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Catalyst Deactivation Reactions

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;
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2010-06-04 # Formatted by publCIF
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# 1. SUBMISSION DETAILS

_publ_contact_author_name      # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address    # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email      A.Meetsma@rug.nl
_publ_contact_author_fax        '+31 50 3634441'
_publ_contact_author_phone      '+31 50 3634368'

_publ_requested_journal         'J. Am. Chem. Soc'
# Publication choose FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
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_publ_requested_coeditor_name   ?

_publ_contact_letter            # Include date of submission
;
  Date of submission : 2010-06-04  14:10:18

  Consider this CIF submission for deposition of the first
  X-ray structure of a manuscript to be submitted to : J. Am. Chem. Soc
  (Our Compound_Identification_Code : q1392)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor     ?
_journal_date_accepted          ?

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_journal_date_printers_final      ?
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_journal_page_last               ?

_journal_suppl_publ_number        ?
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3. TITLE AND AUTHOR LIST

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Title (type here to add)
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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.

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loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
;   # author related footnote
;
;   # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

```

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#=====

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4. TEXT

_publ_section_synopsis

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_publ_section_abstract

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Insert blank lines between paragraphs

_publ_section_comment

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(type here to add)

;

_publ_section_exptl_prep

;

;

_publ_section_exptl_refinement

;

Refinement was frustrated by a disorder problem: from the solution, it was clear that the positions of one of the Cp* ligands were highly disordered: the electron density of the atoms appeared to be spread out. The atoms showed unrealistic displacement parameters when allowed to vary anisotropically, suggesting dynamic disorder (dynamic means that the smeared electron density is due to fluctuations of the atomic positions within each unit cell). A disorder model with two alternative positions of the second Cp* (C111--C220) ligand with bond restraints was used in the final refinement (in which the disorder is compensated by the large displacement parameters). This molecule was fitted- and refined to a regular Cp* ligand. To improve the parameters chemical more reasonable, ultimately restrain instructions (DELU, SIMU)22 were applied in the refinement. Although the disorder model was not satisfactory in all respects, it was the best of several models tested. The s.o.f. of the major fraction of the component of the disorder model refined to a value of 0.555(7). This is in line with the weak scattering power of the crystals investigated.

The hydrogen atoms were generated by geometrical considerations, constrained to idealized geometries, and allowed to ride on the carrier atom with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms, with $U_{iso}(H) = 1.2 U_{eq}(C)$ or $1.5 U_{eq}(methyl\ C)$. The methyl-groups were refined as rigid groups, which were allowed to rotate freely. Assigned values of bond distances: secondary C---H₂ = 0.99 Å and methyl C---H₃ = 0.98 Å.

;

_publ_section_related_literature

;

;

Insert blank lines between references

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;

Beurskens, P. T., Beurskens, G., de Gelder, R., Smits, J. M. M., Garc'ia-Granda, S. & Gould, R. O. (2007). The <i>DIRDIF07</i> program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

Bruker, (2007). <i>SMART</i> (Version 5.632), <i>SAINT-Plus</i> (Version 7.46a) and <i>SADABS</i> (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Meetsma, A. (2007). Extended version of the program *PLUTO*. University of Groningen, The Netherlands. (unpublished).

Sheldrick, G. M. (1997). *SHELXL97*. Program for Crystal Structure Refinement. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7--13.

;

_publ_section_figure_captions

;

Fig. 1. Perspective *PLUTO* drawings of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective *ORTEP* drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

;

_publ_section_acknowledgements

;

?

;

#####

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C₂₈ H₄₆ N O Zr, C₂₄ B F₂₀'

Ex: 'C₁₂ H₁₆ N₂ O₆, H₂ O' and '(Cd²⁺)₃, (C₆ N₆ Cr³⁻)₂, 2(H₂ O)'

_chemical_formula_structural ?

_chemical_formula_sum

'C₅₂ H₄₆ B F₂₀ N O Zr'

_chemical_formula_iupac ?

_chemical_formula_weight 1182.95

_chemical_compound_source 'see text'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

Zr Zr -2.9673 0.5597

'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'

N N 0.0061 0.0033

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

F F 0.0171 0.0103

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

B B 0.0013 0.0007

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H H 0.0000 0.0000

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C C 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

6. CRYSTAL DATA

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_symmetry_space_group_name_Hall '-P 2ybc'
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x, y, z
2 -x, 1/2+y, 1/2-z
3 -x, -y, -z
4 x, 1/2-y, 1/2+z

_cell_length_a 10.744(2)
_cell_length_b 15.660(3)
_cell_length_c 29.067(5)
_cell_angle_alpha 90
_cell_angle_beta 96.143(3)
_cell_angle_gamma 90
_cell_volume 4862.5(15)
_cell_formula_units_Z 4

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 6400
_cell_measurement_theta_min 2.35
_cell_measurement_theta_max 24.07
_cell_special_details

;

The final unit cell was obtained from the xyz centroids of
6400 reflections after integration using the SAINTPLUS
software package (Bruker, 2007).

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)

;

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_exptl_crystal_colour 'yellow'
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_exptl_crystal_size_mid 0.29
_exptl_crystal_size_min 0.10
_exptl_crystal_size_rad ?
_exptl_crystal_density_meas ?
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_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 2392
_exptl_absorpt_coefficient_mu 0.344
_exptl_absorpt_correction_type 'multi-scan'
_exptl_absorpt_process_details '(SADABS, (Bruker, 2006))'
_exptl_absorpt_correction_T_min 0.8524
_exptl_absorpt_correction_T_max 0.9662

#=====

7. EXPERIMENTAL DATA

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;
_diffrn_ambient_temperature          100(1)
_diffrn_radiation_wavelength         0.71073
_diffrn_radiation_type               'MoK\alpha'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method            '\f and \w scans'
_diffrn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2006)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              0
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_diffrn_standards_interval_time       .
_diffrn_standards_decay_%             0

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                 33104
_diffrn_reflns_av_R_equivalents       0.1296
_diffrn_reflns_av_sigmaI/netI        0.1264
_diffrn_reflns_limit_h_min            -12
_diffrn_reflns_limit_h_max            12
_diffrn_reflns_limit_k_min            -18
_diffrn_reflns_limit_k_max            18
_diffrn_reflns_limit_l_min            -34
_diffrn_reflns_limit_l_max            34
_diffrn_reflns_theta_min               2.35
_diffrn_reflns_theta_max              25.03
_diffrn_measured_fraction_theta_max   0.997
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full  0.997

_diffrn_reflns_reduction_process
;
  Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to  $F_o^2$ 
  using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
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_reflns_number_gt                     5557
_reflns_threshold_expression            $I > 2\sigma(I)$ 

_computing_data_collection             'SMART (Bruker, 2006)'
_computing_cell_refinement             'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction              'SAINT-Plus'

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```

_computing_structure_solution
;
DIRDIF-07 (Beurskens et al., 2007)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
  PLATON (Spek, 2003)
  PLUTO (Meetsma, 2007)
;
_computing_publication_material      'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
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Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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_matrix_type            full
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
'calc w=1/[s2(Fo2)+(0.0836P)2+6.7706P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary       heavy
_atom_sites_solution_secondary      direct
_atom_sites_solution_hydrogens      geom
_refine_ls_hydrogen_treatment        constr
_refine_ls_extinction_method         none
_refine_ls_extinction_coef           ?
_refine_ls_abs_structure_details     ?
_chemical_absolute_configuration    '.'

# choose from: rm (reference molecule of known chirality),
# ad (anomalous dispersion - Flack), rmad (rm and ad),
# syn (from synthesis), unk (unknown) or . (not applicable).

_refine_ls_abs_structure_Flack      ?
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_refine_ls_number_restraints         998
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_refine_ls_R_factor_gt               0.0717
_refine_ls_wR_factor_ref             0.1974
_refine_ls_wR_factor_gt              0.1760
_refine_ls_goodness_of_fit_ref       1.044
_refine_ls_restrained_S_all          1.008
_refine_ls_shift/su_max              0.000
_refine_ls_shift/su_mean             0.000
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_refine_diff_density_min             -1.126
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9. ATOMIC COORDINATES AND DISPLACEMENT 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

_atom_site_calc_flag

_atom_site_refinement_flags

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O1 O Uani 0.0417(3) 0.3022(2) 0.09715(13) 1.000 0.0273(12) . .
N1 N Uani 0.0338(4) 0.1094(3) 0.10485(17) 1.000 0.0302(16) . .
C11 C Uani -0.1693(5) 0.1729(4) 0.1701(2) 1.000 0.0319(16) . .
C12 C Uani -0.1007(5) 0.1645(4) 0.2147(2) 1.000 0.0370(16) . .
C13 C Uani -0.0616(5) 0.2473(5) 0.2298(2) 1.000 0.0407(19) . .
C14 C Uani -0.0992(5) 0.3047(4) 0.1943(2) 1.000 0.0341(17) . .
C15 C Uani -0.1683(5) 0.2582(4) 0.1574(2) 1.000 0.0262(16) . .
C16 C Uani -0.2431(6) 0.1043(5) 0.1438(3) 1.000 0.060(3) . .
C17 C Uani -0.0940(7) 0.0861(5) 0.2441(3) 1.000 0.069(3) . .
C18 C Uani -0.0240(7) 0.2707(8) 0.2795(3) 1.000 0.090(4) . .
C19 C Uani -0.0964(8) 0.3997(5) 0.2010(3) 1.000 0.076(3) . .
C110 C Uani -0.2393(6) 0.2973(5) 0.1159(3) 1.000 0.056(3) . .
C111A C Uani 0.2905(6) 0.2573(5) 0.1549(2) 0.456(8) 0.035(3) . .
C111B C Uani 0.2961(5) 0.2333(3) 0.14431(16) 0.545(8) 0.033(3) . .
C112A C Uani 0.2947(9) 0.1675(5) 0.1570(3) 0.456(8) 0.036(2) . .
C112B C Uani 0.2902(6) 0.1513(3) 0.16434(18) 0.545(8) 0.034(2) . .
C113A C Uani 0.2647(8) 0.1425(4) 0.2010(3) 0.456(8) 0.033(3) . .
C113B C Uani 0.2669(5) 0.1618(4) 0.21099(19) 0.545(8) 0.036(2) . .
C114A C Uani 0.2420(7) 0.2168(4) 0.2261(2) 0.456(8) 0.031(2) . .
C114B C Uani 0.2584(5) 0.2503(4) 0.21978(17) 0.545(8) 0.035(3) . .
C115A C Uani 0.2579(8) 0.2878(4) 0.1976(3) 0.456(8) 0.031(3) . .
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C123 C Uani 0.0175(5) 0.3565(4) 0.0199(2) 1.000 0.0304(17) . .
C124 C Uani 0.0205(5) 0.2758(4) 0.04896(19) 1.000 0.0301(17) . .
C125 C Uani 0.0430(5) 0.0729(4) 0.1436(2) 1.000 0.0349(17) . .
C126 C Uani 0.0395(7) -0.0224(4) 0.1519(3) 1.000 0.046(2) . .
C127 C Uani 0.0205(6) 0.0670(4) 0.0600(2) 1.000 0.042(2) . .
C128 C Uani -0.1127(7) 0.0605(6) 0.0384(3) 1.000 0.064(3) . .

H16 H Uiso -0.33166 0.10997 0.14847 1.000 0.0900 . .
H16' H Uiso -0.21234 0.04826 0.15486 1.000 0.0900 . .
H16'' H Uiso -0.23351 0.10979 0.11076 1.000 0.0900 . .
H17 H Uiso -0.16065 0.08768 0.26457 1.000 0.1040 . .
H17' H Uiso -0.01246 0.08361 0.26266 1.000 0.1040 . .
H17'' H Uiso -0.10454 0.03542 0.22420 1.000 0.1040 . .
H18 H Uiso 0.02022 0.32553 0.28096 1.000 0.1349 . .

H18' H Uiso 0.03117 0.22642 0.29420 1.000 0.1349 . .
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H19 H Uiso -0.13770 0.41439 0.22841 1.000 0.1130 . .
H19' H Uiso -0.14022 0.42749 0.17372 1.000 0.1130 . .
H19" H Uiso -0.00927 0.41936 0.20528 1.000 0.1130 . .
H110 H Uiso -0.23064 0.26153 0.08872 1.000 0.0834 . .
H110' H Uiso -0.20606 0.35442 0.11080 1.000 0.0834 . .
H110" H Uiso -0.32795 0.30168 0.12072 1.000 0.0834 . .
H121 H Uiso 0.13698 0.41356 0.09961 1.000 0.0487 . .
H121' H Uiso 0.01019 0.41786 0.12436 1.000 0.0487 . .
H122 H Uiso 0.00466 0.48215 0.04413 1.000 0.0377 . .
H122' H Uiso -0.11362 0.42399 0.05438 1.000 0.0377 . .
H123 H Uiso -0.04392 0.35155 -0.00789 1.000 0.0362 . .
H123' H Uiso 0.10102 0.36925 0.01016 1.000 0.0362 . .
H124 H Uiso -0.05996 0.24474 0.04316 1.000 0.0361 . .
H124' H Uiso 0.08866 0.23761 0.04119 1.000 0.0361 . .
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H1161 H Uiso 0.30482 0.37134 0.12165 0.456(8) 0.0991 . .
H1161' H Uiso 0.25809 0.29517 0.08736 0.456(8) 0.0991 . .
H1161" H Uiso 0.40241 0.30141 0.10746 0.456(8) 0.0991 . .
H1162 H Uiso 0.28221 0.30744 0.08586 0.545(8) 0.0764 . .
H1162' H Uiso 0.28096 0.20732 0.07481 0.545(8) 0.0764 . .
H1162" H Uiso 0.40956 0.25376 0.09299 0.545(8) 0.0764 . .
H1171 H Uiso 0.36686 0.05991 0.13009 0.456(8) 0.0976 . .
H1171' H Uiso 0.36141 0.13958 0.09545 0.456(8) 0.0976 . .
H1171" H Uiso 0.23609 0.08857 0.10294 0.456(8) 0.0976 . .
H1172 H Uiso 0.31900 0.02191 0.16284 0.545(8) 0.0971 . .
H1172' H Uiso 0.37192 0.07087 0.12069 0.545(8) 0.0971 . .
H1172" H Uiso 0.22461 0.05523 0.12030 0.545(8) 0.0971 . .
H1181 H Uiso 0.16566 0.03173 0.20535 0.456(8) 0.0906 . .
H1181' H Uiso 0.25902 0.05075 0.25086 0.456(8) 0.0906 . .
H1181" H Uiso 0.31279 0.01612 0.20511 0.456(8) 0.0906 . .
H1182 H Uiso 0.18673 0.05097 0.23112 0.545(8) 0.0942 . .
H1182' H Uiso 0.22290 0.11535 0.27319 0.545(8) 0.0942 . .
H1182" H Uiso 0.32976 0.06112 0.25221 0.545(8) 0.0942 . .
H1191 H Uiso 0.14087 0.18642 0.27956 0.456(8) 0.1067 . .
H1191' H Uiso 0.20235 0.27949 0.28451 0.456(8) 0.1067 . .
H1191" H Uiso 0.28744 0.19653 0.29536 0.456(8) 0.1067 . .
H1192 H Uiso 0.25503 0.24850 0.29018 0.545(8) 0.1113 . .
H1192' H Uiso 0.15084 0.30990 0.26435 0.545(8) 0.1113 . .
H1192" H Uiso 0.29421 0.33946 0.27117 0.545(8) 0.1113 . .
H1201 H Uiso 0.29638 0.41475 0.19066 0.456(8) 0.0736 . .
H1201' H Uiso 0.29091 0.38647 0.24332 0.456(8) 0.0736 . .
H1201" H Uiso 0.16411 0.39780 0.20962 0.456(8) 0.0736 . .
H1202 H Uiso 0.30970 0.40390 0.14310 0.545(8) 0.0862 . .
