.	.	.	.	no
C10	C11	C12	C13	-.9(3)	.	.	.	.	no
C11	C12	C13	C8	1.0(2)	.	.	.	.	no
C11	C12	C13	C14	-179.33(14)	.	.	.	.	no
C8	C13	C14	O2	-30.90(18)	.	.	.	.	no
C8	C13	C14	O3	149.99(13)	.	.	.	.	no
C12	C13	C14	O2	149.48(12)	.	.	.	.	no
C12	C13	C14	O3	-29.63(19)	.	.	.	.	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
O1      O2      2.9511(13)      .      .      no
O1      N1      2.6535(13)      .      .      no
O1      O2      2.4549(13)      .      2_555      no
O1      C14     3.2959(16)      .      2_555      no
O2      C1      3.2808(16)      .      2_555      no
O2      O1      2.9511(13)      .      .      no
O2      N1      2.6632(14)      .      .      no
O2      C2      3.3742(18)      .      2_555      no
O2      O1      2.4549(13)      .      2_555      no
O3      C9      3.2462(18)      .      4_575      no
O3      C7      3.2532(17)      .      4_575      no
O1      H1'      1.961(18)      .      .      no
O2      H1      1.34(2)      .      2_555      no
O2      H1'      1.896(18)      .      .      no
O2      H2      2.744(16)      .      2_555      no
O3      H1      2.626(19)      .      2_555      no
O3      H12     2.548(18)      .      .      no
O3      H7      2.300(15)      .      4_575      no
O3      H9      2.423(19)      .      4_575      no
N1      O1      2.6535(13)      .      .      no
N1      O2      2.6632(14)      .      .      no
N1      C3      3.3600(18)      .      3_565      no
C1      C6      3.5086(18)      .      3_565      no
C1      O2      3.2807(16)      .      2_555      no
C1      C5      3.4391(19)      .      3_565      no
C1      C6      3.4608(18)      .      3_575      no
C1      C7      3.1893(18)      .      3_575      no
C2      C7      3.5032(19)      .      3_565      no
C2      O2      3.3742(18)      .      2_555      no
C2      C7      3.4333(19)      .      3_575      no
C2      C8      3.5812(19)      .      3_575      no
C3      C13     3.508(2)      .      3_575      no
C3      C8      3.3008(19)      .      3_575      no
C3      N1      3.3600(18)      .      3_565      no
C3      C7      3.4431(19)      .      3_565      no
C4      C14     3.543(2)      .      3_575      no
C5      C1      3.4391(19)      .      3_565      no
C6      C1      3.4608(18)      .      3_575      no
C6      C1      3.5086(18)      .      3_565      no
C6      C6      3.3929(18)      .      3_575      no
C6      C7      3.4479(18)      .      3_575      no
C6      C6      3.5715(18)      .      3_565      no
C7      C2      3.4333(19)      .      3_575      no
C7      C2      3.5032(19)      .      3_565      no
C7      O3      3.2532(17)      .      4_475      no
C7      C1      3.1893(18)      .      3_575      no
C7      C6      3.4479(18)      .      3_575      no
C7      C3      3.4431(19)      .      3_565      no
C8      C2      3.5812(19)      .      3_575      no
C8      C3      3.3008(19)      .      3_575      no
C9      O3      3.2462(18)      .      4_475      no
C12     C12     3.534(2)      .      7_575      no
C12     C12     3.560(2)      .      7_565      no
C13     C3      3.508(2)      .      3_575      no
C14     O1      3.2959(16)      .      2_555      no
C14     C4      3.543(2)      .      3_575      no
C1      H1'      2.646(18)      .      .      no
C2      H10     3.071(18)      .      8_564      no
C7      H9      2.645(18)      .      .      no
C9      H7      2.613(16)      .      .      no

```

C10	H2	3.079(16)	.	8_565	no
C14	H1'	2.457(18)	.	.	no
C14	H1	2.243(19)	.	2_555	no
C14	H2	3.022(16)	.	2_555	no
H1	H2	2.32(3)	.	.	no
H1	O2	1.34(2)	.	2_555	no
H1	O3	2.626(19)	.	2_555	no
H1	C14	2.243(19)	.	2_555	no
H1'	O1	1.961(18)	.	.	no
H1'	O2	1.896(18)	.	.	no
H1'	C1	2.646(18)	.	.	no
H1'	C14	2.457(18)	.	.	no
H2	H1	2.32(3)	.	.	no
H2	O2	2.744(16)	.	2_555	no
H2	C14	3.022(16)	.	2_555	no
H2	C10	3.079(16)	.	8_564	no
H2	H10	2.38(2)	.	8_564	no
H5	H7	2.25(2)	.	.	no
H7	C9	2.613(16)	.	.	no
H7	H5	2.25(2)	.	.	no
H7	H9	2.07(2)	.	.	no
H7	O3	2.300(15)	.	4_475	no
H9	C7	2.645(18)	.	.	no
H9	H7	2.07(2)	.	.	no
H9	O3	2.423(19)	.	4_475	no
H10	C2	3.071(18)	.	8_565	no
H10	H2	2.38(2)	.	8_565	no
H12	O3	2.548(18)	.	.	no

loop_

_geom_hbond_atom_site_label_D

_geom_hbond_atom_site_label_H

_geom_hbond_atom_site_label_A

_geom_hbond_distance_DH

_geom_hbond_distance_HA

_geom_hbond_distance_DA

_geom_hbond_angle_DHA

_geom_hbond_site_symmetry_A

_geom_hbond_publ_flag

#

#D	H	A	D - H	H...A	D...A	D - H...A	symm(A)
----	---	---	-------	-------	-------	-----------	---------

#

O1	H1	O2	1.115(19)	1.34(2)	2.4549(13)	173.1(19)	2_555 yes
N1	H1'	O1	.972(18)	1.961(18)	2.6535(13)	126.2(14)	. yes
N1	H1'	O2	.972(18)	1.896(18)	2.6632(14)	133.9(15)	. yes
C7	H7	O3	.972(15)	2.300(15)	3.2532(17)	166.6(12)	4_475 yes
C9	H9	O3	.927(19)	2.423(19)	3.2462(18)	147.9(17)	4_475 yes

End of Crystallographic Information File

=== END

CIF-file generated for C14H11NO3

CP389B

data_c14h11no2

=====

5. CHEMICAL DATA

_chemical_name_systematic

;

?

;

