

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cuce

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cuce

Bond precision:	C-C = 0.0086 A	Wavelength=0.71073	
Cell:	a=13.9772(17)	b=13.9772(17)	c=22.773(2)
	alpha=90	beta=90	gamma=120
Temperature:	150 K		
	Calculated	Reported	
Volume	3852.9(12)	3852.9(10)	
Space group	P 32 2 1	P 32 2 1	
Hall group	P 32 2"	P 32 2"	
Moiety formula	C30 H34 Ce Cl2 Cu2 N11	C30 H34 Ce Cl2 Cu2 N11	
	O13, 2(C3 H6 N O), H2 O	O13, 2(C3 H6 N O), H2 O	
Sum formula	C36 H48 Ce Cl2 Cu2 N13 O16	C36 H48 Ce Cl2 Cu2 N13 O16	
Mr	1256.99	1256.97	
Dx,g cm-3	1.625	1.625	
Z	3	3	
Mu (mm-1)	1.871	1.871	
F000	1899.0	1899.0	
F000'	1901.77		
h,k,lmax	18,18,29	18,18,29	
Nref	5936[3325]	5931	
Tmin,Tmax	0.669,0.728	0.620,0.746	
Tmin'	0.656		

Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 1.78/1.00 Theta(max)= 27.545

R(reflections)= 0.0372(5369) wR2(reflections)= 0.1011(5931)

S = 1.045 Npar= 305

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

● Alert level B

PLAT220_ALERT_2_B	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	7.2	Ratio
PLAT220_ALERT_2_B	Non-Solvent	Resd 1	N	Ueq(max)/Ueq(min)	Range	6.3	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N2	--C2	.		13.5	s.u.
PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j)	Tensor			4.8	Note
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O8A				0.159	Check

● Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.460
From the CIF: _refine_ls_abs_structure_Flack_su 0.020

PLAT220_ALERT_2_C	Non-Solvent	Resd 1	O	Ueq(max)/Ueq(min)	Range	5.4	Ratio	
PLAT222_ALERT_3_C	Non-Solv.	Resd 1	H	Uiso(max)/Uiso(min)	Range	9.9	Ratio	
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N2	--C3	.		0.20	Ang.	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			01	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			03	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			Ce1	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			N2	Check	
PLAT243_ALERT_4_C	High	'Solvent'	Ueq as Compared to Neighbors of			C16	Check	
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of			N7	Check	
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.00862	Ang.	
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#				1	Note	
		C30	H34	Ce	C12	Cu2	N11	O13
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers				1	Check	
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.04A	From	O1		-0.40	eA-3	
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.					0	Info	

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...				8	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension					3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				3	Report
PLAT012_ALERT_1_G	No	_shelx_res_checksum	Found in CIF		Please	Check
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero	.				0.460	Note
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by	...				2	Units
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records					6	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records					3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records					3	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ce1	--O3	.		5.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of	O2	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	N1	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	O8A	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	O8B	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H10A	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H10B	Constrained at			0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)				3%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)				20%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety				C2	Check
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for	O8A			64.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for	O8B			67.8	Degree
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.				1.26	Ratio

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PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Cu1      --Cu1      ..      9.03 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Cu1      --Cu1      ..      7.04 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Cu1      --Cu1      ..      10.76 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      79 Check
                   N1      -O1      -N1      1.555      1.555      6.556      21.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      82 Check
                   N1      -O2      -N1      1.555      1.555      6.556      31.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      101 Check
                   N1      -N1      -O1      6.556      1.555      6.556      20.60 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #      2 Note
                   C3 H6 N O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #      3 Note
                   H2 O
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1      (II)      .      2.10 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      34 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      4 Note

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0 ALERT level A = Most likely a serious problem - resolve or explain
5 ALERT level B = A potentially serious problem, consider carefully
16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
34 ALERT level G = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
24 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```

# start Validation Reply Form
_vrf_ABSTY02_cuce
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_STRVA01_cuce
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT220_cuce
;
PROBLEM: Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range      5.4 Ratio
RESPONSE: ...
;
_vrf_PLAT222_cuce
;
PROBLEM: Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range      9.9 Ratio
RESPONSE: ...
;
_vrf_PLAT234_cuce
;
PROBLEM: Large Hirshfeld Difference N2      --C3      .      0.20 Ang.
RESPONSE: ...
;

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_vrf_PLAT241_cuce
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      01 Check
RESPONSE: ...
;
_vrf_PLAT242_cuce
;
PROBLEM: Low       'MainMol' Ueq as Compared to Neighbors of      Cε1 Check
RESPONSE: ...
;
_vrf_PLAT243_cuce
;
PROBLEM: High      'Solvent' Ueq as Compared to Neighbors of      C16 Check
RESPONSE: ...
;
_vrf_PLAT244_cuce
;
PROBLEM: Low       'Solvent' Ueq as Compared to Neighbors of      N7 Check
RESPONSE: ...
;
_vrf_PLAT342_cuce
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00862 Ang.
RESPONSE: ...
;
_vrf_PLAT790_cuce
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. #      1 Note
RESPONSE: ...
;
_vrf_PLAT934_cuce
;
PROBLEM: Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....      1 Check
RESPONSE: ...
;
_vrf_PLAT976_cuce
;
PROBLEM: Check Calcd Resid. Dens.  1.04A    From O1      -0.40 eA-3
RESPONSE: ...
;
_vrf_PLAT978_cuce
;
PROBLEM: Number C-C Bonds with Positive Residual Density.      0 Info
RESPONSE: ...
;
# end Validation Reply Form

```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

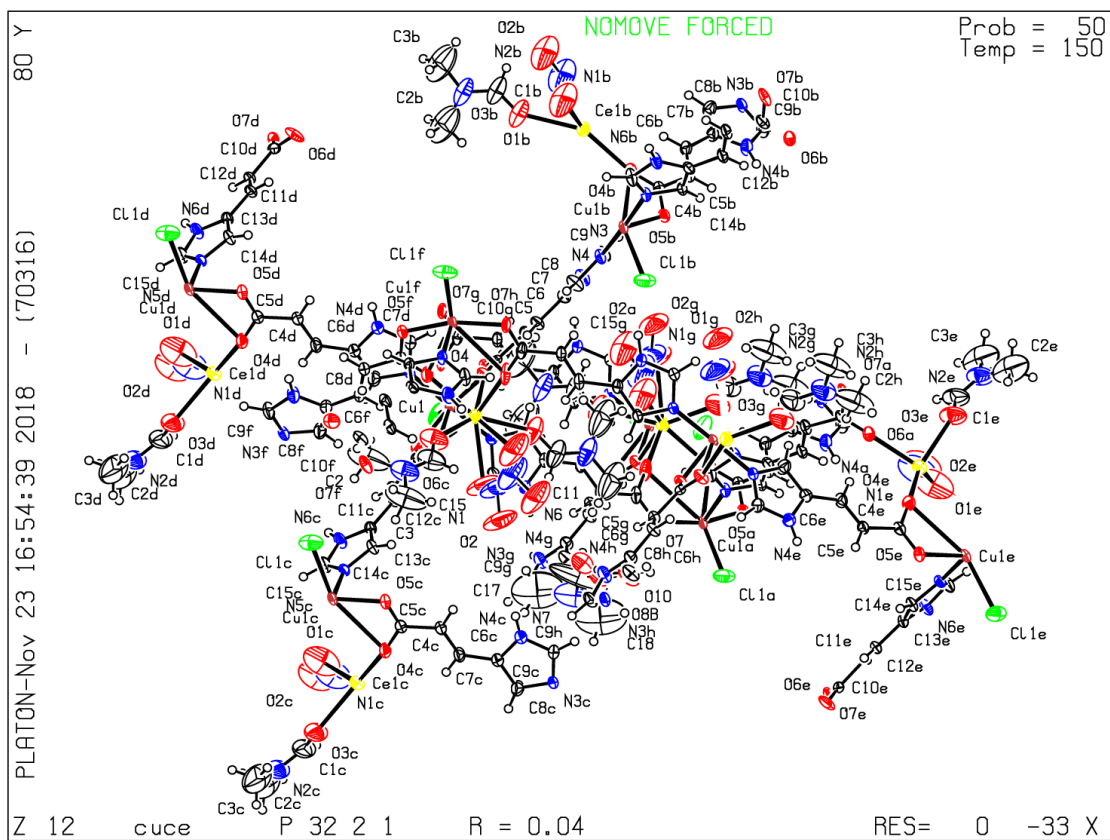
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/10/2018; check.def file version of 15/10/2018