H1202' H Uiso 0.33347 0.41539 0.19804 0.545(8) 0.0862 . .
H1202" H Uiso 0.19350 0.41250 0.17294 0.545(8) 0.0862 . .

F22 F Uani 0.1696(3) 0.57686(19) 0.13769(10) 1.000 0.0249(10) . .
F23 F Uani -0.0781(3) 0.5867(2) 0.13093(11) 1.000 0.0319(10) . .
F24 F Uani -0.2008(3) 0.7244(2) 0.08926(14) 1.000 0.0436(13) . .
F25 F Uani -0.0639(3) 0.8538(2) 0.05696(13) 1.000 0.0399(11) . .
F26 F Uani 0.1834(3) 0.8496(2) 0.06683(12) 1.000 0.0315(10) . .
F28 F Uani 0.2988(3) 0.7329(2) 0.01180(10) 1.000 0.0275(10) . .
F29 F Uani 0.4229(3) 0.8374(3) -0.03998(12) 1.000 0.0461(14) . .
F210 F Uani 0.6194(3) 0.9323(3) -0.00116(13) 1.000 0.0505(14) . .
F211 F Uani 0.6889(3) 0.9203(2) 0.09223(12) 1.000 0.0412(11) . .
F212 F Uani 0.5680(3) 0.8192(2) 0.14442(12) 1.000 0.0313(10) . .
F214 F Uani 0.3238(3) 0.8567(2) 0.16147(12) 1.000 0.0352(11) . .

F215 F Uani 0.3677(3) 0.8808(3) 0.25288(13) 1.000 0.0483(12) . .
 F216 F Uani 0.4327(3) 0.7473(3) 0.31063(12) 1.000 0.0467(13) . .
 F217 F Uani 0.4464(3) 0.5866(3) 0.27393(11) 1.000 0.0422(13) . .
 F218 F Uani 0.4166(3) 0.5619(2) 0.18386(11) 1.000 0.0299(10) . .
 F220 F Uani 0.5982(2) 0.6384(2) 0.13046(11) 1.000 0.0269(10) . .
 F221 F Uani 0.7038(3) 0.5019(2) 0.09697(12) 1.000 0.0357(11) . .
 F222 F Uani 0.5658(3) 0.3912(2) 0.03910(11) 1.000 0.0331(11) . .
 F223 F Uani 0.3192(3) 0.4269(2) 0.01308(11) 1.000 0.0300(10) . .
 F224 F Uani 0.2126(2) 0.5639(2) 0.04411(11) 1.000 0.0268(10) . .
 C21 C Uani 0.1923(4) 0.7106(3) 0.10140(18) 1.000 0.0205(16) . .
 C22 C Uani 0.1161(5) 0.6478(3) 0.11729(19) 1.000 0.0220(16) . .
 C23 C Uani -0.0133(4) 0.6508(3) 0.11415(19) 1.000 0.0227(16) . .
 C24 C Uani -0.0750(5) 0.7205(4) 0.0937(2) 1.000 0.0296(16) . .
 C25 C Uani -0.0049(5) 0.7850(4) 0.0779(2) 1.000 0.0298(17) . .
 C26 C Uani 0.1239(5) 0.7802(3) 0.08254(19) 1.000 0.0225(16) . .
 C27 C Uani 0.4230(4) 0.7715(3) 0.08113(19) 1.000 0.0201(16) . .
 C28 C Uani 0.3959(4) 0.7791(3) 0.03401(19) 1.000 0.0225(16) . .
 C29 C Uani 0.4577(5) 0.8317(4) 0.0057(2) 1.000 0.0309(17) . .
 C210 C Uani 0.5572(5) 0.8797(4) 0.0251(2) 1.000 0.0355(17) . .
 C211 C Uani 0.5901(5) 0.8745(4) 0.0722(2) 1.000 0.0301(17) . .
 C212 C Uani 0.5249(5) 0.8210(4) 0.0989(2) 1.000 0.0261(17) . .
 C213 C Uani 0.3736(4) 0.7088(3) 0.16735(19) 1.000 0.0217(16) . .
 C214 C Uani 0.3581(5) 0.7872(4) 0.1880(2) 1.000 0.0273(16) . .
 C215 C Uani 0.3781(5) 0.8014(4) 0.2352(2) 1.000 0.0350(17) . .
 C216 C Uani 0.4114(5) 0.7342(4) 0.2643(2) 1.000 0.0330(19) . .
 C217 C Uani 0.4211(5) 0.6543(4) 0.2460(2) 1.000 0.0323(17) . .
 C218 C Uani 0.4036(4) 0.6429(4) 0.19846(19) 1.000 0.0233(16) . .
 C219 C Uani 0.3982(4) 0.6090(3) 0.09018(18) 1.000 0.0200(16) . .
 C220 C Uani 0.5250(4) 0.5876(3) 0.10147(19) 1.000 0.0229(16) . .
 C221 C Uani 0.5818(4) 0.5159(4) 0.0848(2) 1.000 0.0266(16) . .
 C222 C Uani 0.5126(5) 0.4616(3) 0.0557(2) 1.000 0.0248(17) . .
 C223 C Uani 0.3880(5) 0.4790(3) 0.04297(19) 1.000 0.0224(16) . .
 C224 C Uani 0.3345(4) 0.5513(3) 0.05999(18) 1.000 0.0198(16) . .
 B2 B Uani 0.3466(5) 0.6997(4) 0.1097(2) 1.000 0.0204(16) . .

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_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

Zr1 0.0222(3) 0.0218(3) 0.0250(3) 0.0050(3) 0.0013(2) -0.0015(2)
 O1 0.036(2) 0.019(2) 0.027(2) 0.0031(17) 0.0035(16) -0.0011(16)
 N1 0.031(2) 0.030(3) 0.030(3) 0.007(2) 0.005(2) -0.001(2)
 C111B 0.022(4) 0.039(5) 0.037(4) 0.007(4) -0.001(4) -0.004(4)
 C112B 0.022(4) 0.035(4) 0.045(4) 0.005(4) 0.003(4) -0.008(4)
 C113B 0.030(4) 0.039(4) 0.040(4) 0.013(4) 0.004(4) 0.001(4)
 C114B 0.027(4) 0.043(5) 0.034(5) 0.005(4) 0.005(4) -0.003(4)
 C115B 0.030(4) 0.033(4) 0.043(5) 0.008(4) 0.000(4) -0.001(4)
 C11 0.020(2) 0.030(3) 0.046(3) 0.004(3) 0.005(2) 0.000(2)
 C12 0.022(2) 0.046(3) 0.044(3) 0.022(3) 0.008(2) 0.006(2)
 C116B 0.049(7) 0.060(9) 0.048(7) 0.016(6) 0.024(6) 0.002(7)
 C13 0.022(3) 0.071(4) 0.029(3) -0.003(3) 0.003(2) -0.005(3)
 C14 0.029(3) 0.034(3) 0.041(3) -0.008(3) 0.011(2) -0.008(2)
 C117B 0.070(8) 0.043(7) 0.084(9) 0.001(7) 0.020(8) 0.005(7)
 C15 0.022(2) 0.030(3) 0.027(3) 0.005(2) 0.005(2) 0.001(2)
 C16 0.038(4) 0.042(4) 0.100(6) -0.027(4) 0.009(4) -0.010(3)
 C118B 0.039(6) 0.072(8) 0.073(9) 0.048(7) -0.016(7) -0.013(7)
 C17 0.045(4) 0.074(5) 0.094(6) 0.057(5) 0.031(4) 0.026(4)
 C18 0.039(4) 0.201(11) 0.031(4) -0.022(5) 0.009(3) -0.012(5)
 C119B 0.068(8) 0.105(10) 0.049(7) -0.035(8) 0.003(7) -0.010(8)
 C19 0.089(6) 0.041(4) 0.106(7) -0.031(4) 0.054(5) -0.024(4)
 C120B 0.063(8) 0.031(6) 0.077(10) 0.000(6) 0.000(7) -0.013(6)
 C110 0.032(3) 0.084(6) 0.051(4) 0.035(4) 0.006(3) 0.018(4)

C121 0.069(4) 0.022(3) 0.031(3) 0.006(3) 0.005(3) -0.001(3)
C122 0.036(3) 0.026(3) 0.033(3) 0.011(3) 0.007(3) 0.004(2)
C123 0.031(3) 0.034(3) 0.027(3) 0.004(3) 0.007(2) 0.001(2)
C124 0.034(3) 0.032(3) 0.025(3) 0.004(3) 0.007(2) 0.005(2)
C125 0.034(3) 0.029(3) 0.042(3) 0.003(3) 0.005(3) 0.000(2)
C126 0.061(4) 0.031(3) 0.047(4) 0.002(3) 0.012(3) 0.003(3)
C127 0.057(4) 0.034(4) 0.036(4) 0.004(3) 0.010(3) 0.002(3)
C128 0.066(5) 0.068(6) 0.057(5) -0.002(4) 0.002(4) -0.008(4)
C111A 0.023(3) 0.042(5) 0.039(5) 0.012(4) 0.003(4) -0.004(4)
C112A 0.022(4) 0.042(4) 0.044(4) 0.000(4) 0.006(4) 0.000(4)
C113A 0.019(4) 0.031(4) 0.046(5) 0.010(4) -0.010(4) -0.016(4)
C114A 0.011(3) 0.047(5) 0.036(4) 0.009(4) 0.003(3) -0.013(4)
C115A 0.020(4) 0.028(4) 0.046(5) 0.004(4) 0.003(4) -0.003(4)
C116A 0.064(8) 0.079(10) 0.055(9) 0.022(8) 0.000(7) -0.028(9)
C117A 0.022(6) 0.086(10) 0.096(10) -0.044(8) 0.044(7) -0.025(7)
C118A 0.050(8) 0.041(7) 0.092(12) 0.021(8) 0.017(9) 0.016(7)
C119A 0.116(12) 0.061(11) 0.037(7) 0.012(8) 0.013(7) 0.007(10)
C120A 0.056(8) 0.023(6) 0.062(9) 0.004(6) -0.024(7) 0.000(6)
F22 0.0264(15) 0.0180(16) 0.0303(19) 0.0035(14) 0.0033(13) 0.0030(13)
F23 0.0202(15) 0.0327(19) 0.044(2) 0.0065(16) 0.0084(14) -0.0065(13)
F24 0.0153(15) 0.048(2) 0.068(3) 0.014(2) 0.0073(16) 0.0058(15)
F25 0.0273(16) 0.034(2) 0.059(2) 0.0162(18) 0.0072(16) 0.0135(15)
F26 0.0259(16) 0.0243(18) 0.046(2) 0.0097(16) 0.0111(14) 0.0016(13)
F28 0.0209(15) 0.035(2) 0.0263(18) -0.0014(15) 0.0019(13) -0.0065(13)
F29 0.044(2) 0.067(3) 0.028(2) 0.0075(19) 0.0076(16) -0.0167(19)
F210 0.051(2) 0.055(3) 0.048(2) 0.011(2) 0.0168(18) -0.0246(19)
F211 0.0339(18) 0.045(2) 0.045(2) -0.0040(18) 0.0056(16) -0.0223(16)
F212 0.0294(16) 0.0313(19) 0.0323(19) -0.0012(16) -0.0002(14) -0.0080(14)
F214 0.0391(18) 0.0232(18) 0.044(2) -0.0063(16) 0.0079(16) 0.0085(15)
F215 0.048(2) 0.046(2) 0.052(2) -0.027(2) 0.0105(18) 0.0020(18)
F216 0.0356(18) 0.079(3) 0.026(2) -0.010(2) 0.0052(15) -0.0019(19)
F217 0.0366(18) 0.062(3) 0.028(2) 0.0149(19) 0.0029(15) 0.0028(17)
F218 0.0295(16) 0.0281(18) 0.0323(19) 0.0014(15) 0.0049(14) 0.0000(14)
F220 0.0164(14) 0.0286(18) 0.0347(19) -0.0076(15) -0.0018(13) -0.0012(13)
F221 0.0199(15) 0.037(2) 0.050(2) -0.0016(17) 0.0035(14) 0.0093(14)
F222 0.0358(17) 0.0268(19) 0.037(2) -0.0025(16) 0.0060(15) 0.0130(14)
F223 0.0305(16) 0.0290(19) 0.0303(19) -0.0075(16) 0.0024(14) -0.0038(14)
F224 0.0166(14) 0.0322(19) 0.0305(19) -0.0032(15) -0.0019(12) 0.0016(13)
C21 0.019(2) 0.019(3) 0.024(3) -0.001(2) 0.004(2) 0.001(2)
C22 0.022(2) 0.020(3) 0.024(3) -0.001(2) 0.002(2) 0.004(2)
C23 0.018(2) 0.023(3) 0.028(3) 0.001(2) 0.007(2) 0.000(2)
C24 0.020(2) 0.034(3) 0.036(3) -0.002(3) 0.008(2) 0.002(2)
C25 0.028(3) 0.028(3) 0.035(3) 0.007(3) 0.011(2) 0.010(2)
C26 0.024(2) 0.020(3) 0.025(3) 0.005(2) 0.009(2) -0.001(2)
C27 0.015(2) 0.020(3) 0.026(3) 0.002(2) 0.006(2) 0.0041(19)
C28 0.016(2) 0.026(3) 0.026(3) -0.006(2) 0.004(2) -0.004(2)
C29 0.036(3) 0.033(3) 0.024(3) 0.004(3) 0.005(2) -0.005(2)
C210 0.036(3) 0.038(3) 0.034(3) 0.006(3) 0.011(2) -0.011(3)
C211 0.023(3) 0.028(3) 0.040(3) -0.003(3) 0.007(2) -0.009(2)
C212 0.028(3) 0.022(3) 0.029(3) 0.001(2) 0.006(2) 0.002(2)
C213 0.012(2) 0.025(3) 0.028(3) -0.003(2) 0.002(2) -0.003(2)
C214 0.023(2) 0.030(3) 0.029(3) -0.005(3) 0.004(2) 0.001(2)
C215 0.028(3) 0.042(3) 0.035(3) -0.014(3) 0.004(2) -0.001(3)
C216 0.025(3) 0.054(4) 0.021(3) -0.008(3) 0.007(2) -0.001(3)
C217 0.025(3) 0.046(3) 0.026(3) 0.005(3) 0.003(2) -0.002(3)
C218 0.013(2) 0.030(3) 0.027(3) -0.004(2) 0.002(2) -0.005(2)
C219 0.017(2) 0.018(3) 0.025(3) 0.005(2) 0.003(2) 0.0000(19)
C220 0.019(2) 0.022(3) 0.028(3) 0.000(2) 0.004(2) 0.000(2)
C221 0.018(2) 0.028(3) 0.034(3) 0.005(2) 0.004(2) 0.006(2)
C222 0.030(3) 0.017(3) 0.029(3) 0.001(2) 0.010(2) 0.005(2)
C223 0.024(2) 0.023(3) 0.021(3) 0.002(2) 0.006(2) -0.005(2)