```

_chemical_name_common          ?
_chemical_melting_point        ?
_chemical_formula_moiety
'C14 H11 N O3'
_chemical_formula_structural    ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C14 H11 N O3'
_chemical_formula_weight        241.25
_chemical_compound_source       'by syntheses'

```

```

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
O   O   .0106   .0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N   N   .0061   .0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H   H   .0000   .0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C   C   .0033   .0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

#=====

6. CRYSTAL DATA

```

_symmetry_cell_setting          Monoclinic
_symmetry_space_group_name_Hall '-I 2ya'
_symmetry_space_group_name_H-M  'I 2/a'

```

```

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
1/2-x,y,-z
-x,-y,-z
1/2+x,-y,z
1/2+x,1/2+y,1/2+z
-x,1/2+y,1/2-z
1/2-x,1/2-y,1/2-z
x,1/2-y,1/2+z

```

```

_cell_length_a                  14.831(1)
_cell_length_b                  6.718(1)
_cell_length_c                  22.660(5)
_cell_angle_alpha               90
_cell_angle_beta                97.610(5)
_cell_angle_gamma               90
_cell_volume                    2237.8(6)
_cell_formula_units_Z           8
_cell_measurement_temperature    130
_cell_measurement_reflns_used    22
_cell_measurement_theta_min      16.63
_cell_measurement_theta_max      21.46
_cell_special_details
;

```

Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting. Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

```

;
_exptl_crystal_description      'block-shaped'

```

```

_exptl_crystal_colour      'oranje-red'
_exptl_crystal_size_max    0.50
_exptl_crystal_size_mid    0.15
_exptl_crystal_size_min    0.10
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas 'Not Measured'
_exptl_crystal_density_diffn 1.432
_exptl_crystal_density_method ?
_exptl_crystal_F_000        1008
_exptl_absorpt_coefficient_mu .10
_exptl_crystal_density_meas_temp ?
_exptl_absorpt_correction_type ' none'
_exptl_absorpt_process_details ?
_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?