```

data_cuce

_audit_update_record
;
2018-11-23 # Formatted by publCIF

;

# publCIF _publ_body_element loop start
loop_
  _publ_body_element
  _publ_body_title
  _publ_body_contents

  section
;
Introduction
;
;

;
  section
;
Experimental
;
;

;
  subsection
;
Synthesis and crystallization
;
;

;
  subsection
;
Refinement
;
;
Crystal data, data collection and structure refinement details are
summarized
in Table 1.
;

  section
;
Results and discussion
;
;

;
# publCIF _publ_body_element loop end
_audit_creation_date          2018-11-23

```

```

_audit_creation_method
;
Olex2 1.2
(compiled 2017.03.28 svn.r3405 for OlexSys, GUI svn.r5335)
;
_shelx_SHELXL_version_number      '2014/7'
_publ_contact_author_address       ?
_publ_contact_author_email         ?
_publ_contact_author_id_orcid      ?
_publ_contact_author_name          ''
_publ_contact_author_phone         ?
_publ_section_references
;
Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G.
L., De
Caro, L., Giacovazzo, C., Polidori, G., Siliqi, D. & Spagna, R. (2007).
<i>J. Appl. Cryst.</i> 40, 609--613.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. &
Puschmann,
H. (2009). <i>J. Appl. Cryst.</i> 42, 339--341.

Sheldrick, G. M. (2015). <i>Acta Cryst.</i> C71, 3--8.
;
_chemical_name_common              ?
_chemical_name_systematic          ?
_chemical_formula_moiety           'C30 H34 Ce Cl2 Cu2 N11 O13, 2(C3 H6 N O), H2 O'
_chemical_formula_sum               'C36 H48 Ce Cl2 Cu2 N13 O16'
_chemical_formula_weight           1256.97
_chemical_absolute_configuration    ?
_chemical_melting_point            ?
loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_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 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
  'Ce' 'Ce' -0.2486 2.6331
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Cl' 'Cl' 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
  'Cu' 'Cu' 0.3201 1.2651 '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'

```


_shelx_space_group_comment

;

The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names. They are only intended as comments.

;

_space_group_crystal_system trigonal
_space_group_IT_number 154
_space_group_name_H-M_alt 'P 32 2 1'
_space_group_name_Hall 'P 32 2'''

loop_

_space_group_symop_operation_xyz

'x, y, z'

'-y, x-y, z+2/3'

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

'y, x, -z'

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

'-x, -x+y, -z+2/3'

_cell_length_a 13.9772(17)
_cell_length_b 13.9772(17)
_cell_length_c 22.773(2)
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 120
_cell_volume 3852.9(10)
_cell_formula_units_Z 3
_cell_measurement_reflns_used 9680
_cell_measurement_temperature 150(2)
_cell_measurement_theta_max 27.42
_cell_measurement_theta_min 2.46
_shelx_estimated_absorpt_T_max ?
_shelx_estimated_absorpt_T_min ?
_exptl_absorpt_coefficient_mu 1.871
_exptl_absorpt_correction_T_max 0.7456
_exptl_absorpt_correction_T_min 0.6198
_exptl_absorpt_correction_type multi-scan
_exptl_absorpt_process_details ?
_exptl_absorpt_special_details ?
_exptl_crystal_colour blue
_exptl_crystal_density_diffn 1.625
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?
_exptl_crystal_description prism
_exptl_crystal_F_000 1899
_exptl_crystal_size_max 0.22
_exptl_crystal_size_mid 0.20
_exptl_crystal_size_min 0.17
_exptl_transmission_factor_max ?
_exptl_transmission_factor_min ?
_diffn_reflns_av_R_equivalents 0.0367
_diffn_reflns_av_unetI/netI 0.0439
_diffn_reflns_Laue_measured_fraction_full 0.999

```

_diffrn_reflns_Laue_measured_fraction_max 0.998
_diffrn_reflns_limit_h_max      18
_diffrn_reflns_limit_h_min     -18
_diffrn_reflns_limit_k_max      18
_diffrn_reflns_limit_k_min     -18
_diffrn_reflns_limit_l_max      29
_diffrn_reflns_limit_l_min      0
_diffrn_reflns_number           17514
_diffrn_reflns_point_group_measured_fraction_full 0.999
_diffrn_reflns_point_group_measured_fraction_max 0.998
_diffrn_reflns_theta_full       25.242
_diffrn_reflns_theta_max        27.545
_diffrn_reflns_theta_min        2.456
_diffrn_ambient_temperature     150.00
_diffrn_detector_area_resol_mean ?
_diffrn_measured_fraction_theta_full 0.999
_diffrn_measured_fraction_theta_max 0.998
_diffrn_measurement_device_type 'D8 VENTURE Bruker AXS'
_diffrn_measurement_method      'rotation images'
_diffrn_radiation_type          MoK\alpha
_diffrn_radiation_wavelength    0.71073
_diffrn_source                  ?
_reflns_Friedel_coverage        0.786
_reflns_Friedel_fraction_full   1.000
_reflns_Friedel_fraction_max    0.998
_reflns_number_gt               5369
_reflns_number_total            5931
_reflns_special_details
;
Reflections were merged by SHELXL according to the crystal
class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique
Friedel pairs measured divided by the number that would be
possible theoretically, ignoring centric projections and
systematic absences.
;
_reflns_threshold_expression     'I > 2\sigma(I)'
_computing_cell_refinement       'APEX3 (Bruker, 2015); SAINT (Bruker,
2014)'
_computing_data_collection       'SAINT (Bruker, 2014)'
_computing_data_reduction        'SAINT (Bruker, 2014)'
_computing_molecular_graphics    'Olex2 (Dolomanov et al., 2009)'
_computing_publication_material 'Olex2 (Dolomanov et al., 2009)'
_computing_structure_refinement  'ShelXL (Sheldrick, 2015)'
_computing_structure_solution    'SIR2004 (Burla et al., 2007)'
_refine_diff_density_max         1.137
_refine_diff_density_min        -0.751
_refine_diff_density_rms        0.102
_refine_ls_abs_structure_details
;
Refined as an inversion twin.
;
_refine_ls_abs_structure_Flack   0.46(2)