C224 0.014(2) 0.021(3) 0.025(3) -0.001(2) 0.005(2) -0.001(2)
B2 0.014(2) 0.019(3) 0.028(3) -0.001(2) 0.002(2) -0.002(2)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's 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

Zr1	O1	2.337(4)	.	.	yes
Zr1	N1	2.259(5)	.	.	yes
Zr1	C111B	2.639(5)	.	.	yes
Zr1	C112B	2.614(6)	.	.	yes
Zr1	C113B	2.623(6)	.	.	yes
Zr1	C114B	2.653(5)	.	.	yes
Zr1	C115B	2.664(5)	.	.	yes
Zr1	C11	2.590(5)	.	.	yes
Zr1	C12	2.568(6)	.	.	yes
Zr1	C13	2.588(6)	.	.	yes
Zr1	C14	2.550(6)	.	.	yes
Zr1	C15	2.575(6)	.	.	yes
Zr1	C125	2.207(6)	.	.	yes
Zr1	C111A	2.591(7)	.	.	yes
Zr1	C112A	2.604(10)	.	.	yes
Zr1	C113A	2.589(8)	.	.	yes
Zr1	C114A	2.567(7)	.	.	yes
Zr1	C115A	2.569(8)	.	.	yes
F22	C22	1.358(6)	.	.	yes
F23	C23	1.343(6)	.	.	yes
F24	C24	1.345(6)	.	.	yes
F25	C25	1.360(7)	.	.	yes
F26	C26	1.364(6)	.	.	yes
F28	C28	1.373(6)	.	.	yes
F29	C29	1.343(7)	.	.	yes
F210	C210	1.348(7)	.	.	yes
F211	C211	1.359(7)	.	.	yes
F212	C212	1.355(7)	.	.	yes
F214	C214	1.362(7)	.	.	yes
F215	C215	1.355(8)	.	.	yes
F216	C216	1.357(7)	.	.	yes
F217	C217	1.345(7)	.	.	yes
F218	C218	1.350(7)	.	.	yes
F220	C220	1.349(6)	.	.	yes
F221	C221	1.339(6)	.	.	yes
F222	C222	1.354(6)	.	.	yes
F223	C223	1.353(6)	.	.	yes
F224	C224	1.356(5)	.	.	yes
O1	C121	1.447(7)	.	.	yes
O1	C124	1.455(7)	.	.	yes
N1	C127	1.456(8)	.	.	yes
N1	C125	1.258(8)	.	.	yes
C111A	C112A	1.408(11)	.	.	no
C111A	C116A	1.498(12)	.	.	no
C111A	C115A	1.409(10)	.	.	no
C111B	C115B	1.414(7)	.	.	no
C111B	C112B	1.414(7)	.	.	no
C111B	C116B	1.504(8)	.	.	no

C112A	C117A	1.498(14)	.	.	no
C112A	C113A	1.408(12)	.	.	no
C112B	C117B	1.505(8)	.	.	no
C112B	C113B	1.415(8)	.	.	no
C113A	C114A	1.408(9)	.	.	no
C113A	C118A	1.499(12)	.	.	no
C113B	C118B	1.503(10)	.	.	no
C113B	C114B	1.414(9)	.	.	no
C114A	C119A	1.499(11)	.	.	no
C114A	C115A	1.408(10)	.	.	no
C114B	C115B	1.415(7)	.	.	no
C114B	C119B	1.504(8)	.	.	no
C115A	C120A	1.497(10)	.	.	no
C115B	C120B	1.504(7)	.	.	no
C11	C12	1.427(8)	.	.	no
C11	C15	1.386(9)	.	.	no
C11	C16	1.496(10)	.	.	no
C12	C17	1.493(10)	.	.	no
C12	C13	1.418(10)	.	.	no
C13	C14	1.395(9)	.	.	no
C13	C18	1.503(11)	.	.	no
C14	C15	1.436(8)	.	.	no
C14	C19	1.500(10)	.	.	no
C15	C110	1.488(10)	.	.	no
C116A	H1161	0.9800	.	.	no
C116A	H1161"	0.9800	.	.	no
C116A	H1161'	0.9800	.	.	no
C116B	H1162"	0.9800	.	.	no
C116B	H1162'	0.9800	.	.	no
C116B	H1162	0.9800	.	.	no
C117A	H1171	0.9800	.	.	no
C117A	H1171"	0.9800	.	.	no
C117A	H1171'	0.9800	.	.	no
C117B	H1172'	0.9800	.	.	no
C117B	H1172"	0.9800	.	.	no
C117B	H1172	0.9800	.	.	no
C118A	H1181"	0.9800	.	.	no
C118A	H1181'	0.9800	.	.	no
C118A	H1181	0.9800	.	.	no
C16	H16"	0.9800	.	.	no
C16	H16'	0.9800	.	.	no
C16	H16	0.9800	.	.	no
C118B	H1182'	0.9800	.	.	no
C118B	H1182"	0.9800	.	.	no
C118B	H1182	0.9800	.	.	no
C17	H17	0.9800	.	.	no
C17	H17"	0.9800	.	.	no
C17	H17'	0.9800	.	.	no
C119A	H1191"	0.9800	.	.	no
C119A	H1191'	0.9800	.	.	no
C119A	H1191	0.9800	.	.	no
C18	H18	0.9800	.	.	no
C18	H18'	0.9800	.	.	no
C18	H18"	0.9800	.	.	no
C119B	H1192"	0.9800	.	.	no
C119B	H1192	0.9800	.	.	no
C119B	H1192'	0.9800	.	.	no
C19	H19'	0.9800	.	.	no
C19	H19	0.9800	.	.	no
C19	H19"	0.9800	.	.	no
C120A	H1201"	0.9800	.	.	no
C120A	H1201'	0.9800	.	.	no
C120A	H1201	0.9800	.	.	no
C120B	H1202'	0.9800	.	.	no
C120B	H1202"	0.9800	.	.	no
C120B	H1202	0.9800	.	.	no

C121	C122	1.510(8)	.	.	no
C122	C123	1.521(8)	.	.	no
C123	C124	1.519(9)	.	.	no
C125	C126	1.513(9)	.	.	no
C127	C128	1.503(10)	.	.	no
C110	H110"	0.9800	.	.	no
C110	H110	0.9800	.	.	no
C110	H110'	0.9800	.	.	no
C121	H121'	0.9900	.	.	no
C21	C22	1.390(7)	.	.	no
C21	C26	1.394(7)	.	.	no
C21	B2	1.658(7)	.	.	yes
C121	H121	0.9900	.	.	no
C22	C23	1.384(7)	.	.	no
C122	H122'	0.9900	.	.	no
C122	H122	0.9900	.	.	no
C123	H123'	0.9900	.	.	no
C123	H123	0.9900	.	.	no
C23	C24	1.378(8)	.	.	no
C124	H124'	0.9900	.	.	no
C124	H124	0.9900	.	.	no
C24	C25	1.368(8)	.	.	no
C25	C26	1.378(8)	.	.	no
C126	H126	0.9800	.	.	no
C126	H126'	0.9800	.	.	no
C126	H126"	0.9800	.	.	no
C127	H127	0.9900	.	.	no
C27	B2	1.665(8)	.	.	yes
C27	C28	1.375(8)	.	.	no
C127	H127'	0.9900	.	.	no
C27	C212	1.395(7)	.	.	no
C128	H128	0.9800	.	.	no
C128	H128'	0.9800	.	.	no
C28	C29	1.383(8)	.	.	no
C128	H128"	0.9800	.	.	no
C29	C210	1.377(8)	.	.	no
C210	C211	1.379(8)	.	.	no
C211	C212	1.383(8)	.	.	no
C213	C214	1.385(8)	.	.	no
C213	C218	1.387(8)	.	.	no
C213	B2	1.676(8)	.	.	yes
C214	C215	1.384(8)	.	.	no
C215	C216	1.373(9)	.	.	no
C216	C217	1.368(9)	.	.	no
C217	C218	1.386(8)	.	.	no
C219	C220	1.407(6)	.	.	no
C219	C224	1.388(7)	.	.	no
C219	B2	1.647(8)	.	.	yes
C220	C221	1.390(7)	.	.	no
C221	C222	1.363(8)	.	.	no
C222	C223	1.377(8)	.	.	no
C223	C224	1.385(7)	.	.	no

loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

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_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O1	Zr1	N1	82.45(15)	.	.	.	yes
O1	Zr1	C111B	77.28(13)	.	.	.	yes
O1	Zr1	C112B	104.78(14)	.	.	.	yes
O1	Zr1	C113B	128.21(15)	.	.	.	yes

O1	Zr1	C114B	111.31(15)	.	.	.	yes
O1	Zr1	C115B	81.42(13)	.	.	.	yes
O1	Zr1	C11	102.36(15)	.	.	.	yes
O1	Zr1	C12	130.06(15)	.	.	.	yes
O1	Zr1	C13	117.55(18)	.	.	.	yes
O1	Zr1	C14	86.24(16)	.	.	.	yes
O1	Zr1	C15	77.45(15)	.	.	.	yes
O1	Zr1	C125	115.11(17)	.	.	.	yes
O1	Zr1	C111A	77.21(17)	.	.	.	yes
O1	Zr1	C112A	97.6(2)	.	.	.	yes
O1	Zr1	C113A	127.7(2)	.	.	.	yes
O1	Zr1	C114A	123.87(17)	.	.	.	yes
O1	Zr1	C115A	92.18(19)	.	.	.	yes
N1	Zr1	C111B	91.26(15)	.	.	.	yes
N1	Zr1	C112B	80.53(16)	.	.	.	yes
N1	Zr1	C113B	103.82(17)	.	.	.	yes
N1	Zr1	C114B	131.77(17)	.	.	.	yes
N1	Zr1	C115B	122.13(15)	.	.	.	yes
N1	Zr1	C11	82.25(17)	.	.	.	yes
N1	Zr1	C12	101.53(18)	.	.	.	yes
N1	Zr1	C13	132.55(19)	.	.	.	yes
N1	Zr1	C14	129.65(17)	.	.	.	yes
N1	Zr1	C15	97.19(17)	.	.	.	yes
N1	Zr1	C125	32.68(19)	.	.	.	yes
N1	Zr1	C111A	101.89(19)	.	.	.	yes
N1	Zr1	C112A	81.2(2)	.	.	.	yes
N1	Zr1	C113A	94.7(2)	.	.	.	yes
N1	Zr1	C114A	126.35(19)	.	.	.	yes
N1	Zr1	C115A	132.1(2)	.	.	.	yes
C111B	Zr1	C112B	31.23(15)	.	.	.	yes
C111B	Zr1	C113B	51.57(16)	.	.	.	yes
C111B	Zr1	C114B	51.24(15)	.	.	.	yes
C111B	Zr1	C115B	30.93(14)	.	.	.	yes
C111B	Zr1	C11	173.48(17)	.	.	.	yes
C111B	Zr1	C12	150.76(16)	.	.	.	yes
C111B	Zr1	C13	133.35(17)	.	.	.	yes
C111B	Zr1	C14	133.44(17)	.	.	.	yes
C111B	Zr1	C15	152.00(17)	.	.	.	yes
C111B	Zr1	C125	99.16(17)	.	.	.	yes
C112B	Zr1	C113B	31.35(17)	.	.	.	yes
C112B	Zr1	C114B	51.49(17)	.	.	.	yes
C112B	Zr1	C115B	51.37(15)	.	.	.	yes
C112B	Zr1	C11	145.44(18)	.	.	.	yes
C112B	Zr1	C12	125.08(17)	.	.	.	yes
C112B	Zr1	C13	127.21(17)	.	.	.	yes
C112B	Zr1	C14	149.48(17)	.	.	.	yes
C112B	Zr1	C15	176.49(18)	.	.	.	yes
C112B	Zr1	C125	74.31(18)	.	.	.	yes
C113B	Zr1	C114B	31.08(19)	.	.	.	yes
C113B	Zr1	C115B	51.29(17)	.	.	.	yes
C113B	Zr1	C11	129.40(18)	.	.	.	yes
C113B	Zr1	C12	99.53(18)	.	.	.	yes
C113B	Zr1	C13	95.87(18)	.	.	.	yes
C113B	Zr1	C14	121.19(18)	.	.	.	yes
C113B	Zr1	C15	148.36(18)	.	.	.	yes
C113B	Zr1	C125	84.1(2)	.	.	.	yes
C114B	Zr1	C115B	30.86(16)	.	.	.	yes
C114B	Zr1	C11	133.72(17)	.	.	.	yes
C114B	Zr1	C12	102.53(17)	.	.	.	yes
C114B	Zr1	C13	83.25(17)	.	.	.	yes
C114B	Zr1	C14	98.01(18)	.	.	.	yes
C114B	Zr1	C15	130.48(18)	.	.	.	yes
C114B	Zr1	C125	115.1(2)	.	.	.	yes
C115B	Zr1	C11	155.59(17)	.	.	.	yes
C115B	Zr1	C12	130.52(17)	.	.	.	yes
C115B	Zr1	C13	103.95(18)	.	.	.	yes

C115B	Zr1	C14	104.17(17)	.	.	.	yes
C115B	Zr1	C15	132.01(17)	.	.	.	yes
C115B	Zr1	C125	125.66(17)	.	.	.	yes
C11	Zr1	C12	32.12(18)	.	.	.	yes
C11	Zr1	C13	52.68(19)	.	.	.	yes
C11	Zr1	C14	52.71(19)	.	.	.	yes
C11	Zr1	C15	31.13(19)	.	.	.	yes
C11	Zr1	C125	75.0(2)	.	.	.	yes
C111A	Zr1	C11	175.7(2)	.	.	.	yes
C112A	Zr1	C11	152.0(2)	.	.	.	yes
C113A	Zr1	C11	129.2(2)	.	.	.	yes
C114A	Zr1	C11	126.0(2)	.	.	.	yes
C115A	Zr1	C11	144.6(2)	.	.	.	yes
C12	Zr1	C13	31.9(2)	.	.	.	yes
C12	Zr1	C14	52.78(19)	.	.	.	yes
C12	Zr1	C15	52.62(19)	.	.	.	yes
C12	Zr1	C125	79.5(2)	.	.	.	yes
C111A	Zr1	C12	146.14(18)	.	.	.	yes
C112A	Zr1	C12	132.3(2)	.	.	.	yes
C113A	Zr1	C12	101.8(2)	.	.	.	yes
C114A	Zr1	C12	93.9(2)	.	.	.	yes
C115A	Zr1	C12	117.2(2)	.	.	.	yes
C13	Zr1	C14	31.5(2)	.	.	.	yes
C13	Zr1	C15	52.73(18)	.	.	.	yes
C13	Zr1	C125	110.7(2)	.	.	.	yes
C111A	Zr1	C13	123.6(2)	.	.	.	yes
C112A	Zr1	C13	131.6(2)	.	.	.	yes
C113A	Zr1	C13	102.6(2)	.	.	.	yes
C114A	Zr1	C13	79.9(2)	.	.	.	yes
C115A	Zr1	C13	92.0(2)	.	.	.	yes
C14	Zr1	C15	32.54(18)	.	.	.	yes
C14	Zr1	C125	127.1(2)	.	.	.	yes
C111A	Zr1	C14	123.0(2)	.	.	.	yes
C112A	Zr1	C14	149.1(2)	.	.	.	yes
C113A	Zr1	C14	129.6(2)	.	.	.	yes
C114A	Zr1	C14	100.4(2)	.	.	.	yes
C115A	Zr1	C14	97.1(2)	.	.	.	yes
C15	Zr1	C125	102.3(2)	.	.	.	yes
C111A	Zr1	C15	145.8(2)	.	.	.	yes
C112A	Zr1	C15	175.0(2)	.	.	.	yes
C113A	Zr1	C15	153.6(2)	.	.	.	yes