```

```

#=====

```

``` # 7. EXPERIMENTAL DATA ```

```

_exptl_special_details
;
?
;
_diffn_ambient_temperature      130
_diffn_radiation_wavelength     .71073
_diffn_radiation_type           'Mo K\alpha'
_diffn_radiation_source         'fine focus sealed Philips Mo tube '
_diffn_radiation_monochromator   'perpendicular mounted graphite'
_diffn_radiation_detector
;
    scintillation NaI crystal with photomultiplier
;
_diffn_measurement_device_type
;
    Enraf Nonius CAD-4F diffractometer
;

_diffn_measurement_method       '\w/2\q'

_diffn_special_details
;
    Crystal into the cold nitrogen stream of the low-temperature unit
    (Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
    Graphite-monochromated Mo K\alpha radiation,
    \w/2\q scan, \D\w = (0.80 + 0.34 tg \q)\%.
;
_diffn_detector_area_resol_mean ?

_diffn_standards_number         3
_diffn_standards_interval_count ?
_diffn_standards_interval_time  180
_diffn_standards_decay_%        0.2

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
-3  2 -1
 4  0 -2
-2 -1 -3
# number of measured reflections (redundant set)
_diffn_reflns_number            2484
_diffn_reflns_av_R_equivalents  0.0061
_diffn_reflns_av_sigmaI/netI    0.0186
_diffn_reflns_limit_h_min       -18
_diffn_reflns_limit_h_max       0

```

```

_diffrn_reflms_limit_k_min      0
_diffrn_reflms_limit_k_max      8
_diffrn_reflms_limit_l_min     -27
_diffrn_reflms_limit_l_max      27
_diffrn_reflms_theta_min       1.55
_diffrn_reflms_theta_max       26.00

_diffrn_reflms_reduction_process
;
  Intensity data were corrected for Lorentz and polarization effects, scale
  variation, but not for absorption and reduced to  $F_o^2$ 
;

# number of unique reflections
_reflms_number_total            2192
_reflms_number_gt               1783
_reflms_threshold_expression    >2sigma(I)

_computing_data_collection      'CAD4-UNIX Software Version 5.1, 1994'
_computing_cell_refinement      'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction       'HELENA (Spek, 1993)'
_computing_structure_solution
;
  The coordinates of the room-temperature structure were used as starting
  positions of the refinement
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
  PLUTO (Meetsma, 1997)
  ORTEP (Burnett et al., 1996)
  PLATON (Spek, 1994, 1996)
;
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_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
 $F^2 > 2\sigma(F^2)$  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.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme
  'calc w=1/[\s^2(Fo^2)+(0.0636P)^2+0.3190P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary    direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment  isotropic
_refine_ls_extinction_method    none
_refine_ls_extinction_coef      ?
_refine_ls_number_reflms       2192
_refine_ls_number_parameters    207
_refine_ls_number_restraints    0
_refine_ls_R_factor_all         0.0482
_refine_ls_R_factor_gt          0.0359
_refine_ls_wR_factor_ref        0.1001

```


_refine_ls_wR_factor_gt	0.0951
_refine_ls_goodness_of_fit_ref	1.050
_refine_ls_restrained_S_all	1.050
_refine_ls_shift/su_max	0.000
_refine_ls_shift/su_mean	0.000

_refine_diff_density_max	.214
_refine_diff_density_min	-.256
_refine_diff_density_rms	.049

#####

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