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```

_refine_ls_extinction_coef      .
_refine_ls_extinction_method    none
_refine_ls_goodness_of_fit_ref  1.045
_refine_ls_hydrogen_treatment  mixed
_refine_ls_matrix_type          full
_refine_ls_number_parameters    305
_refine_ls_number_reflns        5931
_refine_ls_number_restraints    34
_refine_ls_R_factor_all         0.0445
_refine_ls_R_factor_gt          0.0372
_refine_ls_restrained_S_all     1.042
_refine_ls_shift/su_max         0.000
_refine_ls_shift/su_mean        0.000
_refine_ls_structure_factor_coef Fsqd
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0585P)^2^+2.7045P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_weighting_scheme      calc
_refine_ls_wR_factor_gt          0.0979
_refine_ls_wR_factor_ref         0.1011
_refine_special_details
;
  Refined as a 2-component inversion twin.
;
_olex2_refinement_description
;
1. Twinned data refinement
  Scales: 0.54(2)
          0.46(2)
2. Fixed Uiso
  At 1.2 times of:
    All C(H) groups, All N(H) groups
  At 1.5 times of:
    All C(H,H,H) groups, All O(H,H) groups
3. Rigid bond restraints
  O1, N1
  with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
  N2, C1
  with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
  O1, O2, N1
  with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
4. Uiso/Uanis restraints and constraints
  Uanis(C1) \sim Ueq: with sigma of 0.1 and sigma for terminal atoms of
  0.2
  Uanis(N7) \sim Ueq, Uanis(N2) \sim Ueq: with sigma of 0.1 and sigma for
  terminal atoms of 0.2
  Uanis(C2) \sim Ueq, Uanis(C3) \sim Ueq: with sigma of 0.1 and sigma for
  terminal atoms of 0.2
  Uanis(O1) = Uanis(N1)
  Uanis(N2) = Uanis(C1) = Uanis(O3)
  Uanis(C18) = Uanis(C17)
  Uanis(O8B) = Uanis(O8A)
  Uanis(C2) = Uanis(C3)
  Uanis(O2) = Uanis(O1)
5. Others

```

```

Fixed Sof: O2(0.5) H10A(0.5) H10B(0.5) N1(0.5) O8A(0.5) O8B(0.5)
6.a Free rotating group:
  O10(H10A,H10B)
6.b Aromatic/amide H refined with riding coordinates:
  N4(H4), C1(H1), C5(H5), C6(H6A), C8(H8), C9(H9), C11(H11), C12(H12),
  C14(H14),
  C15(H15)
6.c Idealised Me refined as rotating group:
  C2(H2A,H2B,H2C), C3(H3A,H3B,H3C), C17(H17A,H17B,H17C),
  C18(H18A,H18B,H18C)
;
_atom_sites_solution_hydrogens    mixed
_atom_sites_solution_primary       direct
_atom_sites_solution_secondary     ?
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_site_symmetry_order
  _atom_site_calc_flag
  _atom_site_refinement_flags_posn
  _atom_site_refinement_flags_adp
  _atom_site_refinement_flags_occupancy
  _atom_site_disorder_assembly
  _atom_site_disorder_group
Cel Ce 0.0000 0.64408(4) 0.8333 0.02814(13) Uani 1 2 d S T P . .
Cul Cu -0.29061(6) 0.66736(5) 0.83921(2) 0.01851(15) Uani 1 1 d . . . .
.
C11 Cl -0.48442(16) 0.63889(18) 0.84675(9) 0.0520(5) Uani 1 1 d . . . A
1
O1 O -0.0841(12) 0.4372(8) 0.8614(5) 0.127(4) Uani 1 1 d . U . . .
O2 O -0.032(2) 0.3295(13) 0.8655(8) 0.127(4) Uani 0.5 1 d . U . . .
O3 O 0.1037(6) 0.6359(7) 0.9205(3) 0.0764(15) Uani 1 1 d . . . . .
O4 O -0.0783(4) 0.7403(4) 0.78340(17) 0.0301(10) Uani 1 1 d . . . . .
O5 O -0.2286(3) 0.7487(3) 0.76291(15) 0.0237(8) Uani 1 1 d . . . . .
O6 O -0.5910(4) 0.2547(4) 0.56223(18) 0.0389(13) Uani 1 1 d . . . . .
O7 O -0.5856(4) 0.1043(4) 0.58378(16) 0.0294(10) Uani 1 1 d . . . . .
O10 O -0.4974(7) 0.0000 0.6667 0.074(3) Uani 1 2 d S T P . .
H10A H -0.5227 -0.0229 0.6324 0.112 Uiso 0.5 1 d G . . . .
H10B H -0.5436 0.0102 0.6861 0.112 Uiso 0.5 1 d G . . . .
N1 N -0.030(3) 0.422(2) 0.8476(16) 0.127(4) Uani 0.5 1 d . U . . .
N2 N 0.1787(7) 0.5880(8) 0.9932(4) 0.0764(15) Uani 1 1 d . U . . .
N3 N 0.1909(4) 0.9709(4) 0.54904(18) 0.0236(10) Uani 1 1 d . . . . .
N4 N 0.0202(5) 0.9141(5) 0.57585(19) 0.0312(12) Uani 1 1 d . . . . .
H4 H -0.0484 0.9004 0.5742 0.037 Uiso 1 1 calc R . . . .
N5 N -0.3482(4) 0.5291(4) 0.79436(17) 0.0202(10) Uani 1 1 d . . . . .
N6 N -0.4225(5) 0.3532(4) 0.77085(19) 0.0291(11) Uani 1 1 d . . . . .
H6 H -0.451(5) 0.276(6) 0.779(3) 0.022(16) Uiso 1 1 d . . . B 2
C1 C 0.1459(9) 0.5864(10) 0.9421(5) 0.0764(15) Uani 1 1 d . U . . .