C114A	Zr1	C15	131.4(2)	.	.	.	yes
C115A	Zr1	C15	128.2(2)	.	.	.	yes
C111A	Zr1	C125	109.1(2)	.	.	.	yes
C112A	Zr1	C125	78.9(2)	.	.	.	yes
C113A	Zr1	C125	75.9(2)	.	.	.	yes
C114A	Zr1	C125	104.5(2)	.	.	.	yes
C115A	Zr1	C125	127.3(2)	.	.	.	yes
C111A	Zr1	C112A	31.5(2)	.	.	.	yes
C111A	Zr1	C113A	52.2(2)	.	.	.	yes
C111A	Zr1	C114A	52.4(2)	.	.	.	yes
C111A	Zr1	C115A	31.7(2)	.	.	.	yes
C112A	Zr1	C113A	31.5(3)	.	.	.	yes
C112A	Zr1	C114A	52.3(2)	.	.	.	yes
C112A	Zr1	C115A	52.3(2)	.	.	.	yes
C113A	Zr1	C114A	31.7(2)	.	.	.	yes
C113A	Zr1	C115A	52.4(2)	.	.	.	yes
C114A	Zr1	C115A	31.8(2)	.	.	.	yes
Zr1	O1	C121	127.6(3)	.	.	.	yes
Zr1	O1	C124	125.3(3)	.	.	.	yes
C121	O1	C124	107.2(4)	.	.	.	yes
Zr1	N1	C125	71.4(4)	.	.	.	yes
Zr1	N1	C127	162.6(4)	.	.	.	yes
C125	N1	C127	125.8(5)	.	.	.	yes
Zr1	C111A	C116A	117.9(5)	.	.	.	yes
C112A	C111A	C115A	108.1(6)	.	.	.	no

C112A	C111A	C116A	125.9(7)	.	.	.	no
C115A	C111A	C116A	126.0(7)	.	.	.	no
Zr1	C111A	C112A	74.8(5)	.	.	.	yes
Zr1	C111A	C115A	73.3(4)	.	.	.	yes
C112B	C111B	C116B	126.0(5)	.	.	.	no
Zr1	C111B	C112B	73.4(3)	.	.	.	yes
Zr1	C111B	C115B	75.5(3)	.	.	.	yes
Zr1	C111B	C116B	117.2(4)	.	.	.	yes
C112B	C111B	C115B	108.0(4)	.	.	.	no
C115B	C111B	C116B	126.0(5)	.	.	.	no
Zr1	C112A	C111A	73.8(5)	.	.	.	yes
Zr1	C112A	C117A	114.7(6)	.	.	.	yes
C111A	C112A	C113A	107.9(7)	.	.	.	no
Zr1	C112A	C113A	73.7(5)	.	.	.	yes
C113A	C112A	C117A	126.0(7)	.	.	.	no
C111A	C112A	C117A	126.0(8)	.	.	.	no
Zr1	C112B	C113B	74.7(3)	.	.	.	yes
Zr1	C112B	C117B	114.7(5)	.	.	.	yes
C111B	C112B	C117B	126.0(5)	.	.	.	no
C113B	C112B	C117B	126.0(5)	.	.	.	no
C111B	C112B	C113B	108.0(4)	.	.	.	no
Zr1	C112B	C111B	75.4(3)	.	.	.	yes
Zr1	C113A	C112A	74.9(5)	.	.	.	yes
Zr1	C113A	C114A	73.3(4)	.	.	.	yes
Zr1	C113A	C118A	114.1(7)	.	.	.	yes
C112A	C113A	C114A	108.1(6)	.	.	.	no
C112A	C113A	C118A	126.0(8)	.	.	.	no
C114A	C113A	C118A	125.8(8)	.	.	.	no
Zr1	C113B	C112B	74.0(3)	.	.	.	yes
Zr1	C113B	C118B	115.0(5)	.	.	.	yes
C112B	C113B	C114B	108.0(5)	.	.	.	no
C112B	C113B	C118B	126.0(6)	.	.	.	no
C114B	C113B	C118B	126.0(5)	.	.	.	no
Zr1	C113B	C114B	75.7(3)	.	.	.	yes
C113A	C114A	C119A	126.0(7)	.	.	.	no
C115A	C114A	C119A	125.9(7)	.	.	.	no
Zr1	C114A	C113A	75.0(4)	.	.	.	yes
Zr1	C114A	C115A	74.2(4)	.	.	.	yes
Zr1	C114A	C119A	120.6(7)	.	.	.	yes
C113A	C114A	C115A	108.0(6)	.	.	.	no
Zr1	C114B	C113B	73.3(3)	.	.	.	yes
Zr1	C114B	C115B	75.0(3)	.	.	.	yes
C113B	C114B	C119B	126.1(5)	.	.	.	no
Zr1	C114B	C119B	119.2(5)	.	.	.	yes
C113B	C114B	C115B	108.0(5)	.	.	.	no
C115B	C114B	C119B	125.9(6)	.	.	.	no
Zr1	C115A	C111A	75.0(4)	.	.	.	yes
C114A	C115A	C120A	126.0(8)	.	.	.	no
Zr1	C115A	C120A	120.7(6)	.	.	.	yes
C111A	C115A	C114A	107.9(6)	.	.	.	no
Zr1	C115A	C114A	74.0(4)	.	.	.	yes
C111A	C115A	C120A	125.9(8)	.	.	.	no
Zr1	C115B	C114B	74.2(3)	.	.	.	yes
Zr1	C115B	C120B	119.6(4)	.	.	.	yes
Zr1	C115B	C111B	73.6(3)	.	.	.	yes
C111B	C115B	C120B	126.0(5)	.	.	.	no
C114B	C115B	C120B	126.0(5)	.	.	.	no
C111B	C115B	C114B	108.0(4)	.	.	.	no
C15	C11	C16	125.1(6)	.	.	.	no
C12	C11	C16	126.3(6)	.	.	.	no
Zr1	C11	C12	73.1(3)	.	.	.	yes
Zr1	C11	C15	73.8(3)	.	.	.	yes
Zr1	C11	C16	124.6(4)	.	.	.	yes
C12	C11	C15	108.2(5)	.	.	.	no
Zr1	C12	C11	74.8(3)	.	.	.	yes
C11	C12	C13	107.7(5)	.	.	.	no

Zr1	C12	C13	74.8(3)	.	.	.	yes
Zr1	C12	C17	125.7(4)	.	.	.	yes
C11	C12	C17	125.8(6)	.	.	.	no
C13	C12	C17	125.5(6)	.	.	.	no
Zr1	C13	C14	72.8(3)	.	.	.	yes
Zr1	C13	C12	73.3(3)	.	.	.	yes
C12	C13	C18	124.1(7)	.	.	.	no
Zr1	C13	C18	133.9(4)	.	.	.	yes
C12	C13	C14	107.9(5)	.	.	.	no
C14	C13	C18	125.5(8)	.	.	.	no
C13	C14	C15	108.1(6)	.	.	.	no
Zr1	C14	C13	75.7(3)	.	.	.	yes
Zr1	C14	C15	74.7(3)	.	.	.	yes
Zr1	C14	C19	128.5(5)	.	.	.	yes
C13	C14	C19	122.9(6)	.	.	.	no
C15	C14	C19	127.0(6)	.	.	.	no
C11	C15	C110	126.5(6)	.	.	.	no
Zr1	C15	C11	75.1(3)	.	.	.	yes
Zr1	C15	C14	72.8(3)	.	.	.	yes
Zr1	C15	C110	123.9(4)	.	.	.	yes
C11	C15	C14	107.9(5)	.	.	.	no
C14	C15	C110	125.2(6)	.	.	.	no
C111A	C116A	H1161"	109.00	.	.	.	no
H1161'	C116A	H1161"	110.00	.	.	.	no
C111A	C116A	H1161'	109.00	.	.	.	no
C111A	C116A	H1161	109.00	.	.	.	no
H1161	C116A	H1161"	109.00	.	.	.	no
H1161	C116A	H1161'	109.00	.	.	.	no
C111B	C116B	H1162"	109.00	.	.	.	no
C111B	C116B	H1162	109.00	.	.	.	no
C111B	C116B	H1162'	109.00	.	.	.	no
H1162'	C116B	H1162"	109.00	.	.	.	no
H1162	C116B	H1162'	110.00	.	.	.	no
H1162	C116B	H1162"	109.00	.	.	.	no
C112A	C117A	H1171	109.00	.	.	.	no
C112A	C117A	H1171'	109.00	.	.	.	no
C112A	C117A	H1171"	109.00	.	.	.	no
H1171	C117A	H1171'	110.00	.	.	.	no
H1171	C117A	H1171"	109.00	.	.	.	no
H1171'	C117A	H1171"	109.00	.	.	.	no
C112B	C117B	H1172'	109.00	.	.	.	no
H1172	C117B	H1172"	110.00	.	.	.	no
C112B	C117B	H1172"	109.00	.	.	.	no
H1172	C117B	H1172'	109.00	.	.	.	no
C112B	C117B	H1172	109.00	.	.	.	no
H1172'	C117B	H1172"	110.00	.	.	.	no
C113A	C118A	H1181	109.00	.	.	.	no
C113A	C118A	H1181"	109.00	.	.	.	no
H1181	C118A	H1181'	110.00	.	.	.	no
C113A	C118A	H1181'	110.00	.	.	.	no
H1181	C118A	H1181"	109.00	.	.	.	no
H1181'	C118A	H1181"	110.00	.	.	.	no
C11	C16	H16"	109.00	.	.	.	no
H16'	C16	H16"	109.00	.	.	.	no
H16	C16	H16'	110.00	.	.	.	no
H16	C16	H16"	109.00	.	.	.	no
C11	C16	H16	109.00	.	.	.	no
C11	C16	H16'	110.00	.	.	.	no
H1182'	C118B	H1182"	109.00	.	.	.	no
H1182	C118B	H1182'	109.00	.	.	.	no
H1182	C118B	H1182"	109.00	.	.	.	no
C113B	C118B	H1182"	110.00	.	.	.	no
C113B	C118B	H1182	110.00	.	.	.	no
C113B	C118B	H1182'	110.00	.	.	.	no
C12	C17	H17"	109.00	.	.	.	no
H17	C17	H17'	110.00	.	.	.	no

H17	C17	H17"	109.00	.	.	.	no
H17'	C17	H17"	109.00	.	.	.	no
C12	C17	H17'	109.00	.	.	.	no
C12	C17	H17	109.00	.	.	.	no
H1191	C119A	H1191"	110.00	.	.	.	no
H1191'	C119A	H1191"	110.00	.	.	.	no
C114A	C119A	H1191	109.00	.	.	.	no
C114A	C119A	H1191'	109.00	.	.	.	no
C114A	C119A	H1191"	109.00	.	.	.	no
H1191	C119A	H1191'	110.00	.	.	.	no
C13	C18	H18'	110.00	.	.	.	no
C13	C18	H18"	109.00	.	.	.	no
C13	C18	H18	110.00	.	.	.	no
H18	C18	H18"	109.00	.	.	.	no
H18'	C18	H18"	109.00	.	.	.	no
H18	C18	H18'	109.00	.	.	.	no
C114B	C119B	H1192	109.00	.	.	.	no
H1192'	C119B	H1192"	110.00	.	.	.	no
C114B	C119B	H1192"	110.00	.	.	.	no
H1192	C119B	H1192"	109.00	.	.	.	no
H1192	C119B	H1192'	109.00	.	.	.	no
C114B	C119B	H1192'	110.00	.	.	.	no
C14	C19	H19	109.00	.	.	.	no
H19	C19	H19'	109.00	.	.	.	no
H19'	C19	H19"	109.00	.	.	.	no
H19	C19	H19"	109.00	.	.	.	no
C14	C19	H19'	110.00	.	.	.	no
C14	C19	H19"	109.00	.	.	.	no
C115A	C120A	H1201'	109.00	.	.	.	no
H1201	C120A	H1201"	109.00	.	.	.	no
C115A	C120A	H1201"	110.00	.	.	.	no
C115A	C120A	H1201	110.00	.	.	.	no
H1201'	C120A	H1201"	109.00	.	.	.	no
H1201	C120A	H1201'	109.00	.	.	.	no
C115B	C120B	H1202	109.00	.	.	.	no
H1202'	C120B	H1202"	110.00	.	.	.	no
C115B	C120B	H1202"	109.00	.	.	.	no
H1202	C120B	H1202'	109.00	.	.	.	no
C115B	C120B	H1202'	110.00	.	.	.	no
H1202	C120B	H1202"	109.00	.	.	.	no
O1	C121	C122	106.3(5)	.	.	.	yes
C121	C122	C123	100.2(5)	.	.	.	no
C122	C123	C124	102.9(5)	.	.	.	no
O1	C124	C123	106.9(5)	.	.	.	yes
Zr1	C125	N1	75.9(4)	.	.	.	yes
Zr1	C125	C126	157.9(5)	.	.	.	yes
N1	C125	C126	126.2(6)	.	.	.	yes
N1	C127	C128	113.7(6)	.	.	.	yes
C15	C110	H110"	110.00	.	.	.	no
C15	C110	H110'	110.00	.	.	.	no
H110'	C110	H110"	109.00	.	.	.	no
H110'	C110	H110	109.00	.	.	.	no
C15	C110	H110	109.00	.	.	.	no
H110"	C110	H110	109.00	.	.	.	no
H121'	C121	H121	109.00	.	.	.	no
C22	C21	B2	119.6(4)	.	.	.	yes
O1	C121	H121'	111.00	.	.	.	no
O1	C121	H121	110.00	.	.	.	no
C122	C121	H121'	110.00	.	.	.	no
C122	C121	H121	110.00	.	.	.	no
C22	C21	C26	112.3(4)	.	.	.	no
C26	C21	B2	127.9(4)	.	.	.	yes
C123	C122	H122'	112.00	.	.	.	no
C123	C122	H122	112.00	.	.	.	no
H122'	C122	H122	110.00	.	.	.	no
C21	C22	C23	125.3(5)	.	.	.	no

F22	C22	C23	115.6(4)	.	.	.	yes
C121	C122	H122'	112.00	.	.	.	no
C121	C122	H122	112.00	.	.	.	no
F22	C22	C21	119.2(5)	.	.	.	yes
C124	C123	H123'	111.00	.	.	.	no
C124	C123	H123	111.00	.	.	.	no
H123'	C123	H123	109.00	.	.	.	no
C122	C123	H123	111.00	.	.	.	no
C122	C123	H123'	111.00	.	.	.	no
F23	C23	C22	120.5(4)	.	.	.	yes
F23	C23	C24	120.3(4)	.	.	.	yes
C22	C23	C24	119.3(5)	.	.	.	no
O1	C124	H124	110.00	.	.	.	no
C123	C124	H124'	110.00	.	.	.	no
C123	C124	H124	110.00	.	.	.	no
H124'	C124	H124	109.00	.	.	.	no
F24	C24	C23	120.6(5)	.	.	.	yes
F24	C24	C25	121.2(5)	.	.	.	yes
O1	C124	H124'	110.00	.	.	.	no
C23	C24	C25	118.2(5)	.	.	.	no
C24	C25	C26	120.7(5)	.	.	.	no
F25	C25	C26	120.1(5)	.	.	.	yes
F25	C25	C24	119.2(5)	.	.	.	yes
C125	C126	H126"	109.00	.	.	.	no
C125	C126	H126'	110.00	.	.	.	no
F26	C26	C21	120.6(5)	.	.	.	yes
C125	C126	H126	109.00	.	.	.	no
H126'	C126	H126"	110.00	.	.	.	no
H126'	C126	H126	110.00	.	.	.	no
H126"	C126	H126	109.00	.	.	.	no
F26	C26	C25	115.2(5)	.	.	.	yes
C21	C26	C25	124.3(5)	.	.	.	no
N1	C127	H127'	109.00	.	.	.	no