```

loop_
_atom_site_label
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
O1      Uani      .12980(6)  .78538(15)  -.01551(4)  1.000  .0248(3)
O2      Uani      .26662(6)  .80206(15)  .09128(4)  1.000  .0280(3)
O3      Uani      .33983(7)  1.05781(17) .13936(5)  1.000  .0346(3)
N1      Uani      .08788(8)  .83165(16)  .09402(5)  1.000  .0200(3)
C1      Uani      .04360(9)  .74642(18)  -.03433(6)  1.000  .0202(4)
C2      Uani      .01177(10) .6979(2)    -.09385(6)  1.000  .0247(4)
C3      Uani      -.07892(10) .6580(2)    -.11074(6)  1.000  .0268(4)
C4      Uani      -.14234(10) .6674(2)    -.07030(6)  1.000  .0280(4)
C5      Uani      -.11313(10) .7184(2)    -.01226(6)  1.000  .0251(4)
C6      Uani      -.02015(9)  .75678(19)  .00711(6)  1.000  .0202(4)
C7      Uani      .00482(9)   .80837(19)  .06808(6)  1.000  .0208(4)
C8      Uani      .11423(9)   .88418(19)  .15485(5)  1.000  .0198(4)
C9      Uani      .05096(10)   .8894(2)    .19506(6)  1.000  .0265(4)
C10     Uani      .07777(10)   .9499(2)    .25296(6)  1.000  .0313(5)
C11     Uani      .16672(11)   1.0065(2)   .27150(6)  1.000  .0313(5)
C12     Uani      .22920(10)   1.0016(2)   .23128(6)  1.000  .0275(4)
C13     Uani      .20474(9)    .9394(2)    .17287(6)  1.000  .0215(4)
C14     Uani      .27718(9)    .9368(2)    .13160(6)  1.000  .0234(4)
H1      Uiso      .1731(14)    .801(3)     -.0511(9)  1.000  .067(7)
H1'     Uiso      .1348(12)    .813(3)     .0699(8)  1.000  .041(5)
H2      Uiso      .0572(11)    .695(2)     -.1231(7)  1.000  .031(4)
H3      Uiso      -.1012(11)   .620(2)     -.1522(7)  1.000  .033(4)
H4      Uiso      -.2039(13)   .637(3)     -.0824(8)  1.000  .042(5)
H5      Uiso      -.1556(12)   .725(3)     .0185(8)  1.000  .037(4)
H7      Uiso      -.0467(11)   .826(2)     .0917(7)  1.000  .036(4)
H9      Uiso      -.0093(13)   .855(3)     .1822(8)  1.000  .041(5)
H10     Uiso      .0309(11)    .952(3)     .2805(7)  1.000  .035(4)
H11     Uiso      .1864(11)    1.053(2)    .3110(8)  1.000  .035(4)
H12     Uiso      .2899(12)    1.039(2)    .2435(7)  1.000  .032(4)