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H1 H 0.1555 0.5390 0.9159 0.092 Uiso 1 1 calc R
 C2 C 0.1736(13) 0.6598(15) 1.0384(8) 0.146(6) Uani 1 1 d . U . . .
 H2A H 0.1231 0.6144 1.0697 0.218 Uiso 1 1 calc GR
 H2B H 0.1468 0.7062 1.0210 0.218 Uiso 1 1 calc GR
 H2C H 0.2475 0.7069 1.0549 0.218 Uiso 1 1 calc GR
 C3 C 0.2171(14) 0.5174(15) 1.0128(8) 0.146(6) Uani 1 1 d . U . . .
 H3A H 0.2878 0.5610 1.0331 0.218 Uiso 1 1 calc GR
 H3B H 0.2272 0.4799 0.9790 0.218 Uiso 1 1 calc GR
 H3C H 0.1631 0.4624 1.0398 0.218 Uiso 1 1 calc GR
 C4 C -0.1357(5) 0.7621(5) 0.7499(2) 0.0200(10) Uani 1 1 d
 C5 C -0.0896(5) 0.8115(5) 0.6912(2) 0.0230(11) Uani 1 1 d
 H5 H -0.1337 0.8258 0.6649 0.028 Uiso 1 1 calc R
 C6 C 0.0109(5) 0.8359(5) 0.6750(2) 0.0266(12) Uani 1 1 d
 H6A H 0.0510 0.8179 0.7021 0.032 Uiso 1 1 calc R
 C7 C 0.0666(5) 0.8870(5) 0.6207(2) 0.0249(12) Uani 1 1 d
 C8 C 0.1721(6) 0.9226(6) 0.6042(3) 0.0336(16) Uani 1 1 d
 H8 H 0.2252 0.9156 0.6269 0.040 Uiso 1 1 calc R
 C9 C 0.0986(5) 0.9657(6) 0.5344(3) 0.0310(15) Uani 1 1 d
 H9 H 0.0876 0.9946 0.4989 0.037 Uiso 1 1 calc R
 C10 C -0.5667(5) 0.1990(6) 0.5959(2) 0.0259(12) Uani 1 1 d
 C11 C -0.5110(5) 0.2486(5) 0.6530(2) 0.0249(12) Uani 1 1 d
 H11 H -0.4971 0.2051 0.6799 0.030 Uiso 1 1 calc R
 C12 C -0.4808(5) 0.3515(6) 0.6668(2) 0.0262(12) Uani 1 1 d
 H12 H -0.4927 0.3938 0.6381 0.031 Uiso 1 1 calc R
 C13 C -0.4309(5) 0.4057(5) 0.7219(2) 0.0234(12) Uani 1 1 d
 C14 C -0.3835(5) 0.5145(5) 0.7370(2) 0.0233(12) Uani 1 1 d
 H14 H -0.3759 0.5718 0.7116 0.028 Uiso 1 1 calc R
 C15 C -0.3751(6) 0.4286(5) 0.8130(2) 0.0300(14) Uani 1 1 d
 H15 H -0.3619 0.4125 0.8517 0.036 Uiso 1 1 calc R
 O8A O -0.0661(11) 0.1219(13) 0.7679(6) 0.054(3) Uani 0.5 1 d
 O8B O -0.1035(13) 0.0651(14) 0.7473(6) 0.054(3) Uani 0.5 1 d
 N7 N -0.2522(10) 0.0214(14) 0.7830(10) 0.140(7) Uani 1 1 d . U . . .
 C16 C -0.1515(13) 0.078(2) 0.7767(12) 0.219(15) Uani 1 1 d
 C17 C -0.283(3) 0.072(3) 0.8353(14) 0.242(11) Uani 1 1 d
 H17A H -0.3017 0.0227 0.8694 0.363 Uiso 1 1 calc GR
 H17B H -0.3463 0.0796 0.8247 0.363 Uiso 1 1 calc GR
 H17C H -0.2198 0.1442 0.8450 0.363 Uiso 1 1 calc GR
 C18 C -0.332(2) -0.072(2) 0.7543(14) 0.242(11) Uani 1 1 d
 H18A H -0.3004 -0.0843 0.7188 0.363 Uiso 1 1 calc GR
 H18B H -0.3940 -0.0609 0.7435 0.363 Uiso 1 1 calc GR
 H18C H -0.3587 -0.1358 0.7804 0.363 Uiso 1 1 calc GR

loop_

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 Cl1 0.0366(10) 0.0591(12) 0.0701(11) -0.0329(10) -0.0111(8) 0.0312(9)
 O1 0.176(11) 0.041(3) 0.164(8) -0.009(4) -0.072(8) 0.053(5)

O2 0.176(11) 0.041(3) 0.164(8) -0.009(4) -0.072(8) 0.053(5)
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 O4 0.031(3) 0.038(3) 0.0219(18) 0.0094(17) 0.0039(16) 0.018(2)
 O5 0.031(2) 0.026(2) 0.0156(16) 0.0041(14) 0.0035(15) 0.0155(18)
 O6 0.045(3) 0.059(4) 0.026(2) -0.023(2) -0.022(2) 0.036(3)
 O7 0.028(2) 0.031(2) 0.0128(16) -0.0074(15) -0.0006(15) 0.0026(18)
 O10 0.067(4) 0.117(9) 0.056(5) 0.017(6) 0.009(3) 0.059(5)
 N1 0.176(11) 0.041(3) 0.164(8) -0.009(4) -0.072(8) 0.053(5)
 N2 0.055(3) 0.082(4) 0.084(3) 0.028(3) -0.018(2) 0.029(3)
 N3 0.022(3) 0.032(3) 0.0134(19) -0.0005(18) 0.0007(17) 0.011(2)
 N4 0.025(3) 0.045(3) 0.021(2) 0.006(2) 0.0001(19) 0.015(2)
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 C2 0.096(8) 0.150(11) 0.178(12) 0.104(10) 0.018(8) 0.052(8)
 C3 0.096(8) 0.150(11) 0.178(12) 0.104(10) 0.018(8) 0.052(8)
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 C6 0.032(3) 0.031(3) 0.019(2) 0.007(2) 0.002(2) 0.017(3)
 C7 0.025(3) 0.028(3) 0.021(2) 0.003(2) 0.000(2) 0.013(2)
 C8 0.029(3) 0.048(4) 0.028(3) 0.014(3) 0.006(2) 0.022(3)
 C9 0.026(3) 0.041(4) 0.020(3) 0.008(2) 0.004(2) 0.012(3)
 C10 0.016(3) 0.038(4) 0.019(2) -0.010(3) 0.000(2) 0.009(2)
 C11 0.023(3) 0.031(3) 0.015(2) -0.005(2) -0.003(2) 0.009(3)
 C12 0.025(3) 0.038(3) 0.015(2) -0.006(2) -0.004(2) 0.015(3)
 C13 0.026(3) 0.028(3) 0.016(2) -0.005(2) 0.000(2) 0.014(3)
 C14 0.035(3) 0.026(3) 0.014(2) -0.002(2) -0.004(2) 0.019(3)
 C15 0.042(4) 0.023(3) 0.016(2) 0.001(2) -0.004(2) 0.009(3)
 O8A 0.042(7) 0.075(9) 0.056(7) 0.015(5) 0.012(5) 0.037(7)
 O8B 0.042(7) 0.075(9) 0.056(7) 0.015(5) 0.012(5) 0.037(7)
 N7 0.054(7) 0.121(12) 0.239(18) 0.075(12) -0.013(9) 0.040(7)
 C16 0.067(10) 0.27(3) 0.32(3) 0.25(2) 0.066(14) 0.088(14)
 C17 0.18(2) 0.22(2) 0.37(3) 0.06(2) -0.04(2) 0.13(2)
 C18 0.18(2) 0.22(2) 0.37(3) 0.06(2) -0.04(2) 0.13(2)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are
 only

used when they are defined by crystal symmetry. An approximate
 (isotropic)

treatment of cell esds is used for estimating esds involving l.s.
 planes.