C128	C127	H127	109.00	.	.	.	no
N1	C127	H127	109.00	.	.	.	no
C128	C127	H127'	109.00	.	.	.	no
C28	C27	C212	113.3(5)	.	.	.	no
C28	C27	B2	119.5(4)	.	.	.	yes
C212	C27	B2	126.9(5)	.	.	.	yes
H127'	C127	H127	108.00	.	.	.	no
H128'	C128	H128	109.00	.	.	.	no
H128"	C128	H128	110.00	.	.	.	no
C127	C128	H128'	109.00	.	.	.	no
C127	C128	H128"	110.00	.	.	.	no
C127	C128	H128	110.00	.	.	.	no
H128'	C128	H128"	109.00	.	.	.	no
F28	C28	C27	119.5(4)	.	.	.	yes
F28	C28	C29	115.0(5)	.	.	.	yes
C27	C28	C29	125.5(5)	.	.	.	no
F29	C29	C28	121.8(5)	.	.	.	yes
F29	C29	C210	119.4(5)	.	.	.	yes
C28	C29	C210	118.8(5)	.	.	.	no
F210	C210	C29	120.8(5)	.	.	.	yes
F210	C210	C211	120.6(5)	.	.	.	yes
C29	C210	C211	118.7(5)	.	.	.	no
F211	C211	C210	120.0(5)	.	.	.	yes
F211	C211	C212	119.9(5)	.	.	.	yes
C210	C211	C212	120.1(5)	.	.	.	no
F212	C212	C27	121.5(5)	.	.	.	yes
F212	C212	C211	114.9(5)	.	.	.	yes
C27	C212	C211	123.6(5)	.	.	.	no
C214	C213	C218	114.1(5)	.	.	.	no
C214	C213	B2	119.5(5)	.	.	.	yes
C218	C213	B2	126.3(5)	.	.	.	yes
F214	C214	C213	120.1(5)	.	.	.	yes
F214	C214	C215	115.9(5)	.	.	.	yes

C213	C214	C215	124.0(6)	.	.	.	no
F215	C215	C214	120.9(5)	.	.	.	yes
F215	C215	C216	119.8(5)	.	.	.	yes
C214	C215	C216	119.4(6)	.	.	.	no
F216	C216	C215	120.0(6)	.	.	.	yes
F216	C216	C217	120.8(5)	.	.	.	yes
C215	C216	C217	119.2(5)	.	.	.	no
F217	C217	C216	120.3(5)	.	.	.	yes
F217	C217	C218	119.8(5)	.	.	.	yes
C216	C217	C218	119.8(6)	.	.	.	no
F218	C218	C213	121.3(5)	.	.	.	yes
F218	C218	C217	115.3(5)	.	.	.	yes
C213	C218	C217	123.5(6)	.	.	.	no
C220	C219	C224	113.1(4)	.	.	.	no
C220	C219	B2	118.6(4)	.	.	.	yes
C224	C219	B2	128.2(4)	.	.	.	yes
F220	C220	C219	119.4(4)	.	.	.	yes
F220	C220	C221	116.5(4)	.	.	.	yes
C219	C220	C221	124.2(5)	.	.	.	no
F221	C221	C220	119.6(5)	.	.	.	yes
F221	C221	C222	121.0(5)	.	.	.	yes
C220	C221	C222	119.3(4)	.	.	.	no
F222	C222	C221	120.4(5)	.	.	.	yes
F222	C222	C223	120.0(5)	.	.	.	yes
C221	C222	C223	119.6(5)	.	.	.	no
F223	C223	C222	120.1(4)	.	.	.	yes
F223	C223	C224	120.2(5)	.	.	.	yes
C222	C223	C224	119.6(5)	.	.	.	no
F224	C224	C219	120.9(4)	.	.	.	yes
F224	C224	C223	114.8(4)	.	.	.	yes
C219	C224	C223	124.2(4)	.	.	.	no
C21	B2	C27	113.4(4)	.	.	.	yes
C21	B2	C213	101.5(4)	.	.	.	yes
C21	B2	C219	114.0(4)	.	.	.	yes
C27	B2	C213	113.5(4)	.	.	.	yes
C27	B2	C219	102.0(4)	.	.	.	yes
C213	B2	C219	112.9(4)	.	.	.	yes

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N1	Zr1	O1	C121	-179.2(4)	.	.	.	.	no
N1	Zr1	O1	C124	0.3(3)	.	.	.	.	no
C111B	Zr1	O1	C121	-86.1(4)	.	.	.	.	no
C111B	Zr1	O1	C124	93.4(4)	.	.	.	.	no
C112B	Zr1	O1	C121	-101.1(4)	.	.	.	.	no
C112B	Zr1	O1	C124	78.4(4)	.	.	.	.	no
C113B	Zr1	O1	C121	-77.5(4)	.	.	.	.	no
C113B	Zr1	O1	C124	102.0(4)	.	.	.	.	no
C114B	Zr1	O1	C121	-47.1(4)	.	.	.	.	no
C114B	Zr1	O1	C124	132.4(4)	.	.	.	.	no
C115B	Zr1	O1	C121	-54.9(4)	.	.	.	.	no
C115B	Zr1	O1	C124	124.6(4)	.	.	.	.	no
C11	Zr1	O1	C121	100.5(4)	.	.	.	.	no
C11	Zr1	O1	C124	-80.0(4)	.	.	.	.	no
C12	Zr1	O1	C121	82.1(4)	.	.	.	.	no
C12	Zr1	O1	C124	-98.4(4)	.	.	.	.	no
C13	Zr1	O1	C121	46.4(4)	.	.	.	.	no

C13	Zr1	O1	C124	-134.1(4)	.	.	.	.	no
C14	Zr1	O1	C121	50.0(4)	.	.	.	.	no
C14	Zr1	O1	C124	-130.5(4)	.	.	.	.	no
C15	Zr1	O1	C121	81.7(4)	.	.	.	.	no
C15	Zr1	O1	C124	-98.8(4)	.	.	.	.	no
C125	Zr1	O1	C121	179.6(4)	.	.	.	.	no
C125	Zr1	O1	C124	-0.9(4)	.	.	.	.	no
O1	Zr1	N1	C125	-177.9(3)	.	.	.	.	no
C111B	Zr1	N1	C125	105.1(3)	.	.	.	.	no
C112B	Zr1	N1	C125	75.7(3)	.	.	.	.	no
C113B	Zr1	N1	C125	54.5(3)	.	.	.	.	no
C114B	Zr1	N1	C125	70.2(4)	.	.	.	.	no
C115B	Zr1	N1	C125	107.2(3)	.	.	.	.	no
C11	Zr1	N1	C125	-74.3(3)	.	.	.	.	no
C12	Zr1	N1	C125	-48.4(3)	.	.	.	.	no
C13	Zr1	N1	C125	-57.1(4)	.	.	.	.	no
C14	Zr1	N1	C125	-99.2(4)	.	.	.	.	no
C15	Zr1	N1	C125	-101.7(3)	.	.	.	.	no
O1	Zr1	C111B	C112B	-151.3(3)	.	.	.	.	no
O1	Zr1	C111B	C115B	94.6(3)	.	.	.	.	no
O1	Zr1	C111B	C116B	-28.8(4)	.	.	.	.	no
N1	Zr1	C111B	C112B	-69.3(3)	.	.	.	.	no
N1	Zr1	C111B	C115B	176.5(3)	.	.	.	.	no
N1	Zr1	C111B	C116B	53.2(4)	.	.	.	.	no
C112B	Zr1	C111B	C115B	-114.2(4)	.	.	.	.	no
C112B	Zr1	C111B	C116B	122.4(5)	.	.	.	.	no
C113B	Zr1	C111B	C112B	37.4(3)	.	.	.	.	no
C113B	Zr1	C111B	C115B	-76.8(3)	.	.	.	.	no
C113B	Zr1	C111B	C116B	159.9(5)	.	.	.	.	no
C114B	Zr1	C111B	C112B	77.5(3)	.	.	.	.	no
C114B	Zr1	C111B	C115B	-36.7(3)	.	.	.	.	no
C114B	Zr1	C111B	C116B	-160.0(5)	.	.	.	.	no
C115B	Zr1	C111B	C112B	114.2(4)	.	.	.	.	no
C115B	Zr1	C111B	C116B	-123.4(5)	.	.	.	.	no
C12	Zr1	C111B	C112B	47.4(5)	.	.	.	.	no
C12	Zr1	C111B	C115B	-66.8(5)	.	.	.	.	no
C12	Zr1	C111B	C116B	169.8(4)	.	.	.	.	no
C13	Zr1	C111B	C112B	92.7(4)	.	.	.	.	no
C13	Zr1	C111B	C115B	-21.5(4)	.	.	.	.	no
C13	Zr1	C111B	C116B	-144.9(4)	.	.	.	.	no
C14	Zr1	C111B	C112B	136.6(3)	.	.	.	.	no
C14	Zr1	C111B	C115B	22.4(4)	.	.	.	.	no
C14	Zr1	C111B	C116B	-101.0(5)	.	.	.	.	no
C15	Zr1	C111B	C112B	-177.2(4)	.	.	.	.	no
C15	Zr1	C111B	C115B	68.6(5)	.	.	.	.	no
C15	Zr1	C111B	C116B	-54.8(6)	.	.	.	.	no
C125	Zr1	C111B	C112B	-37.4(3)	.	.	.	.	no
C125	Zr1	C111B	C115B	-151.6(3)	.	.	.	.	no
C125	Zr1	C111B	C116B	85.0(4)	.	.	.	.	no
O1	Zr1	C112B	C111B	29.0(3)	.	.	.	.	no
O1	Zr1	C112B	C113B	142.8(3)	.	.	.	.	no
O1	Zr1	C112B	C117B	-94.2(4)	.	.	.	.	no
N1	Zr1	C112B	C111B	108.6(3)	.	.	.	.	no
N1	Zr1	C112B	C113B	-137.7(3)	.	.	.	.	no
N1	Zr1	C112B	C117B	-14.7(4)	.	.	.	.	no
C111B	Zr1	C112B	C113B	113.8(4)	.	.	.	.	no
C111B	Zr1	C112B	C117B	-123.3(6)	.	.	.	.	no
C113B	Zr1	C112B	C111B	-113.8(4)	.	.	.	.	no
C113B	Zr1	C112B	C117B	123.0(6)	.	.	.	.	no
C114B	Zr1	C112B	C111B	-76.7(3)	.	.	.	.	no
C114B	Zr1	C112B	C113B	37.1(3)	.	.	.	.	no
C114B	Zr1	C112B	C117B	160.1(5)	.	.	.	.	no
C115B	Zr1	C112B	C111B	-36.9(3)	.	.	.	.	no
C115B	Zr1	C112B	C113B	76.9(3)	.	.	.	.	no
C115B	Zr1	C112B	C117B	-160.1(5)	.	.	.	.	no
C11	Zr1	C112B	C111B	169.7(3)	.	.	.	.	no

C11	Zr1	C112B	C113B	-76.6(4)	.	.	.	.	no
C11	Zr1	C112B	C117B	46.4(6)	.	.	.	.	no
C12	Zr1	C112B	C111B	-153.9(3)	.	.	.	.	no
C12	Zr1	C112B	C113B	-40.2(4)	.	.	.	.	no
C12	Zr1	C112B	C117B	82.8(5)	.	.	.	.	no
C13	Zr1	C112B	C111B	-114.2(3)	.	.	.	.	no
C13	Zr1	C112B	C113B	-0.4(4)	.	.	.	.	no
C13	Zr1	C112B	C117B	122.5(5)	.	.	.	.	no
C14	Zr1	C112B	C111B	-79.3(4)	.	.	.	.	no
C14	Zr1	C112B	C113B	34.5(5)	.	.	.	.	no
C14	Zr1	C112B	C117B	157.5(5)	.	.	.	.	no
C125	Zr1	C112B	C111B	141.5(3)	.	.	.	.	no
C125	Zr1	C112B	C113B	-104.8(4)	.	.	.	.	no
C125	Zr1	C112B	C117B	18.2(4)	.	.	.	.	no
O1	Zr1	C113B	C112B	-48.1(4)	.	.	.	.	no
O1	Zr1	C113B	C114B	65.8(3)	.	.	.	.	no
O1	Zr1	C113B	C118B	-170.8(4)	.	.	.	.	no
N1	Zr1	C113B	C112B	43.2(3)	.	.	.	.	no
N1	Zr1	C113B	C114B	157.0(3)	.	.	.	.	no
N1	Zr1	C113B	C118B	-79.6(5)	.	.	.	.	no
C111B	Zr1	C113B	C112B	-37.3(3)	.	.	.	.	no
C111B	Zr1	C113B	C114B	76.6(3)	.	.	.	.	no
C111B	Zr1	C113B	C118B	-160.0(6)	.	.	.	.	no
C112B	Zr1	C113B	C114B	113.9(5)	.	.	.	.	no
C112B	Zr1	C113B	C118B	-122.7(6)	.	.	.	.	no
C114B	Zr1	C113B	C112B	-113.9(5)	.	.	.	.	no
C114B	Zr1	C113B	C118B	123.4(6)	.	.	.	.	no
C115B	Zr1	C113B	C112B	-77.2(3)	.	.	.	.	no
C115B	Zr1	C113B	C114B	36.7(3)	.	.	.	.	no
C115B	Zr1	C113B	C118B	160.1(5)	.	.	.	.	no
C11	Zr1	C113B	C112B	134.4(3)	.	.	.	.	no
C11	Zr1	C113B	C114B	-111.7(3)	.	.	.	.	no
C11	Zr1	C113B	C118B	11.7(6)	.	.	.	.	no
C12	Zr1	C113B	C112B	147.6(3)	.	.	.	.	no
C12	Zr1	C113B	C114B	-98.5(3)	.	.	.	.	no
C12	Zr1	C113B	C118B	24.9(5)	.	.	.	.	no
C13	Zr1	C113B	C112B	179.7(3)	.	.	.	.	no
C13	Zr1	C113B	C114B	-66.5(3)	.	.	.	.	no
C13	Zr1	C113B	C118B	57.0(5)	.	.	.	.	no
C14	Zr1	C113B	C112B	-160.4(3)	.	.	.	.	no
C14	Zr1	C113B	C114B	-46.5(4)	.	.	.	.	no
C14	Zr1	C113B	C118B	77.0(5)	.	.	.	.	no
C15	Zr1	C113B	C112B	173.3(3)	.	.	.	.	no
C15	Zr1	C113B	C114B	-72.8(5)	.	.	.	.	no
C15	Zr1	C113B	C118B	50.6(7)	.	.	.	.	no
C125	Zr1	C113B	C112B	69.4(3)	.	.	.	.	no
C125	Zr1	C113B	C114B	-176.7(3)	.	.	.	.	no
C125	Zr1	C113B	C118B	-53.3(5)	.	.	.	.	no
O1	Zr1	C114B	C113B	-129.7(3)	.	.	.	.	no
O1	Zr1	C114B	C115B	-15.2(3)	.	.	.	.	no
O1	Zr1	C114B	C119B	107.9(5)	.	.	.	.	no
N1	Zr1	C114B	C113B	-30.5(4)	.	.	.	.	no
N1	Zr1	C114B	C115B	84.0(4)	.	.	.	.	no
N1	Zr1	C114B	C119B	-153.0(4)	.	.	.	.	no
C111B	Zr1	C114B	C113B	-77.8(3)	.	.	.	.	no
C111B	Zr1	C114B	C115B	36.8(3)	.	.	.	.	no
C111B	Zr1	C114B	C119B	159.8(6)	.	.	.	.	no
C112B	Zr1	C114B	C113B	-37.4(3)	.	.	.	.	no
C112B	Zr1	C114B	C115B	77.1(3)	.	.	.	.	no
C112B	Zr1	C114B	C119B	-159.9(6)	.	.	.	.	no
C113B	Zr1	C114B	C115B	114.5(4)	.	.	.	.	no
C113B	Zr1	C114B	C119B	-122.4(6)	.	.	.	.	no
C115B	Zr1	C114B	C113B	-114.5(4)	.	.	.	.	no
C115B	Zr1	C114B	C119B	123.1(6)	.	.	.	.	no
C11	Zr1	C114B	C113B	96.6(4)	.	.	.	.	no
C11	Zr1	C114B	C115B	-148.9(3)	.	.	.	.	no

C11	Zr1	C114B	C119B	-25.8(6)	.	.	.	.	no
C12	Zr1	C114B	C113B	87.7(3)	.	.	.	.	no
C12	Zr1	C114B	C115B	-157.8(3)	.	.	.	.	no
C12	Zr1	C114B	C119B	-34.7(5)	.	.	.	.	no