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loop_
_atom_site_aniso_label
_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
O1      .0184(5)  .0354(6)  .0209(5)  .0005(4)  .0034(4)  -.0034(4)
O2      .0206(5)  .0399(6)  .0243(5)  -.0068(4)  .0061(4)  -.0026(4)
O3      .0228(5)  .0445(7)  .0376(6)  -.0085(5)  .0084(4)  -.0102(5)
N1      .0178(6)  .0226(6)  .0198(5)  .0016(5)  .0035(4)  .0004(5)
C1      .0197(7)  .0179(6)  .0225(6)  .0030(5)  .0007(5)  -.0010(5)
C2      .0269(7)  .0239(7)  .0232(7)  -.0003(5)  .0026(6)  -.0001(6)
C3      .0310(8)  .0236(7)  .0241(7)  -.0010(6)  -.0031(6)  -.0012(6)

```

C4	.0227(7)	.0277(8)	.0319(8)	.0009(6)	-.0026(6)	-.0035(6)
C5	.0208(7)	.0260(7)	.0286(7)	.0038(6)	.0031(6)	-.0017(6)
C6	.0202(7)	.0182(6)	.0224(6)	.0021(5)	.0033(5)	-.0001(5)
C7	.0189(6)	.0202(7)	.0235(7)	.0041(5)	.0038(5)	.0007(5)
C8	.0209(7)	.0202(6)	.0185(6)	.0032(5)	.0030(5)	.0013(5)
C9	.0219(7)	.0341(8)	.0239(7)	.0040(6)	.0045(6)	.0005(6)
C10	.0300(8)	.0422(9)	.0230(7)	.0030(6)	.0087(6)	.0041(7)
C11	.0360(9)	.0383(8)	.0192(7)	-.0034(6)	.0027(6)	.0019(7)
C12	.0245(7)	.0323(8)	.0247(7)	-.0015(6)	.0000(6)	-.0007(6)
C13	.0205(7)	.0223(7)	.0219(6)	.0018(5)	.0041(5)	.0015(5)
C14	.0167(6)	.0314(7)	.0219(6)	.0012(6)	.0013(5)	.0002(6)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

;

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

O1	C1	1.3192(16)	.	.	yes
O2	C14	1.2809(17)	.	.	yes
O3	C14	1.2296(18)	.	.	yes
O1	H1	1.10(2)	.	.	no
N1	C7	1.3022(18)	.	.	yes
N1	C8	1.4264(16)	.	.	yes
N1	H1'	.948(18)	.	.	no
C1	C2	1.4070(19)	.	.	no
C1	C6	1.4198(19)	.	.	no
C2	C3	1.375(2)	.	.	no
C3	C4	1.399(2)	.	.	no
C4	C5	1.3725(19)	.	.	no
C5	C6	1.414(2)	.	.	no
C6	C7	1.4250(19)	.	.	no
C8	C13	1.4004(19)	.	.	no
C8	C9	1.3923(19)	.	.	no
C9	C10	1.3808(19)	.	.	no
C10	C11	1.384(2)	.	.	no
C11	C12	1.383(2)	.	.	no
C12	C13	1.3896(19)	.	.	no
C13	C14	1.5150(19)	.	.	no
C2	H2	1.006(16)	.	.	no
C3	H3	.987(16)	.	.	no
C4	H4	.940(19)	.	.	no
C5	H5	1.000(18)	.	.	no
C7	H7	.996(16)	.	.	no
C9	H9	.932(19)	.	.	no
C10	H10	.994(16)	.	.	no
C11	H11	.956(18)	.	.	no
C12	H12	.940(18)	.	.	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							
C1	O1	H1	114.6(11)	.	.	.	no
C7	N1	C8	125.99(12)	.	.	.	yes
C7	N1	H1'	116.5(11)	.	.	.	no
C8	N1	H1'	117.5(11)	.	.	.	no
O1	C1	C2	122.93(12)	.	.	.	yes
O1	C1	C6	118.57(12)	.	.	.	yes
C2	C1	C6	118.50(12)	.	.	.	no
C1	C2	C3	120.24(13)	.	.	.	no
C2	C3	C4	121.78(13)	.	.	.	no
C3	C4	C5	118.99(14)	.	.	.	no
C4	C5	C6	120.92(13)	.	.	.	no
C1	C6	C5	119.55(12)	.	.	.	no
C1	C6	C7	122.88(12)	.	.	.	no
C5	C6	C7	117.56(12)	.	.	.	no
N1	C7	C6	125.15(12)	.	.	.	yes
C9	C8	C13	120.37(11)	.	.	.	no
N1	C8	C13	118.47(11)	.	.	.	yes
N1	C8	C9	121.10(12)	.	.	.	yes
C8	C9	C10	119.67(13)	.	.	.	no
C9	C10	C11	120.82(13)	.	.	.	no