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loop_

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_geom_bond_site_symmetry_2

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 Ce1 O4 2.403(4) . ?
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 Cu1 Cu1 7.0406(17) 6_556 ?
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 Cu1 O5 2.019(4) . ?
 Cu1 O7 2.053(4) 3_455 ?
 Cu1 N3 1.978(5) 3_465 ?
 Cu1 N5 1.967(5) . ?
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 O2 N1 1.82(3) 6_556 ?
 O2 N1 1.34(3) . ?
 O3 C1 1.217(12) . ?
 O4 C4 1.250(7) . ?
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 O6 C10 1.255(8) . ?
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 N3 C9 1.298(9) . ?
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 N4 C9 1.349(8) . ?
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 N6 C15 1.331(7) . ?
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 C3 H3B 0.9800 . ?

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 C13 C14 1.364(9) . ?
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 C15 H15 0.9500 . ?
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 O8B C16 1.02(3) . ?
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 N7 C17 1.55(3) . ?
 N7 C18 1.38(3) . ?
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 C17 H17B 0.9800 . ?
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loop_

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 O1 Ce1 N1 18.3(9) 6_556 6_556 ?
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 Cl1 Cu1 Cu1 117.13(6) . 3_455 ?
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 N1 O2 N1 31(2) . 6_556 ?
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 C10 O7 Cu1 114.8(4) . 2_564 ?
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 C1 N2 C3 123.1(14) . . ?
 C3 N2 C2 115.0(12) . . ?
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 C9 N3 Cu1 128.2(4) . 2_674 ?
 C9 N3 C8 105.3(5) . . ?
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 C9 N4 H4 126.2 . . ?
 C9 N4 C7 107.5(5) . . ?
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 C15 N5 Cu1 129.3(4) . . ?
 C15 N5 C14 104.8(5) . . ?
 C13 N6 H6 131(4) . . ?
 C15 N6 H6 121(4) . . ?
 C15 N6 C13 107.7(5) . . ?
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 O3 C1 H1 114.9 . . ?
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 N2 C2 H2B 109.5 . . ?
 N2 C2 H2C 109.5 . . ?

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H2A C2 H2C 109.5 . . ?
H2B C2 H2C 109.5 . . ?
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N2 C3 H3B 109.5 . . ?
N2 C3 H3C 109.5 . . ?
H3A C3 H3B 109.5 . . ?
H3A C3 H3C 109.5 . . ?
H3B C3 H3C 109.5 . . ?
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O4 C4 C5 118.5(6) . . ?
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C5 C6 C7 127.5(5) . . ?
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C8 C7 N4 105.8(5) . . ?
C8 C7 C6 129.8(6) . . ?
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C7 C8 H8 125.1 . . ?
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C16 N7 C18 132(3) . . ?
C18 N7 C17 121(2) . . ?
O8A C16 N7 175(4) . . ?
O8B C16 O8A 47.8(12) . . ?
O8B C16 N7 127(4) . . ?
N7 C17 H17A 109.5 . . ?

N7 C17 H17B 109.5 . . ?
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15 -2 10 -1.1 10.17
15 -2 11 23.12 5.94

15 -2 12 38.42 8.43
15 -2 13 7.53 7.05
15 -1 1 -0.89 11.89
15 -1 2 35.72 16.44
15 -1 3 15.84 4.68
15 -1 4 1.71 12.47
15 -1 5 47.35 6.29
15 -1 6 16.55 5.51
15 -1 7 2.21 5.62
15 -1 8 49.88 6.66
15 -1 9 5.72 5.48
15 -1 10 5.2 5.63
15 -1 11 33.01 9.2
15 0 0 19.81 5.26
15 0 1 6.29 4.89
15 0 2 1.7 4.84
15 0 3 3.23 10.9
15 0 4 15.48 5.86
15 0 5 -4.12 12.88
15 0 6 5.47 5.26
15 0 7 22.07 5.94
15 0 8 -2.14 10.21
15 1 0 17.71 7.68
15 1 1 6.4 17.56
15 1 2 51.11 18.47
15 1 3 28.45 6.3
15 1 4 4.37 5.47
16 -15 1 33.24 6.96
16 -15 2 -8.85 13.55
16 -15 3 19.07 6.45
16 -15 4 24.4 13.4
16 -14 1 -3.08 7.39
16 -14 2 73.45 7.91
16 -14 3 14.82 5.75
16 -14 4 4.1 5.56
16 -14 5 80.19 8.89
16 -14 6 3.45 10.14
16 -14 7 -14.69 7.47
16 -14 8 90.84 15.1
16 -13 1 38.62 10.53
16 -13 2 2.38 4.89
16 -13 3 20.25 6.98
16 -13 4 52.13 6.66
16 -13 5 2.98 5.29
16 -13 6 7.59 8.38
16 -13 7 34 18.41
16 -13 8 10.04 8.12
16 -13 9 3.3 4.36
16 -13 10 27.97 5.06
16 -12 1 63.86 14.57
16 -12 2 -0.95 7.7
16 -12 3 18.83 7.38
16 -12 4 50.25 10.3
16 -12 5 12.17 5.32

16 -12 6 40.86 9.69
16 -12 7 27.35 5.88
16 -12 8 20.54 6.93
16 -12 9 25.15 4.79
16 -12 10 52.83 7.38
16 -12 11 16.35 6.21
16 -11 1 1.98 4.4
16 -11 2 51.52 22.48
16 -11 3 47.69 8.01
16 -11 4 -1.77 6.25
16 -11 5 46.67 6.08
16 -11 6 44.21 11.44
16 -11 7 15.52 4.28
16 -11 8 37.08 4.84
16 -11 9 39.92 5.01
16 -11 10 -3.32 7.02
16 -11 11 62.97 5.82
16 -11 12 31.43 5.02
16 -10 1 94.33 8.29
16 -10 2 -0.42 9.9
16 -10 3 30.13 5.32
16 -10 4 65.44 7.17
16 -10 5 6 4.42
16 -10 6 25.57 5.07
16 -10 7 59.38 9.69
16 -10 8 -3.94 6.3
16 -10 9 2.85 3.9
16 -10 10 53.05 10.32
16 -10 11 -2.4 11.29
16 -10 12 7.45 4.34
16 -10 13 104.01 12.95
16 -9 1 -3.15 11.75
16 -9 2 40.19 5.41
16 -9 3 15.17 4.54
16 -9 4 13.52 4.51
16 -9 5 22.55 7.8
16 -9 6 17.2 4.74
16 -9 7 2.56 3.57
16 -9 8 11.31 3.86
16 -9 9 20.9 4.14
16 -9 10 3.47 3.85
16 -9 11 9.54 4.29
16 -9 12 21.99 9.65
16 -9 13 17.68 4.69
16 -8 1 34.07 7.65
16 -8 2 17.58 4.48
16 -8 3 100.27 17.02
16 -8 4 16.69 9.8
16 -8 5 36.15 4.33
16 -8 6 86.79 12.61
16 -8 7 29.8 4.31
16 -8 8 15.6 4.07
16 -8 9 90 7.31
16 -8 10 37.01 4.87