C13	Zr1	C114B	C113B	113.3(3)	.	.	.	.	no
C13	Zr1	C114B	C115B	-132.2(3)	.	.	.	.	no
C13	Zr1	C114B	C119B	-9.1(5)	.	.	.	.	no
C14	Zr1	C114B	C113B	141.2(3)	.	.	.	.	no
C14	Zr1	C114B	C115B	-104.3(3)	.	.	.	.	no
C14	Zr1	C114B	C119B	18.8(5)	.	.	.	.	no
C15	Zr1	C114B	C113B	138.8(3)	.	.	.	.	no
C15	Zr1	C114B	C115B	-106.7(3)	.	.	.	.	no
C15	Zr1	C114B	C119B	16.4(6)	.	.	.	.	no
C125	Zr1	C114B	C113B	3.6(4)	.	.	.	.	no
C125	Zr1	C114B	C115B	118.1(3)	.	.	.	.	no
C125	Zr1	C114B	C119B	-118.9(5)	.	.	.	.	no
O1	Zr1	C115B	C111B	-79.5(3)	.	.	.	.	no
O1	Zr1	C115B	C114B	165.7(3)	.	.	.	.	no
O1	Zr1	C115B	C120B	43.0(5)	.	.	.	.	no
N1	Zr1	C115B	C111B	-4.1(3)	.	.	.	.	no
N1	Zr1	C115B	C114B	-118.9(3)	.	.	.	.	no
N1	Zr1	C115B	C120B	118.4(5)	.	.	.	.	no
C111B	Zr1	C115B	C114B	-114.8(4)	.	.	.	.	no
C111B	Zr1	C115B	C120B	122.5(6)	.	.	.	.	no
C112B	Zr1	C115B	C111B	37.3(3)	.	.	.	.	no
C112B	Zr1	C115B	C114B	-77.5(3)	.	.	.	.	no
C112B	Zr1	C115B	C120B	159.8(5)	.	.	.	.	no
C113B	Zr1	C115B	C111B	77.7(3)	.	.	.	.	no
C113B	Zr1	C115B	C114B	-37.0(3)	.	.	.	.	no
C113B	Zr1	C115B	C120B	-159.7(5)	.	.	.	.	no
C114B	Zr1	C115B	C111B	114.8(4)	.	.	.	.	no
C114B	Zr1	C115B	C120B	-122.7(6)	.	.	.	.	no
C11	Zr1	C115B	C111B	179.4(4)	.	.	.	.	no
C11	Zr1	C115B	C114B	64.7(5)	.	.	.	.	no
C11	Zr1	C115B	C120B	-58.1(7)	.	.	.	.	no
C12	Zr1	C115B	C111B	143.8(3)	.	.	.	.	no
C12	Zr1	C115B	C114B	29.1(4)	.	.	.	.	no
C12	Zr1	C115B	C120B	-93.7(5)	.	.	.	.	no
C13	Zr1	C115B	C111B	164.1(3)	.	.	.	.	no
C13	Zr1	C115B	C114B	49.3(3)	.	.	.	.	no
C13	Zr1	C115B	C120B	-73.4(5)	.	.	.	.	no
C14	Zr1	C115B	C111B	-163.4(3)	.	.	.	.	no
C14	Zr1	C115B	C114B	81.8(3)	.	.	.	.	no
C14	Zr1	C115B	C120B	-40.9(5)	.	.	.	.	no
C15	Zr1	C115B	C111B	-144.0(3)	.	.	.	.	no
C15	Zr1	C115B	C114B	101.3(4)	.	.	.	.	no
C15	Zr1	C115B	C120B	-21.5(6)	.	.	.	.	no
C125	Zr1	C115B	C111B	35.3(4)	.	.	.	.	no
C125	Zr1	C115B	C114B	-79.5(4)	.	.	.	.	no
C125	Zr1	C115B	C120B	157.8(5)	.	.	.	.	no
O1	Zr1	C11	C12	-152.9(3)	.	.	.	.	no
O1	Zr1	C11	C15	-37.5(4)	.	.	.	.	no
O1	Zr1	C11	C16	84.3(5)	.	.	.	.	no
N1	Zr1	C11	C12	126.6(4)	.	.	.	.	no
N1	Zr1	C11	C15	-118.0(4)	.	.	.	.	no
N1	Zr1	C11	C16	3.8(5)	.	.	.	.	no
C112B	Zr1	C11	C12	66.0(5)	.	.	.	.	no
C112B	Zr1	C11	C15	-178.6(3)	.	.	.	.	no
C112B	Zr1	C11	C16	-56.8(7)	.	.	.	.	no
C113B	Zr1	C11	C12	25.1(4)	.	.	.	.	no
C113B	Zr1	C11	C15	140.5(3)	.	.	.	.	no
C113B	Zr1	C11	C16	-97.8(6)	.	.	.	.	no
C114B	Zr1	C11	C12	-16.5(5)	.	.	.	.	no
C114B	Zr1	C11	C15	98.9(4)	.	.	.	.	no
C114B	Zr1	C11	C16	-139.3(5)	.	.	.	.	no
C115B	Zr1	C11	C12	-56.4(6)	.	.	.	.	no

C115B	Zr1	C11	C15	59.0(6)	.	.	.	.	no
C115B	Zr1	C11	C16	-179.2(5)	.	.	.	.	no
C12	Zr1	C11	C15	115.4(5)	.	.	.	.	no
C12	Zr1	C11	C16	-122.8(7)	.	.	.	.	no
C13	Zr1	C11	C12	-37.6(4)	.	.	.	.	no
C13	Zr1	C11	C15	77.8(4)	.	.	.	.	no
C13	Zr1	C11	C16	-160.4(6)	.	.	.	.	no
C14	Zr1	C11	C12	-77.5(4)	.	.	.	.	no
C14	Zr1	C11	C15	37.9(3)	.	.	.	.	no
C14	Zr1	C11	C16	159.7(6)	.	.	.	.	no
C15	Zr1	C11	C12	-115.4(5)	.	.	.	.	no
C15	Zr1	C11	C16	121.8(7)	.	.	.	.	no
C125	Zr1	C11	C12	94.1(4)	.	.	.	.	no
C125	Zr1	C11	C15	-150.6(4)	.	.	.	.	no
C125	Zr1	C11	C16	-28.8(5)	.	.	.	.	no
O1	Zr1	C12	C11	35.5(4)	.	.	.	.	no
O1	Zr1	C12	C13	-78.1(4)	.	.	.	.	no
O1	Zr1	C12	C17	158.9(5)	.	.	.	.	no
N1	Zr1	C12	C11	-54.3(4)	.	.	.	.	no
N1	Zr1	C12	C13	-167.9(3)	.	.	.	.	no
N1	Zr1	C12	C17	69.1(6)	.	.	.	.	no
C111B	Zr1	C12	C11	-168.5(3)	.	.	.	.	no
C111B	Zr1	C12	C13	77.9(5)	.	.	.	.	no
C111B	Zr1	C12	C17	-45.1(7)	.	.	.	.	no
C112B	Zr1	C12	C11	-140.7(3)	.	.	.	.	no
C112B	Zr1	C12	C13	105.7(4)	.	.	.	.	no
C112B	Zr1	C12	C17	-17.3(6)	.	.	.	.	no
C113B	Zr1	C12	C11	-160.6(4)	.	.	.	.	no
C113B	Zr1	C12	C13	85.8(4)	.	.	.	.	no
C113B	Zr1	C12	C17	-37.2(6)	.	.	.	.	no
C114B	Zr1	C12	C11	167.9(3)	.	.	.	.	no
C114B	Zr1	C12	C13	54.3(4)	.	.	.	.	no
C114B	Zr1	C12	C17	-68.8(6)	.	.	.	.	no
C115B	Zr1	C12	C11	153.1(3)	.	.	.	.	no
C115B	Zr1	C12	C13	39.5(4)	.	.	.	.	no
C115B	Zr1	C12	C17	-83.6(6)	.	.	.	.	no
C11	Zr1	C12	C13	-113.6(5)	.	.	.	.	no
C11	Zr1	C12	C17	123.4(7)	.	.	.	.	no
C13	Zr1	C12	C11	113.6(5)	.	.	.	.	no
C13	Zr1	C12	C17	-123.0(7)	.	.	.	.	no
C14	Zr1	C12	C11	77.2(4)	.	.	.	.	no
C14	Zr1	C12	C13	-36.4(3)	.	.	.	.	no
C14	Zr1	C12	C17	-159.4(6)	.	.	.	.	no
C15	Zr1	C12	C11	36.0(3)	.	.	.	.	no
C15	Zr1	C12	C13	-77.6(4)	.	.	.	.	no
C15	Zr1	C12	C17	159.4(6)	.	.	.	.	no
C125	Zr1	C12	C11	-78.5(4)	.	.	.	.	no
C125	Zr1	C12	C13	167.9(4)	.	.	.	.	no
C125	Zr1	C12	C17	44.9(5)	.	.	.	.	no
O1	Zr1	C13	C12	122.4(3)	.	.	.	.	no
O1	Zr1	C13	C14	6.9(4)	.	.	.	.	no
O1	Zr1	C13	C18	-116.1(8)	.	.	.	.	no
N1	Zr1	C13	C12	16.2(5)	.	.	.	.	no
N1	Zr1	C13	C14	-99.2(4)	.	.	.	.	no
N1	Zr1	C13	C18	137.8(8)	.	.	.	.	no
C111B	Zr1	C13	C12	-139.0(3)	.	.	.	.	no
C111B	Zr1	C13	C14	105.6(4)	.	.	.	.	no
C111B	Zr1	C13	C18	-17.4(10)	.	.	.	.	no
C112B	Zr1	C13	C12	-98.4(3)	.	.	.	.	no
C112B	Zr1	C13	C14	146.2(3)	.	.	.	.	no
C112B	Zr1	C13	C18	23.2(10)	.	.	.	.	no
C113B	Zr1	C13	C12	-98.6(3)	.	.	.	.	no
C113B	Zr1	C13	C14	146.0(4)	.	.	.	.	no
C113B	Zr1	C13	C18	23.0(9)	.	.	.	.	no
C114B	Zr1	C13	C12	-127.1(4)	.	.	.	.	no
C114B	Zr1	C13	C14	117.5(4)	.	.	.	.	no

C114B	Zr1	C13	C18	-5.5(9)	.	.	.	.	no
C115B	Zr1	C13	C12	-150.1(3)	.	.	.	.	no
C115B	Zr1	C13	C14	94.4(4)	.	.	.	.	no
C115B	Zr1	C13	C18	-28.6(9)	.	.	.	.	no
C11	Zr1	C13	C12	37.8(3)	.	.	.	.	no
C11	Zr1	C13	C14	-77.7(4)	.	.	.	.	no
C11	Zr1	C13	C18	159.3(10)	.	.	.	.	no
C12	Zr1	C13	C14	-115.4(5)	.	.	.	.	no
C12	Zr1	C13	C18	121.6(10)	.	.	.	.	no
C14	Zr1	C13	C12	115.4(5)	.	.	.	.	no
C14	Zr1	C13	C18	-123.0(10)	.	.	.	.	no
C15	Zr1	C13	C12	77.2(4)	.	.	.	.	no
C15	Zr1	C13	C14	-38.2(3)	.	.	.	.	no
C15	Zr1	C13	C18	-161.2(10)	.	.	.	.	no
C125	Zr1	C13	C12	-12.8(4)	.	.	.	.	no
C125	Zr1	C13	C14	-128.2(4)	.	.	.	.	no
C125	Zr1	C13	C18	108.8(9)	.	.	.	.	no
O1	Zr1	C14	C13	-173.8(4)	.	.	.	.	no
O1	Zr1	C14	C15	72.4(3)	.	.	.	.	no
O1	Zr1	C14	C19	-53.0(6)	.	.	.	.	no
N1	Zr1	C14	C13	109.2(4)	.	.	.	.	no
N1	Zr1	C14	C15	-4.6(4)	.	.	.	.	no
N1	Zr1	C14	C19	-129.9(6)	.	.	.	.	no
C111B	Zr1	C14	C13	-105.3(4)	.	.	.	.	no
C111B	Zr1	C14	C15	141.0(3)	.	.	.	.	no
C111B	Zr1	C14	C19	15.6(7)	.	.	.	.	no
C112B	Zr1	C14	C13	-60.8(5)	.	.	.	.	no
C112B	Zr1	C14	C15	-174.5(3)	.	.	.	.	no
C112B	Zr1	C14	C19	60.1(7)	.	.	.	.	no
C113B	Zr1	C14	C13	-40.6(4)	.	.	.	.	no
C113B	Zr1	C14	C15	-154.4(3)	.	.	.	.	no
C113B	Zr1	C14	C19	80.3(6)	.	.	.	.	no
C114B	Zr1	C14	C13	-62.8(4)	.	.	.	.	no
C114B	Zr1	C14	C15	-176.6(3)	.	.	.	.	no
C114B	Zr1	C14	C19	58.1(6)	.	.	.	.	no
C115B	Zr1	C14	C13	-93.7(4)	.	.	.	.	no
C115B	Zr1	C14	C15	152.6(3)	.	.	.	.	no
C115B	Zr1	C14	C19	27.2(6)	.	.	.	.	no
C11	Zr1	C14	C13	77.5(4)	.	.	.	.	no
C11	Zr1	C14	C15	-36.2(3)	.	.	.	.	no
C11	Zr1	C14	C19	-161.6(7)	.	.	.	.	no
C12	Zr1	C14	C13	36.9(4)	.	.	.	.	no
C12	Zr1	C14	C15	-76.9(4)	.	.	.	.	no
C12	Zr1	C14	C19	157.7(7)	.	.	.	.	no
C13	Zr1	C14	C15	-113.7(5)	.	.	.	.	no
C13	Zr1	C14	C19	120.9(7)	.	.	.	.	no
C15	Zr1	C14	C13	113.7(5)	.	.	.	.	no
C15	Zr1	C14	C19	-125.4(7)	.	.	.	.	no
C125	Zr1	C14	C13	67.2(4)	.	.	.	.	no
C125	Zr1	C14	C15	-46.5(4)	.	.	.	.	no
C125	Zr1	C14	C19	-171.9(5)	.	.	.	.	no
O1	Zr1	C15	C11	142.4(4)	.	.	.	.	no
O1	Zr1	C15	C14	-103.0(3)	.	.	.	.	no
O1	Zr1	C15	C110	18.3(5)	.	.	.	.	no
N1	Zr1	C15	C11	61.9(4)	.	.	.	.	no
N1	Zr1	C15	C14	176.5(3)	.	.	.	.	no
N1	Zr1	C15	C110	-62.3(5)	.	.	.	.	no
C111B	Zr1	C15	C11	168.4(3)	.	.	.	.	no
C111B	Zr1	C15	C14	-77.0(5)	.	.	.	.	no
C111B	Zr1	C15	C110	44.2(7)	.	.	.	.	no
C113B	Zr1	C15	C11	-69.7(5)	.	.	.	.	no
C113B	Zr1	C15	C14	44.9(5)	.	.	.	.	no
C113B	Zr1	C15	C110	166.1(5)	.	.	.	.	no
C114B	Zr1	C15	C11	-110.1(4)	.	.	.	.	no
C114B	Zr1	C15	C14	4.5(4)	.	.	.	.	no
C114B	Zr1	C15	C110	125.7(5)	.	.	.	.	no

C115B	Zr1	C15	C11	-151.5(3)	.	.	.	.	no
C115B	Zr1	C15	C14	-36.9(4)	.	.	.	.	no
C115B	Zr1	C15	C110	84.3(6)	.	.	.	.	no
C11	Zr1	C15	C14	114.6(5)	.	.	.	.	no
C11	Zr1	C15	C110	-124.2(7)	.	.	.	.	no
C12	Zr1	C15	C11	-37.2(3)	.	.	.	.	no
C12	Zr1	C15	C14	77.4(4)	.	.	.	.	no
C12	Zr1	C15	C110	-161.4(6)	.	.	.	.	no
C13	Zr1	C15	C11	-77.7(4)	.	.	.	.	no
C13	Zr1	C15	C14	37.0(4)	.	.	.	.	no
C13	Zr1	C15	C110	158.2(6)	.	.	.	.	no
C14	Zr1	C15	C11	-114.6(5)	.	.	.	.	no
C14	Zr1	C15	C110	121.2(7)	.	.	.	.	no
C125	Zr1	C15	C11	29.1(4)	.	.	.	.	no
C125	Zr1	C15	C14	143.7(4)	.	.	.	.	no
C125	Zr1	C15	C110	-95.1(5)	.	.	.	.	no
O1	Zr1	C125	N1	2.3(4)	.	.	.	.	no
O1	Zr1	C125	C126	179.2(11)	.	.	.	.	no
N1	Zr1	C125	C126	176.9(14)	.	.	.	.	no
C111B	Zr1	C125	N1	-77.9(3)	.	.	.	.	no
C111B	Zr1	C125	C126	99.1(12)	.	.	.	.	no
C112B	Zr1	C125	N1	-97.0(3)	.	.	.	.	no
C112B	Zr1	C125	C126	80.0(12)	.	.	.	.	no
C113B	Zr1	C125	N1	-127.4(3)	.	.	.	.	no
C113B	Zr1	C125	C126	49.6(12)	.	.	.	.	no
C114B	Zr1	C125	N1	-129.2(3)	.	.	.	.	no
C114B	Zr1	C125	C126	47.7(12)	.	.	.	.	no
C115B	Zr1	C125	N1	-95.4(3)	.	.	.	.	no
C115B	Zr1	C125	C126	81.6(12)	.	.	.	.	no