C10	C11	C12	119.23(13)	.	.	.	no
C11	C12	C13	121.43(13)	.	.	.	no
C12	C13	C14	118.32(12)	.	.	.	no
C8	C13	C12	118.47(12)	.	.	.	no
C8	C13	C14	123.21(12)	.	.	.	no
O2	C14	O3	126.01(13)	.	.	.	yes
O2	C14	C13	114.75(11)	.	.	.	yes
O3	C14	C13	119.23(12)	.	.	.	yes
C1	C2	H2	117.8(9)	.	.	.	no
C3	C2	H2	121.9(9)	.	.	.	no
C2	C3	H3	120.5(10)	.	.	.	no
C4	C3	H3	117.8(10)	.	.	.	no
C3	C4	H4	120.7(11)	.	.	.	no
C5	C4	H4	120.3(11)	.	.	.	no
C4	C5	H5	122.1(10)	.	.	.	no
C6	C5	H5	117.0(10)	.	.	.	no
N1	C7	H7	119.4(9)	.	.	.	no
C6	C7	H7	115.5(9)	.	.	.	no
C8	C9	H9	119.4(11)	.	.	.	no
C10	C9	H9	120.9(11)	.	.	.	no
C9	C10	H10	117.6(10)	.	.	.	no
C11	C10	H10	121.6(10)	.	.	.	no
C10	C11	H11	122.3(10)	.	.	.	no
C12	C11	H11	118.4(10)	.	.	.	no
C11	C12	H12	119.9(10)	.	.	.	no
C13	C12	H12	118.7(10)	.	.	.	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								
_geom_torsion_site_symmetry_1								
_geom_torsion_site_symmetry_2								
_geom_torsion_site_symmetry_3								
_geom_torsion_site_symmetry_4								
_geom_torsion_publ_flag								
C7	N1	C8	C13	-168.22(13)	.	.	.	no
C7	N1	C8	C9	9.0(2)	.	.	.	no
C8	N1	C7	C6	179.67(12)	.	.	.	no
C2	C1	C6	C5	.03(18)	.	.	.	no

C2	C1	C6	C7	-178.76(12)	.	.	.	.	no
O1	C1	C2	C3	179.75(15)	.	.	.	.	no
C6	C1	C2	C3	-1.22(19)	.	.	.	.	no
O1	C1	C6	C5	179.10(12)	.	.	.	.	no
O1	C1	C6	C7	.3(2)	.	.	.	.	no
C1	C2	C3	C4	1.1(2)	.	.	.	.	no
C2	C3	C4	C5	.2(2)	.	.	.	.	no
C3	C4	C5	C6	-1.4(2)	.	.	.	.	no
C4	C5	C6	C1	1.3(2)	.	.	.	.	no
C4	C5	C6	C7	-179.85(12)	.	.	.	.	no
C1	C6	C7	N1	-7.3(2)	.	.	.	.	no
C5	C6	C7	N1	173.91(13)	.	.	.	.	no
N1	C8	C13	C12	176.34(12)	.	.	.	.	no
N1	C8	C9	C10	-176.95(12)	.	.	.	.	no
C13	C8	C9	C10	.2(2)	.	.	.	.	no
C9	C8	C13	C14	179.83(13)	.	.	.	.	no
N1	C8	C13	C14	-2.98(19)	.	.	.	.	no
C9	C8	C13	C12	-.8(2)	.	.	.	.	no
C8	C9	C10	C11	.3(2)	.	.	.	.	no
C9	C10	C11	C12	-.1(2)	.	.	.	.	no
C10	C11	C12	C13	-.6(2)	.	.	.	.	no
C11	C12	C13	C8	1.1(2)	.	.	.	.	no
C11	C12	C13	C14	-179.58(12)	.	.	.	.	no
C8	C13	C14	O2	-31.70(19)	.	.	.	.	no
C8	C13	C14	O3	149.09(14)	.	.	.	.	no
C12	C13	C14	O2	148.98(13)	.	.	.	.	no
C12	C13	C14	O3	-30.23(19)	.	.	.	.	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

O1	O2	2.9471(14)	.	.	.	no
O1	N1	2.6555(16)	.	.	.	no
O1	C5	3.4075(18)	.	3_575	.	no
O1	O2	2.4534(14)	.	2_555	.	no
O1	C14	3.2893(18)	.	2_555	.	no
O2	O1	2.4534(14)	.	2_555	.	no
O2	O1	2.9471(14)	.	.	.	no
O2	N1	2.6672(16)	.	.	.	no
O2	C2	3.3533(19)	.	2_555	.	no
O2	C1	3.2694(18)	.	2_555	.	no
O3	C9	3.237(2)	.	4_575	.	no
O3	C7	3.2329(19)	.	4_575	.	no
O1	H1'	1.936(18)	.	.	.	no
O2	H1	1.36(2)	.	2_555	.	no
O2	H1'	1.952(18)	.	.	.	no
O2	H2	2.714(16)	.	2_555	.	no
O3	H1	2.63(2)	.	2_555	.	no
O3	H12	2.568(16)	.	.	.	no
O3	H7	2.256(16)	.	4_575	.	no
O3	H9	2.391(19)	.	4_575	.	no
O3	H11	2.893(14)	.	7_575	.	no
N1	O1	2.6555(16)	.	.	.	no