16 -8 11 14.5 4.39
16 -8 12 63.58 6.11
16 -8 13 21.04 5.5
16 -8 14 9.01 9.33
16 -7 1 81.34 7.57
16 -7 2 -4 5.05
16 -7 3 19.46 4.55
16 -7 4 74.29 6.36
16 -7 5 22.39 6.83
16 -7 6 17.36 4.15
16 -7 7 61.75 8.91
16 -7 8 27.46 4.4
16 -7 9 18.69 4.28
16 -7 10 44.05 5.1
16 -7 11 11.18 5.32
16 -7 12 16.27 6.59
16 -7 13 54.46 5.78
16 -6 1 2.23 6
16 -6 2 70.07 8.54
16 -6 3 12.85 3.58
16 -6 4 0.66 3.16
16 -6 5 57.27 15.87
16 -6 6 17.79 4.54
16 -6 7 5.99 5.23
16 -6 8 34.47 4.54
16 -6 9 15.08 4.62
16 -6 10 5.4 5.12
16 -6 11 46.81 5.42
16 -6 12 15.26 4.54
16 -6 13 3.09 4.46
16 -5 1 44.86 5.7
16 -5 2 15.36 3.66
16 -5 3 75.31 10.81
16 -5 4 44.18 5.44
16 -5 5 8.76 3.5
16 -5 6 36.75 4.48
16 -5 7 30.06 7.73
16 -5 8 5.98 4.53
16 -5 9 57.68 5.64
16 -5 10 29.18 4.64
16 -5 11 1.96 7.85
16 -5 12 21.29 7.51
16 -4 1 4.37 3.37
16 -4 2 43.14 7.98
16 -4 3 43.05 4.57
16 -4 4 12.38 5.98
16 -4 5 11.99 3.93
16 -4 6 54.36 5.22
16 -4 7 25.97 4.48
16 -4 8 37.24 4.86
16 -4 9 28.94 4.64
16 -4 10 6.86 5.57
16 -4 11 22.43 4.83
16 -3 1 2.91 4.69

16 -3 2 36.14 5.79
16 -3 3 11.04 4.7
16 -3 4 9.57 4.03
16 -3 5 57.04 6.6
16 -3 6 13.19 4.15
16 -3 7 0.43 3.99
16 -3 8 44.23 6.7
16 -3 9 27.14 5.02
16 -3 10 -3.81 15.45
16 -2 1 57.38 9.36
16 -2 2 2.06 5.12
16 -2 3 14.02 5.58
16 -2 4 47.84 6.88
16 -2 5 3.66 8.37
16 -2 6 19.08 6.97
16 -2 7 25.77 7.3
16 -2 8 14.85 8.07
16 -1 1 6.62 5.37
16 -1 2 58.68 7.46
16 -1 3 31.41 13.43
16 -1 4 0.84 5.72
17 -14 1 14.94 6.55
17 -13 1 8.06 5.56
17 -13 2 41.03 7.05
17 -13 3 -1.08 8.12
17 -13 4 11.61 6.04
17 -13 5 55.73 11.27
17 -13 6 6.47 6.42
17 -12 1 50.2 6.89
17 -12 2 20.51 9.75
17 -12 3 4.99 5.54
17 -12 4 72.89 14.24
17 -12 5 11.89 5.89
17 -12 6 17.14 9
17 -12 7 55.38 8.95
17 -12 8 3.46 8.57
17 -11 1 3.1 5.26
17 -11 2 14.41 5.52
17 -11 3 23.61 5.95
17 -11 4 -1.79 24.47
17 -11 5 12.61 7.51
17 -11 6 22.17 4.75
17 -11 7 10.03 6.73
17 -11 8 11.11 5.28
17 -11 9 31.21 6.87
17 -10 1 17.19 7.08
17 -10 2 16.61 5.67
17 -10 3 62.11 7.01
17 -10 4 8.3 5.45
17 -10 5 21.27 5.76
17 -10 6 51.76 10.41
17 -10 7 8.06 7.96
17 -10 8 40.73 7.6
17 -10 9 20.46 4.82

17 -10 10 1.24 6.38
17 -9 1 44.19 6.24
17 -9 2 22.63 5.51
17 -9 3 26.47 5.53
17 -9 4 79.46 8.28
17 -9 5 12.21 7.71
17 -9 6 12.13 6.2
17 -9 7 104.42 7.78
17 -9 8 6.67 4.38
17 -9 9 25.36 5.11
17 -9 10 91.94 9.48
17 -8 1 31.49 9.41
17 -8 2 53.11 6.47
17 -8 3 64.63 11.75
17 -8 4 6.82 4.13
17 -8 5 18.88 4.49
17 -8 6 31.77 4.83
17 -8 7 7.84 4.28
17 -8 8 15.99 4.55
17 -8 9 7.91 4.7
17 -8 10 14.91 4.97
17 -7 1 47.02 6.13
17 -7 2 30.83 5.33
17 -7 3 37.2 4.86
17 -7 4 22.56 4.57
17 -7 5 13.66 6.35
17 -7 6 29.33 4.8
17 -7 7 29.36 4.91
17 -7 8 3.66 5.67
17 -7 9 24.99 5.04
17 -7 10 18.99 6.34
17 -6 1 38.44 4.98
17 -6 2 9.49 6.51
17 -6 3 24.97 7.07
17 -6 4 19.47 4.53
17 -6 5 14.34 4.39
17 -6 6 22.7 6.43
17 -6 7 19.54 4.68
17 -6 8 16.22 6.44
17 -6 9 8.65 4.58
17 -5 1 7.47 6.9
17 -5 2 48.98 6.21
17 -5 3 3.92 6.27
17 -5 4 1.18 4.16
17 -5 5 57.74 8.16
17 -5 6 32.18 6.82
17 -5 7 -1.8 9.38
17 -5 8 24.49 7.71
17 -4 1 58.87 5.7
17 -4 2 4.78 5.88
17 -4 3 25.24 4.96
17 -4 4 35.85 8.93
17 -4 5 12.32 5.08
17 -4 6 25.19 7.86

17 -3 1 4.91 10.27
18 -11 1 -3.58 6.98
18 -10 1 8.16 6.98
18 -10 2 -2.23 10.58
18 -10 3 18.54 7.57
18 -9 1 20.19 7.34
18 -9 2 21.48 8.11
18 -9 3 29.13 5.66
18 -8 1 -6.03 6.23
18 -8 2 -6.65 10.27
18 -8 3 25.93 5.65
18 -7 1 13.2 7.05

_iucr_refine_instructions_details
;

cuce.res created by SHELXL-2014/7

TITL shelxs86_a.res in P3(2)21
CELL 0.71073 13.9772 13.9772 22.773 90 90 120
ZERR 3 0.0017 0.0017 0.002 0 0 0
LATT -1
SYMM -Y,+X-Y,0.667+Z
SYMM +Y-X,-X,0.333+Z
SYMM +Y,+X,-Z
SYMM -Y+X,-Y,0.333-Z
SYMM -X,-X+Y,0.667-Z
SFAC C H Ce Cl Cu N O
UNIT 108 144 3 6 6 39 48
EQIV \$1 1-Y+X,1-Y,1.333-Z
EQIV \$2 -X,-X+Y,1.667-Z
EQIV \$3 -1+Y-X,-X,0.333+Z
EQIV \$4 -Y+X,1-Y,1.333-Z
DELU O1 N1
DELU N2 C1
DELU O1 O2 N1
ISOR C1
ISOR N7 N2
ISOR C2 C3
EADP O1 N1
EADP N2 C1 O3
EADP C18 C17
EADP O8B O8A
EADP C2 C3
EADP O2 O1