C11	Zr1	C125	N1	99.1(3)	.	.	.	.	no
C11	Zr1	C125	C126	-83.9(12)	.	.	.	.	no
C12	Zr1	C125	N1	131.8(3)	.	.	.	.	no
C12	Zr1	C125	C126	-51.3(12)	.	.	.	.	no
C13	Zr1	C125	N1	138.6(3)	.	.	.	.	no
C13	Zr1	C125	C126	-44.5(12)	.	.	.	.	no
C14	Zr1	C125	N1	107.6(3)	.	.	.	.	no
C14	Zr1	C125	C126	-75.5(12)	.	.	.	.	no
C15	Zr1	C125	N1	84.1(3)	.	.	.	.	no
C15	Zr1	C125	C126	-99.0(12)	.	.	.	.	no
Zr1	O1	C121	C122	-156.4(3)	.	.	.	.	no
C124	O1	C121	C122	24.0(5)	.	.	.	.	no
Zr1	O1	C124	C123	-178.5(3)	.	.	.	.	no
C121	O1	C124	C123	1.1(5)	.	.	.	.	no
Zr1	N1	C125	C126	-178.6(6)	.	.	.	.	no
C127	N1	C125	Zr1	177.2(5)	.	.	.	.	no
C127	N1	C125	C126	-1.4(9)	.	.	.	.	no
C125	N1	C127	C128	96.8(7)	.	.	.	.	no
Zr1	C111B	C112B	C113B	-68.2(4)	.	.	.	.	no
Zr1	C111B	C112B	C117B	110.1(7)	.	.	.	.	no
C115B	C111B	C112B	Zr1	68.2(4)	.	.	.	.	no
C115B	C111B	C112B	C113B	0.0(6)	.	.	.	.	no
C115B	C111B	C112B	C117B	178.3(7)	.	.	.	.	no
C116B	C111B	C112B	Zr1	-111.8(6)	.	.	.	.	no
C116B	C111B	C112B	C113B	-180.0(6)	.	.	.	.	no
C116B	C111B	C112B	C117B	-1.8(11)	.	.	.	.	no
Zr1	C111B	C115B	C114B	66.7(3)	.	.	.	.	no
Zr1	C111B	C115B	C120B	-115.0(6)	.	.	.	.	no
C112B	C111B	C115B	Zr1	-66.8(4)	.	.	.	.	no
C112B	C111B	C115B	C114B	0.0(6)	.	.	.	.	no
C112B	C111B	C115B	C120B	178.2(6)	.	.	.	.	no
C116B	C111B	C115B	Zr1	113.3(6)	.	.	.	.	no
C116B	C111B	C115B	C114B	180.0(6)	.	.	.	.	no
C116B	C111B	C115B	C120B	-1.8(9)	.	.	.	.	no
Zr1	C112B	C113B	C114B	-68.6(4)	.	.	.	.	no
Zr1	C112B	C113B	C118B	109.6(7)	.	.	.	.	no
C111B	C112B	C113B	Zr1	68.6(4)	.	.	.	.	no

C111B	C112B	C113B	C114B	0.0(7)	.	.	.	.	no
C111B	C112B	C113B	C118B	178.2(6)	.	.	.	.	no
C117B	C112B	C113B	Zr1	-109.6(7)	.	.	.	.	no
C117B	C112B	C113B	C114B	-178.2(7)	.	.	.	.	no
C117B	C112B	C113B	C118B	0.0(11)	.	.	.	.	no
Zr1	C113B	C114B	C115B	-67.5(4)	.	.	.	.	no
Zr1	C113B	C114B	C119B	114.2(7)	.	.	.	.	no
C112B	C113B	C114B	Zr1	67.5(4)	.	.	.	.	no
C112B	C113B	C114B	C115B	0.0(6)	.	.	.	.	no
C112B	C113B	C114B	C119B	-178.3(7)	.	.	.	.	no
C118B	C113B	C114B	Zr1	-110.7(6)	.	.	.	.	no
C118B	C113B	C114B	C115B	-178.3(6)	.	.	.	.	no
C118B	C113B	C114B	C119B	3.5(11)	.	.	.	.	no
Zr1	C114B	C115B	C111B	-66.3(3)	.	.	.	.	no
Zr1	C114B	C115B	C120B	115.4(6)	.	.	.	.	no
C113B	C114B	C115B	Zr1	66.4(4)	.	.	.	.	no
C113B	C114B	C115B	C111B	0.0(6)	.	.	.	.	no
C113B	C114B	C115B	C120B	-178.2(6)	.	.	.	.	no
C119B	C114B	C115B	Zr1	-115.4(7)	.	.	.	.	no
C119B	C114B	C115B	C111B	178.3(7)	.	.	.	.	no
C119B	C114B	C115B	C120B	0.0(10)	.	.	.	.	no
Zr1	C11	C12	C13	68.2(4)	.	.	.	.	no
Zr1	C11	C12	C17	-123.3(6)	.	.	.	.	no
C15	C11	C12	Zr1	-66.0(4)	.	.	.	.	no
C15	C11	C12	C13	2.2(6)	.	.	.	.	no
C15	C11	C12	C17	170.7(6)	.	.	.	.	no
C16	C11	C12	Zr1	120.9(6)	.	.	.	.	no
C16	C11	C12	C13	-170.9(6)	.	.	.	.	no
C16	C11	C12	C17	-2.4(10)	.	.	.	.	no
Zr1	C11	C15	C14	-65.9(4)	.	.	.	.	no
Zr1	C11	C15	C110	121.3(6)	.	.	.	.	no
C12	C11	C15	Zr1	65.5(4)	.	.	.	.	no
C12	C11	C15	C14	-0.4(6)	.	.	.	.	no
C12	C11	C15	C110	-173.2(6)	.	.	.	.	no
C16	C11	C15	Zr1	-121.3(6)	.	.	.	.	no
C16	C11	C15	C14	172.9(6)	.	.	.	.	no
C16	C11	C15	C110	0.1(10)	.	.	.	.	no
Zr1	C12	C13	C14	65.0(4)	.	.	.	.	no
Zr1	C12	C13	C18	-132.2(6)	.	.	.	.	no
C11	C12	C13	Zr1	-68.2(4)	.	.	.	.	no
C11	C12	C13	C14	-3.2(6)	.	.	.	.	no
C11	C12	C13	C18	159.7(6)	.	.	.	.	no
C17	C12	C13	Zr1	123.3(6)	.	.	.	.	no
C17	C12	C13	C14	-171.7(6)	.	.	.	.	no
C17	C12	C13	C18	-8.9(10)	.	.	.	.	no
Zr1	C13	C14	C15	68.3(4)	.	.	.	.	no
Zr1	C13	C14	C19	-126.9(6)	.	.	.	.	no
C12	C13	C14	Zr1	-65.4(4)	.	.	.	.	no
C12	C13	C14	C15	3.0(6)	.	.	.	.	no
C12	C13	C14	C19	167.8(6)	.	.	.	.	no
C18	C13	C14	Zr1	132.1(6)	.	.	.	.	no
C18	C13	C14	C15	-159.6(6)	.	.	.	.	no
C18	C13	C14	C19	5.3(9)	.	.	.	.	no
Zr1	C14	C15	C11	67.4(4)	.	.	.	.	no
Zr1	C14	C15	C110	-119.7(6)	.	.	.	.	no
C13	C14	C15	Zr1	-69.0(4)	.	.	.	.	no
C13	C14	C15	C11	-1.6(6)	.	.	.	.	no
C13	C14	C15	C110	171.3(6)	.	.	.	.	no
C19	C14	C15	Zr1	127.0(6)	.	.	.	.	no
C19	C14	C15	C11	-165.7(6)	.	.	.	.	no
C19	C14	C15	C110	7.3(10)	.	.	.	.	no
O1	C121	C122	C123	-38.8(5)	.	.	.	.	no
C121	C122	C123	C124	38.0(5)	.	.	.	.	no
C122	C123	C124	O1	-25.3(5)	.	.	.	.	no
C26	C21	C22	F22	-178.4(4)	.	.	.	.	no
C26	C21	C22	C23	1.7(8)	.	.	.	.	no

B2	C21	C22	F22	-2.7(7)	.	.	.	.	no
B2	C21	C22	C23	177.4(5)	.	.	.	.	no
C22	C21	C26	F26	177.4(5)	.	.	.	.	no
C22	C21	C26	C25	-3.1(8)	.	.	.	.	no
B2	C21	C26	F26	2.2(8)	.	.	.	.	no
B2	C21	C26	C25	-178.3(5)	.	.	.	.	no
C22	C21	B2	C27	170.3(5)	.	.	.	.	no
C22	C21	B2	C213	-67.5(6)	.	.	.	.	no
C22	C21	B2	C219	54.2(6)	.	.	.	.	no
C26	C21	B2	C27	-14.7(7)	.	.	.	.	no
C26	C21	B2	C213	107.4(6)	.	.	.	.	no
C26	C21	B2	C219	-130.9(6)	.	.	.	.	no
F22	C22	C23	F23	0.5(7)	.	.	.	.	no
F22	C22	C23	C24	-179.7(5)	.	.	.	.	no
C21	C22	C23	F23	-179.6(5)	.	.	.	.	no
C21	C22	C23	C24	0.2(9)	.	.	.	.	no
F23	C23	C24	F24	-1.6(8)	.	.	.	.	no
F23	C23	C24	C25	178.8(5)	.	.	.	.	no
C22	C23	C24	F24	178.6(5)	.	.	.	.	no
C22	C23	C24	C25	-1.1(8)	.	.	.	.	no
F24	C24	C25	F25	-0.6(9)	.	.	.	.	no
F24	C24	C25	C26	-179.8(5)	.	.	.	.	no
C23	C24	C25	F25	179.0(5)	.	.	.	.	no
C23	C24	C25	C26	-0.2(9)	.	.	.	.	no
F25	C25	C26	F26	2.8(8)	.	.	.	.	no
F25	C25	C26	C21	-176.7(5)	.	.	.	.	no
C24	C25	C26	F26	-178.0(5)	.	.	.	.	no
C24	C25	C26	C21	2.5(9)	.	.	.	.	no
C212	C27	C28	F28	179.1(4)	.	.	.	.	no
C212	C27	C28	C29	-2.1(7)	.	.	.	.	no
B2	C27	C28	F28	5.8(6)	.	.	.	.	no
B2	C27	C28	C29	-175.4(5)	.	.	.	.	no
C28	C27	B2	C21	-55.7(6)	.	.	.	.	no
C28	C27	B2	C213	-170.9(4)	.	.	.	.	no
C28	C27	B2	C219	67.4(5)	.	.	.	.	no
C212	C27	B2	C21	132.0(5)	.	.	.	.	no
C212	C27	B2	C213	16.8(7)	.	.	.	.	no
C212	C27	B2	C219	-105.0(6)	.	.	.	.	no
C28	C27	C212	C211	1.9(8)	.	.	.	.	no
C28	C27	C212	F212	-177.6(5)	.	.	.	.	no
B2	C27	C212	F212	-4.8(8)	.	.	.	.	no
B2	C27	C212	C211	174.6(5)	.	.	.	.	no
F28	C28	C29	F29	1.0(7)	.	.	.	.	no
C27	C28	C29	C210	1.8(8)	.	.	.	.	no
F28	C28	C29	C210	-179.4(5)	.	.	.	.	no
C27	C28	C29	F29	-177.9(5)	.	.	.	.	no
C28	C29	C210	F210	-179.5(5)	.	.	.	.	no
F29	C29	C210	C211	178.7(5)	.	.	.	.	no
C28	C29	C210	C211	-1.1(9)	.	.	.	.	no
F29	C29	C210	F210	0.2(9)	.	.	.	.	no
F210	C210	C211	F211	-2.4(9)	.	.	.	.	no
F210	C210	C211	C212	179.3(5)	.	.	.	.	no
C29	C210	C211	F211	179.2(5)	.	.	.	.	no
C29	C210	C211	C212	0.9(9)	.	.	.	.	no
F211	C211	C212	C27	-179.7(5)	.	.	.	.	no
C210	C211	C212	F212	178.1(5)	.	.	.	.	no
C210	C211	C212	C27	-1.4(9)	.	.	.	.	no
F211	C211	C212	F212	-0.2(8)	.	.	.	.	no
C218	C213	C214	F214	-177.5(4)	.	.	.	.	no
C218	C213	C214	C215	4.0(7)	.	.	.	.	no
B2	C213	C214	F214	-1.4(7)	.	.	.	.	no
B2	C213	C214	C215	-179.9(5)	.	.	.	.	no
C214	C213	C218	F218	177.2(4)	.	.	.	.	no
C214	C213	C218	C217	-2.2(7)	.	.	.	.	no
B2	C213	C218	F218	1.4(7)	.	.	.	.	no
B2	C213	C218	C217	-177.9(5)	.	.	.	.	no

C214	C213	B2	C21	-70.0(5)	.	.	.	.	no
C214	C213	B2	C27	52.0(6)	.	.	.	.	no
C214	C213	B2	C219	167.5(4)	.	.	.	.	no
C218	C213	B2	C21	105.6(5)	.	.	.	.	no
C218	C213	B2	C27	-132.4(5)	.	.	.	.	no
C218	C213	B2	C219	-16.9(6)	.	.	.	.	no
F214	C214	C215	F215	-2.2(7)	.	.	.	.	no
F214	C214	C215	C216	179.2(5)	.	.	.	.	no
C213	C214	C215	F215	176.4(5)	.	.	.	.	no
C213	C214	C215	C216	-2.3(8)	.	.	.	.	no
F215	C215	C216	F216	0.6(8)	.	.	.	.	no
F215	C215	C216	C217	179.8(5)	.	.	.	.	no
C214	C215	C216	F216	179.3(5)	.	.	.	.	no
C214	C215	C216	C217	-1.6(8)	.	.	.	.	no
F216	C216	C217	F217	3.1(8)	.	.	.	.	no
F216	C216	C217	C218	-177.6(5)	.	.	.	.	no
C215	C216	C217	F217	-176.1(5)	.	.	.	.	no
C215	C216	C217	C218	3.3(8)	.	.	.	.	no
F217	C217	C218	F218	-1.4(7)	.	.	.	.	no
F217	C217	C218	C213	178.0(4)	.	.	.	.	no
C216	C217	C218	F218	179.3(5)	.	.	.	.	no
C216	C217	C218	C213	-1.4(8)	.	.	.	.	no
C224	C219	C220	F220	179.8(4)	.	.	.	.	no
C224	C219	C220	C221	-0.6(8)	.	.	.	.	no
B2	C219	C220	F220	4.7(7)	.	.	.	.	no
B2	C219	C220	C221	-175.7(5)	.	.	.	.	no
C220	C219	C224	F224	-177.5(4)	.	.	.	.	no
C220	C219	C224	C223	1.0(7)	.	.	.	.	no
B2	C219	C224	F224	-3.0(8)	.	.	.	.	no
B2	C219	C224	C223	175.6(5)	.	.	.	.	no
C220	C219	B2	C21	-170.7(4)	.	.	.	.	no
C220	C219	B2	C27	66.8(5)	.	.	.	.	no
C220	C219	B2	C213	-55.5(6)	.	.	.	.	no
C224	C219	B2	C21	15.1(7)	.	.	.	.	no
C224	C219	B2	C27	-107.5(5)	.	.	.	.	no
C224	C219	B2	C213	130.3(5)	.	.	.	.	no
F220	C220	C221	F221	-1.6(8)	.	.	.	.	no
F220	C220	C221	C222	179.4(5)	.	.	.	.	no
C219	C220	C221	F221	178.8(5)	.	.	.	.	no
C219	C220	C221	C222	-0.2(9)	.	.	.	.	no
F221	C221	C222	F222	1.2(8)	.	.	.	.	no
F221	C221	C222	C223	-178.4(5)	.	.	.	.	no
C220	C221	C222	F222	-179.8(5)	.	.	.	.	no
C220	C221	C222	C223	0.6(8)	.	.	.	.	no
F222	C222	C223	F223	-1.5(8)	.	.	.	.	no
F222	C222	C223	C224	-179.8(5)	.	.	.	.	no
C221	C222	C223	F223	178.1(5)	.	.	.	.	no
C221	C222	C223	C224	-0.2(8)	.	.	.	.	no
F223	C223	C224	F224	-0.4(7)	.	.	.	.	no
F223	C223	C224	C219	-179.0(5)	.	.	.	.	no
C222	C223	C224	F224	177.9(5)	.	.	.	.	no