N1	O2	2.6672(16)	.	.	.	no
N1	C3	3.3159(19)	.	3_565	.	no
C1	C6	3.4621(19)	.	3_565	.	no
C1	O2	3.2694(18)	.	2_555	.	no
C1	C5	3.412(2)	.	3_565	.	no
C1	C6	3.4201(19)	.	3_575	.	no
C1	C7	3.1465(19)	.	3_575	.	no
C2	C7	3.465(2)	.	3_565	.	no
C2	O2	3.3533(19)	.	2_555	.	no
C2	C7	3.382(2)	.	3_575	.	no

C2	C8	3.550(2)	.	3_575	no
C3	C13	3.476(2)	.	3_575	no
C3	C8	3.255(2)	.	3_575	no
C3	N1	3.3159(19)	.	3_565	no
C3	C7	3.417(2)	.	3_565	no
C4	C14	3.502(2)	.	3_575	no
C4	C13	3.559(2)	.	3_575	no
C5	C1	3.412(2)	.	3_565	no
C5	O1	3.4075(18)	.	3_575	no
C6	C1	3.4201(19)	.	3_575	no
C6	C6	3.345(2)	.	3_575	no
C6	C1	3.4621(19)	.	3_565	no
C6	C7	3.405(2)	.	3_575	no
C6	C6	3.524(2)	.	3_565	no
C7	O3	3.2329(19)	.	4_475	no
C7	C1	3.1465(19)	.	3_575	no
C7	C2	3.382(2)	.	3_575	no
C7	C3	3.417(2)	.	3_565	no
C7	C2	3.465(2)	.	3_565	no
C7	C6	3.405(2)	.	3_575	no
C8	C2	3.550(2)	.	3_575	no
C8	C3	3.255(2)	.	3_575	no
C9	O3	3.237(2)	.	4_475	no
C12	C12	3.520(2)	.	7_565	no
C12	C12	3.479(2)	.	7_575	no
C13	C4	3.559(2)	.	3_575	no
C13	C3	3.476(2)	.	3_575	no
C14	O1	3.2893(18)	.	2_555	no
C14	C4	3.502(2)	.	3_575	no
C1	H1'	2.600(18)	.	.	no
C2	H10	3.068(16)	.	8_564	no
C7	H9	2.641(18)	.	.	no
C9	H7	2.620(16)	.	.	no
C10	H2	3.026(16)	.	8_565	no
C14	H1'	2.515(18)	.	.	no
C14	H1	2.25(2)	.	2_555	no
C14	H2	2.972(16)	.	2_555	no
H1	H2	2.32(3)	.	.	no
H1	O2	1.36(2)	.	2_555	no
H1	O3	2.63(2)	.	2_555	no
H1	C14	2.25(2)	.	2_555	no
H1'	O1	1.936(18)	.	.	no
H1'	O2	1.952(18)	.	.	no
H1'	C1	2.600(18)	.	.	no
H1'	C14	2.515(18)	.	.	no
H2	H1	2.32(3)	.	.	no
H2	O2	2.714(16)	.	2_555	no
H2	C14	2.972(16)	.	2_555	no
H2	C10	3.026(16)	.	8_564	no
H2	H10	2.38(2)	.	8_564	no
H5	H7	2.26(2)	.	.	no
H7	C9	2.620(16)	.	.	no
H7	H5	2.26(2)	.	.	no
H7	H9	2.06(2)	.	.	no
H7	O3	2.256(16)	.	4_475	no
H9	C7	2.641(18)	.	.	no
H9	H7	2.06(2)	.	.	no
H9	O3	2.391(19)	.	4_475	no
H10	C2	3.068(16)	.	8_565	no
H10	H2	2.38(2)	.	8_565	no
H11	O3	2.893(14)	.	7_575	no
H12	O3	2.568(16)	.	.	no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A

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_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag

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#
#D      H      A      D - H      H...A      D...A      D - H...A      symm(A)
#
O1      H1      O2      1.10(2)      1.36(2)  2.4534(14)  172.7(19)  2_555 yes
N1      H1'     O1      .948(18)  1.936(18)  2.6555(16)  130.9(15)  . yes
N1      H1'     O2      .948(18)  1.952(18)  2.6672(16)  130.5(15)  . yes
C7      H7      O3      .996(16)  2.256(16)  3.2329(19)  166.4(11)  4_475 yes
C9      H9      O3      .932(19)  2.391(19)   3.237(2)   150.9(17)  4_475 yes

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# End of Crystallographic Information File

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