L.S. 40
PLAN 40
TEMP -123
HTAB N4 O8A_\$4
HTAB N4 O8B_\$4
BIND Ce1 O4
BIND Ce1 O1
BIND Ce1 Cu1_\$1

```

BIND O3 Ce1
CONN 3 0.7 N6
BIND Cu1 Cu1_$2
BIND Cu1 Cu1_$3
CONN 3 C9
CONN 3 0.77 N3
BOND $H
LIST 4
fmap -2
acta
TWIN -1 0 0 0 -1 0 0 0 -1 2
REM <olex2.extras>
REM <HklSrc "%.\cuce.hkl">
REM </olex2.extras>

WGHT      0.058500      2.704500
BASF      0.45520
FVAR      0.17813
CE1   3      0.000000      0.644083      0.833333      10.50000      0.03094
0.02784 =
      0.02669      -0.00279      -0.00559      0.01547
CU1   5      -0.290614      0.667359      0.839205      11.00000      0.02668
0.01785 =
      0.01015      -0.00039      -0.00170      0.01051
PART 1
CL1   4      -0.484425      0.638892      0.846746      11.00000      0.03659
0.05907 =
      0.07012      -0.03291      -0.01111      0.03121
PART 0
O1    7      -0.084126      0.437211      0.861449      11.00000      0.17602
0.04080 =
      0.16367      -0.00872      -0.07166      0.05286
O2    7      -0.032239      0.329515      0.865515      10.50000      0.17602
0.04080 =
      0.16367      -0.00872      -0.07166      0.05286
O3    7      0.103667      0.635950      0.920465      11.00000      0.05548
0.08211 =
      0.08415      0.02781      -0.01821      0.02875
O4    7      -0.078320      0.740309      0.783403      11.00000      0.03082
0.03814 =
      0.02188      0.00940      0.00391      0.01758
O5    7      -0.228603      0.748750      0.762909      11.00000      0.03080
0.02622 =
      0.01564      0.00412      0.00351      0.01547
O6    7      -0.591022      0.254661      0.562235      11.00000      0.04455
0.05933 =
      0.02615      -0.02321      -0.02247      0.03596
O7    7      -0.585600      0.104281      0.583775      11.00000      0.02848
0.03061 =
      0.01280      -0.00737      -0.00063      0.00260

AFIX      6
O10   7      -0.497441      0.000000      0.666667      10.50000      0.06701
0.11711 =

```

		0.05596	0.01702	0.00851	0.05856	
H10A	2	-0.522691	-0.022902	0.632420	10.50000	-1.50000
H10B	2	-0.543594	0.010166	0.686080	10.50000	-1.50000
AFIX	0					
N1	6	-0.029703	0.422147	0.847591	10.50000	0.17602
		0.04080				
		0.16367	-0.00872	-0.07166	0.05286	
N2	6	0.178656	0.588042	0.993231	11.00000	0.05548
		0.08211				
		0.08415	0.02781	-0.01821	0.02875	
N3	6	0.190877	0.970946	0.549040	11.00000	0.02231
		0.03166				
		0.01338	-0.00051	0.00072	0.01102	
N4	6	0.020219	0.914081	0.575850	11.00000	0.02451
		0.04532				
		0.02118	0.00644	0.00010	0.01547	
AFIX	43					
H4	2	-0.048393	0.900408	0.574175	11.00000	-1.20000
AFIX	0					
N5	6	-0.348225	0.529082	0.794361	11.00000	0.02255
		0.01966				
		0.01445	0.00044	-0.00309	0.00768	
N6	6	-0.422517	0.353218	0.770855	11.00000	0.04257
		0.02072				
		0.01694	-0.00418	-0.00602	0.01053	
PART	2					
H6	2	-0.450837	0.276314	0.778685	11.00000	0.02223
PART	0					
C1	1	0.145926	0.586382	0.942063	11.00000	0.05548
		0.08211				
		0.08415	0.02781	-0.01821	0.02875	
AFIX	43					
H1	2	0.155515	0.538956	0.915852	11.00000	-1.20000
AFIX	0					
C2	1	0.173593	0.659817	1.038447	11.00000	0.09592
		0.14977				
		0.17795	0.10398	0.01813	0.05174	
AFIX	137					
H2A	2	0.123085	0.614404	1.069721	11.00000	-1.50000
H2B	2	0.146819	0.706183	1.021002	11.00000	-1.50000
H2C	2	0.247486	0.706917	1.054891	11.00000	-1.50000
AFIX	0					
C3	1	0.217117	0.517422	1.012795	11.00000	0.09592
		0.14977				
		0.17795	0.10398	0.01813	0.05174	
AFIX	137					
H3A	2	0.287845	0.560975	1.033125	11.00000	-1.50000
H3B	2	0.227160	0.479877	0.979019	11.00000	-1.50000
H3C	2	0.163050	0.462385	1.039824	11.00000	-1.50000
AFIX	0					
C4	1	-0.135740	0.762089	0.749944	11.00000	0.02663
		0.01177				
		0.01770	-0.00080	-0.00186	0.00673	

C5	1	-0.089571	0.811530	0.691205	11.00000	0.02606
0.02648 =						
		0.01695	0.00107	0.00041	0.01356	
AFIX	43					
H5	2	-0.133690	0.825760	0.664857	11.00000	-1.20000
AFIX	0					
C6	1	0.010869	0.835948	0.674962	11.00000	0.03196
0.03117 =						
		0.01888	0.00748	0.00243	0.01742	
AFIX	43					
H6A	2	0.051046	0.817850	0.702070	11.00000	-1.20000
AFIX	0					
C7	1	0.066620	0.887001	0.620722	11.00000	0.02483
0.02848 =						
		0.02071	0.00300	-0.00030	0.01273	
C8	1	0.172060	0.922636	0.604185	11.00000	0.02866
0.04838 =						
		0.02771	0.01386	0.00574	0.02219	
AFIX	43					
H8	2	0.225249	0.915648	0.626903	11.00000	-1.20000
AFIX	0					
C9	1	0.098565	0.965683	0.534431	11.00000	0.02580
0.04126 =						
		0.01969	0.00820	0.00367	0.01218	
AFIX	43					
H9	2	0.087563	0.994612	0.498942	11.00000	-1.20000
AFIX	0					
C10	1	-0.566665	0.199008	0.595913	11.00000	0.01584
0.03772 =						
		0.01852	-0.00961	-0.00025	0.00910	
C11	1	-0.511004	0.248640	0.652995	11.00000	0.02317
0.03106 =						
		0.01472	-0.00536	-0.00333	0.00930	
AFIX	43					
H11	2	-0.497119	0.205071	0.679914	11.00000	-1.20000
AFIX	0					
C12	1	-0.480809	0.351479	0.666757	11.00000	0.02531
0.03758 =						
		0.01470	-0.00646	-0.00432	0.01503	
AFIX	43					
H12	2	-0.492711	0.393847	0.638109	11.00000	-1.20000
AFIX	0					
C13	1	-0.430914	0.405738	0.721904	11.00000	0.02642
0.02837 =						
		0.01562	-0.00484	-0.00003	0.01395	
C14	1	-0.383478	0.514469	0.737013	11.00000	0.03487
0.02644 =						
		0.01396	-0.00223	-0.00385	0.01925	
AFIX	43					
H14	2	-0.375902	0.571762	0.711605	11.00000	-1.20000
AFIX	0					
C15	1	-0.375064	0.428603	0.812953	11.00000	0.04241
0.02263 =						
		0.01555	0.00069	-0.00411	0.00911	

AFIX 43
H15 2 -0.361945 0.412516 0.851662 11.00000 -1.20000
AFIX 0

O8A 7 -0.066118 0.121901 0.767877 10.50000 0.04156
0.07497 =

0.05553 0.01497 0.01240 0.03733
O8B 7 -0.103547 0.065083 0.747336 10.50000 0.04156
0.07497 =

0.05553 0.01497 0.01240 0.03733
N7 6 -0.252201 0.021411 0.783013 11.00000 0.05427
0.12142 =

0.23905 0.07484 -0.01295 0.04006
C16 1 -0.151547 0.077551 0.776689 11.00000 0.06687
0.27156 =

0.32499 0.24780 0.06628 0.08833
C17 1 -0.282809 0.071574 0.835321 11.00000 0.17978
0.21589 =

0.36605 0.06319 -0.04360 0.12564

AFIX 137
H17A 2 -0.301681 0.022664 0.869442 11.00000 -1.50000
H17B 2 -0.346342 0.079648 0.824664 11.00000 -1.50000
H17C 2 -0.219792 0.144186 0.844990 11.00000 -1.50000
AFIX 0

C18 1 -0.332156 -0.071709 0.754349 11.00000 0.17978
0.21589 =
0.36605 0.06319 -0.04360 0.12564

AFIX 137
H18A 2 -0.300418 -0.084337 0.718834 11.00000 -1.50000
H18B 2 -0.393959 -0.060898 0.743517 11.00000 -1.50000
H18C 2 -0.358722 -0.135844 0.780394 11.00000 -1.50000
AFIX 0

HKLF 4

REM shelxs86_a.res in P3(2)21
REM R1 = 0.0372 for 5369 Fo > 4sig(Fo) and 0.0445 for all 5931
data
REM 305 parameters refined using 34 restraints

END

WGHT 0.0585 2.7045

REM Highest difference peak 1.137, deepest hole -0.751, 1-sigma level
0.102

Q1	1	-0.0514	0.2986	0.9342	11.00000	0.05	1.14
Q2	1	0.1363	0.6611	0.9660	11.00000	0.05	0.96
Q3	1	0.0000	0.3928	0.8333	10.50000	0.05	-0.75
Q4	1	0.0297	0.6900	0.8088	11.00000	0.05	-0.58
Q5	1	-0.3430	-0.0340	0.8133	11.00000	0.05	0.56
Q6	1	0.2096	0.5321	0.9585	11.00000	0.05	0.48
Q7	1	-0.2492	-0.0265	0.7209	11.00000	0.05	0.46
Q8	1	-0.2593	0.7212	0.8166	11.00000	0.05	-0.45
Q9	1	-0.0449	0.6102	0.8118	11.00000	0.05	-0.44

Q10	1	0.1771	0.6882	1.0598	11.00000	0.05	-0.44
Q11	1	-0.1341	0.4303	0.8951	11.00000	0.05	-0.44
Q12	1	0.0270	0.6292	0.8113	11.00000	0.05	-0.41
Q13	1	0.0936	0.6575	0.9450	11.00000	0.05	-0.38
Q14	1	0.1088	0.5904	0.9005	11.00000	0.05	-0.38
Q15	1	-0.2709	0.6396	0.8113	11.00000	0.05	-0.37
Q16	1	-0.1311	0.1399	0.8099	11.00000	0.05	-0.37
Q17	1	-0.2568	0.0871	0.8059	11.00000	0.05	-0.37
Q18	1	-0.2912	0.3709	0.8044	11.00000	0.05	-0.37
Q19	1	0.0000	0.4599	0.8333	10.50000	0.05	-0.37
Q20	1	-0.2387	0.6923	0.8357	11.00000	0.05	0.37
Q21	1	-0.3655	-0.0241	0.9376	11.00000	0.05	0.36
Q22	1	-0.3498	0.0580	0.8034	11.00000	0.05	0.36
Q23	1	-0.1824	0.7850	0.7290	11.00000	0.05	-0.35
Q24	1	0.1034	0.6098	0.9871	11.00000	0.05	-0.35
Q25	1	-0.3242	-0.0251	0.9348	11.00000	0.05	0.34
Q26	1	0.0182	0.3482	0.8559	11.00000	0.05	-0.34
Q27	1	0.0968	1.0791	0.4786	11.00000	0.05	-0.34
Q28	1	0.0159	1.0138	0.4800	11.00000	0.05	-0.34
Q29	1	-0.0170	0.7442	0.8174	11.00000	0.05	-0.34
Q30	1	-0.1311	0.8184	0.7183	11.00000	0.05	-0.33
Q31	1	0.2887	0.8014	1.1069	11.00000	0.05	-0.33
Q32	1	0.0000	0.7155	0.8333	10.50000	0.05	0.32
Q33	1	0.2205	0.6143	1.0508	11.00000	0.05	0.32
Q34	1	-0.4720	0.1165	0.6691	11.00000	0.05	-0.32
Q35	1	-0.1076	0.0857	0.7275	11.00000	0.05	-0.32
Q36	1	0.0496	0.3824	0.9243	11.00000	0.05	0.32
Q37	1	-0.3059	0.0362	0.8041	11.00000	0.05	-0.32
Q38	1	-0.2309	0.3908	0.8339	11.00000	0.05	-0.32
Q39	1	-0.3516	0.6195	0.8168	11.00000	0.05	-0.31
Q40	1	0.0893	0.4311	0.9613	11.00000	0.05	0.31

REM The information below was added by Olex2.

REM

REM R1 = 0.0372 for 5369 Fo > 4sig(Fo) and 0.0445 for all 17532 data

REM n/a parameters refined using n/a restraints

REM Highest difference peak 1.14, deepest hole -0.75

REM Mean Shift 0, Max Shift 0.000.

REM +++ Tabular Listing of Refinement Information +++

REM R1_all = 0.0445

REM R1_gt = 0.0372

REM wR_ref = 0.1011

REM GOOF = 1.045

REM Shift_max = 0.000

REM Shift_mean = 0

REM Reflections_all = 17532

REM Reflections_gt = 5369

REM Parameters = n/a

REM Hole = -0.75

REM Peak = 1.14

REM Flack = n/a

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received'  
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  _twin_individual_mass_fraction_refined  
1 0.54(2)  
2 0.46(2)  
loop_  
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