C222	C223	C224	C219	-0.7(8)	.	.	.	.	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

Zr1	C19	3.675(8)	.	.	.	.	no
Zr1	C117A	3.506(11)	.	.	.	.	no
Zr1	C118A	3.480(11)	.	.	.	.	no
Zr1	C116A	3.549(11)	.	.	.	.	no
Zr1	C120A	3.573(9)	.	.	.	.	no
Zr1	C119A	3.572(10)	.	.	.	.	no

Zr1	H110	3.6700	.	.	no
Zr1	H19"	3.6400	.	.	no
Zr1	H1161'	3.4300	.	.	no
Zr1	H1171"	3.2600	.	.	no
Zr1	H1181	3.2300	.	.	no
Zr1	H1191	3.4900	.	.	no
Zr1	H1201"	3.4000	.	.	no
F22	C121	3.298(7)	.	.	no
F22	C213	3.068(6)	.	.	no
F22	C218	3.092(6)	.	.	no
F22	F23	2.652(5)	.	.	no
F22	F218	2.852(5)	.	.	no
F22	F224	2.815(4)	.	.	no
F22	C120B	3.274(6)	.	.	no
F22	C219	2.986(6)	.	.	no
F22	C224	3.042(6)	.	.	no
F23	F22	2.652(5)	.	.	no
F23	F221	2.781(5)	.	1_455	no
F23	F24	2.741(5)	.	.	no
F24	F23	2.741(5)	.	.	no
F24	C211	3.253(7)	.	1_455	no
F24	C212	3.351(6)	.	1_455	no
F24	F220	2.910(4)	.	1_455	no
F24	F25	2.729(5)	.	.	no
F25	F26	2.643(5)	.	.	no
F25	F211	3.126(5)	.	1_455	no
F25	F24	2.729(5)	.	.	no
F25	C128	3.314(10)	.	1_565	no
F26	C28	2.794(6)	.	.	no
F26	F25	2.643(5)	.	.	no
F26	F214	2.995(5)	.	.	no
F26	C27	2.840(6)	.	.	no
F26	F28	2.804(5)	.	.	no
F28	C219	3.094(6)	.	.	no
F28	C21	2.975(6)	.	.	no
F28	F26	2.804(5)	.	.	no
F28	F222	2.923(4)	.	3_665	no
F28	C224	3.175(6)	.	.	no
F28	C26	3.022(6)	.	.	no
F28	F29	2.674(5)	.	.	no
F28	F224	2.988(4)	.	.	no
F29	F28	2.674(5)	.	.	no
F29	F210	2.726(5)	.	.	no
F22	H1202"	2.7700	.	.	no
F22	H121	2.7900	.	.	no
F22	H17	2.8600	.	2_555	no
F23	H121'	2.8200	.	.	no
F25	H127	2.7500	.	1_565	no
F25	H126	2.8400	.	1_565	no
F25	H128	2.8300	.	1_565	no
F26	H127	2.8400	.	1_565	no
F26	H128'	2.8100	.	3_565	no
F26	H126"	2.7700	.	1_565	no
F29	H110	2.8400	.	3_565	no
F29	H16"	2.8600	.	3_565	no
F210	F29	2.726(5)	.	.	no
F210	F211	2.744(5)	.	.	no
F211	F25	3.126(5)	.	1_655	no
F211	C16	3.294(9)	.	1_665	no
F211	F210	2.744(5)	.	.	no
F211	F212	2.630(5)	.	.	no
F212	C119B	3.204(8)	.	2_655	no
F212	F214	2.784(5)	.	.	no
F212	F220	2.884(4)	.	.	no
F212	F211	2.630(5)	.	.	no
F212	C214	2.748(6)	.	.	no

F212	C213	2.845 (6)	.	.	no
F214	C21	3.123 (6)	.	.	no
F214	C117B	3.363 (7)	.	1_565	no
F214	F215	2.675 (5)	.	.	no
F214	C27	2.984 (6)	.	.	no
F214	F26	2.995 (5)	.	.	no
F214	C26	3.203 (6)	.	.	no
F214	F212	2.784 (5)	.	.	no
F214	C212	3.022 (7)	.	.	no
F215	F214	2.675 (5)	.	.	no
F215	F216	2.725 (6)	.	.	no
F215	C118A	3.107 (11)	.	1_565	no
F215	C19	3.349 (9)	.	2_555	no
F216	C115B	3.193 (6)	.	2_655	no
F216	F217	2.743 (6)	.	.	no
F216	C11	3.165 (7)	.	2_555	no
F216	F215	2.725 (6)	.	.	no
F216	C110	3.231 (8)	.	2_555	no
F216	C111A	3.039 (7)	.	2_655	no
F216	C112A	3.230 (10)	.	2_655	no
F216	C112B	3.345 (7)	.	2_655	no
F216	C15	3.087 (6)	.	2_555	no
F216	C111B	3.072 (6)	.	2_655	no
F217	F218	2.632 (5)	.	.	no
F217	C112B	3.342 (7)	.	2_655	no
F217	C118A	3.296 (13)	.	2_655	no
F217	F216	2.743 (6)	.	.	no
F217	C118B	3.364 (10)	.	2_655	no
F217	C113A	3.232 (9)	.	2_655	no
F217	C113B	3.283 (7)	.	2_655	no
F218	F220	2.881 (4)	.	.	no
F218	F22	2.852 (5)	.	.	no
F218	C220	2.802 (6)	.	.	no
F218	C219	2.808 (6)	.	.	no
F218	F217	2.632 (5)	.	.	no
F218	C120B	3.076 (7)	.	.	no
F220	C27	3.060 (6)	.	.	no
F220	F24	2.910 (4)	.	1_655	no
F220	F221	2.653 (4)	.	.	no
F220	F218	2.881 (4)	.	.	no
F220	C213	2.957 (5)	.	.	no
F220	C212	3.080 (7)	.	.	no
F220	C218	3.028 (6)	.	.	no
F220	F212	2.884 (4)	.	.	no
F221	F220	2.653 (4)	.	.	no
F221	C110	3.297 (8)	.	1_655	no
F221	F23	2.781 (5)	.	1_655	no
F221	F222	2.739 (5)	.	.	no
F222	C224	3.304 (6)	.	3_665	no
F222	F28	2.923 (4)	.	3_665	no
F222	C110	3.245 (8)	.	1_655	no
F222	F221	2.739 (5)	.	.	no
F222	C223	3.213 (6)	.	3_665	no
F222	F223	2.734 (5)	.	.	no
F223	C221	3.267 (6)	.	3_665	no
F223	F224	2.636 (4)	.	.	no
F223	C222	3.329 (6)	.	3_665	no
F223	F222	2.734 (5)	.	.	no
F224	F28	2.988 (4)	.	.	no
F224	C122	3.365 (6)	.	.	no
F224	C123	3.185 (6)	.	3_565	no
F224	F223	2.636 (4)	.	.	no
F224	F22	2.815 (4)	.	.	no
F224	C22	2.793 (6)	.	.	no
F224	C122	3.306 (6)	.	3_565	no
F224	C21	2.859 (6)	.	.	no

F211	H128	2.5700	.	1_665	no
F211	H16'	2.8400	.	1_665	no
F212	H1192"	2.7400	.	2_655	no
F212	H1192	2.7700	.	2_655	no
F214	H1181"	2.8100	.	1_565	no
F214	H1172	2.5900	.	1_565	no
F214	H126"	2.7800	.	1_565	no
F215	H19	2.6400	.	2_555	no
F215	H1182"	2.8500	.	1_565	no
F215	H1181"	2.5700	.	1_565	no
F216	H16	2.7400	.	2_555	no
F216	H110"	2.5400	.	2_555	no
F217	H1181"	2.8200	.	2_655	no
F217	H1182"	2.6300	.	2_655	no
F217	H16	2.7100	.	2_555	no
F218	H1202'	2.5100	.	.	no
F218	H1201	2.6600	.	.	no
F220	H1191"	2.5300	.	2_655	no
F221	H122'	2.7200	.	1_655	no
F221	H110'	2.5200	.	1_655	no
F223	H123'	2.5000	.	.	no
F224	H122	2.5700	.	.	no
F224	H123	2.4000	.	3_565	no
O1	N1	3.029(6)	.	.	no
O1	C110	3.126(7)	.	.	no
O1	C15	3.079(7)	.	.	no
O1	C111A	3.082(7)	.	.	no
O1	C116A	2.941(11)	.	.	no
O1	C111B	3.116(6)	.	.	no
O1	C115B	3.272(6)	.	.	no
O1	C116B	3.089(8)	.	.	no
O1	C14	3.344(7)	.	.	no
O1	H1162	2.6400	.	.	no
O1	H110'	2.8500	.	.	no
O1	H1161'	2.3700	.	.	no
N1	C124	3.066(8)	.	.	no
N1	O1	3.029(6)	.	.	no
N1	C112B	3.161(8)	.	.	no
N1	C11	3.199(7)	.	.	no
N1	C117B	3.029(10)	.	.	no
N1	C16	3.295(8)	.	.	no
N1	C112A	3.174(10)	.	.	no
N1	C117A	3.023(12)	.	.	no
N1	C126	2.473(9)	.	.	no
N1	H1171"	2.2000	.	.	no
N1	H124'	2.8300	.	.	no
N1	H16"	2.9000	.	.	no
N1	H1172"	2.2200	.	.	no
N1	H124	2.8900	.	.	no
C111A	C117A	2.589(13)	.	.	no
C111A	C120A	2.587(12)	.	.	no
C111A	C113A	2.277(10)	.	.	no
C111A	F216	3.039(7)	.	2_645	no
C111A	O1	3.082(7)	.	.	no
C111A	C114A	2.278(9)	.	.	no
C111B	O1	3.116(6)	.	.	no
C111B	C117B	2.601(8)	.	.	no
C111B	C120B	2.601(7)	.	.	no
C111B	F216	3.072(6)	.	2_645	no
C111B	C113B	2.289(7)	.	.	no
C111B	C114B	2.289(7)	.	.	no
C112A	N1	3.174(10)	.	.	no
C112A	C125	3.072(11)	.	.	no
C112A	F216	3.230(10)	.	2_645	no
C112A	C118A	2.590(14)	.	.	no
C112A	C116A	2.588(13)	.	.	no

C112A	C114A	2.279(11)	.	.	no
C112A	C115A	2.280(11)	.	.	no
C112B	F217	3.342(7)	.	2_645	no
C112B	F216	3.345(7)	.	2_645	no
C112B	N1	3.161(8)	.	.	no
C112B	C114B	2.288(8)	.	.	no
C112B	C118B	2.599(10)	.	.	no
C112B	C115B	2.288(7)	.	.	no
C112B	C116B	2.600(8)	.	.	no
C112B	C125	2.930(8)	.	.	no
C113A	C119A	2.590(13)	.	.	no
C113A	F217	3.232(9)	.	2_645	no
C113A	C217	3.562(10)	.	2_645	no
C113A	C117A	2.588(14)	.	.	no
C113A	C115A	2.278(9)	.	.	no
C113A	C125	2.966(10)	.	.	no
C113A	C111A	2.277(10)	.	.	no
C113B	C119B	2.601(9)	.	.	no
C113B	F217	3.283(7)	.	2_645	no
C113B	C117B	2.601(10)	.	.	no
C113B	C111B	2.289(7)	.	.	no
C113B	C115B	2.289(8)	.	.	no
C113B	C217	3.452(8)	.	2_645	no
C113B	C125	3.249(8)	.	.	no
C114A	C112A	2.279(11)	.	.	no
C114A	C120A	2.589(10)	.	.	no
C114A	C111A	2.278(9)	.	.	no
C114A	C13	3.310(9)	.	.	no
C114A	C18	3.498(11)	.	.	no
C114A	C118A	2.589(11)	.	.	no
C114B	C111B	2.289(7)	.	.	no
C114B	C112B	2.288(8)	.	.	no
C114B	C13	3.482(8)	.	.	no
C114B	C118B	2.600(10)	.	.	no
C114B	C120B	2.600(9)	.	.	no
C114B	C216	3.537(8)	.	2_645	no
C115A	C112A	2.280(11)	.	.	no
C115A	C113A	2.278(9)	.	.	no
C115A	C116A	2.590(12)	.	.	no
C115A	C119A	2.589(13)	.	.	no
C115B	C121	3.571(8)	.	.	no
C115B	C112B	2.288(7)	.	.	no
C115B	O1	3.272(6)	.	.	no
C115B	C119B	2.599(8)	.	.	no
C115B	F216	3.193(6)	.	2_645	no
C115B	C113B	2.289(8)	.	.	no
C115B	C116B	2.601(8)	.	.	no
C11	C216	3.519(8)	.	2_545	no
C11	N1	3.199(7)	.	.	no
C11	C13	2.297(9)	.	.	no
C11	C110	2.567(10)	.	.	no
C11	F216	3.165(7)	.	2_545	no
C11	C14	2.282(9)	.	.	no
C11	C125	2.937(8)	.	.	no
C11	C17	2.599(10)	.	.	no
C116A	C223	3.488(11)	.	.	no
C116A	C124	3.565(12)	.	.	no
C116A	C121	3.148(13)	.	.	no
C116A	Zr1	3.549(11)	.	.	no
C116A	O1	2.941(11)	.	.	no
C12	C18	2.581(12)	.	.	no
C12	C14	2.275(9)	.	.	no
C12	C125	3.065(8)	.	.	no
C12	C16	2.608(10)	.	.	no
C12	C15	2.279(8)	.	.	no
C116B	C124	3.365(9)	.	.	no

C13	C119A	3.162(14)	.	.	no
C13	C114A	3.310(9)	.	.	no
C13	C15	2.293(8)	.	.	no
C13	C17	2.588(11)	.	.	no
C13	C119B	3.341(12)	.	.	no
C13	C114B	3.482(8)	.	.	no
C13	C11	2.297(9)	.	.	no
C13	C19	2.544(11)	.	.	no
C117A	C127	3.500(13)	.	.	no
C117A	N1	3.023(12)	.	.	no
C117A	Zr1	3.506(11)	.	.	no
C117A	C125	3.160(12)	.	.	no
C14	C110	2.596(10)	.	.	no
C14	C18	2.577(11)	.	.	no
C14	C11	2.282(9)	.	.	no
C14	C12	2.275(9)	.	.	no
C14	O1	3.344(7)	.	.	no
C117B	C126	3.209(12)	.	.	no
C117B	F214	3.363(7)	.	1_545	no
C15	O1	3.079(7)	.	.	no
C15	C13	2.293(8)	.	.	no
C15	C12	2.279(8)	.	.	no
C15	F216	3.087(6)	.	2_545	no
C15	C19	2.628(10)	.	.	no
C15	C16	2.558(10)	.	.	no
C118A	Zr1	3.480(11)	.	.	no
C118A	C125	2.924(13)	.	.	no
C118A	F217	3.296(13)	.	2_645	no
C118A	F215	3.107(11)	.	1_545	no
C118A	C126	3.020(14)	.	.	no
C16	C128	3.569(12)	.	.	no
C16	F211	3.294(9)	.	1_445	no
C118B	F217	3.364(10)	.	2_645	no
C17	C126	3.599(11)	.	.	no
C119A	C18	2.710(16)	.	.	no
C119A	C13	3.162(14)	.	.	no
C119A	Zr1	3.572(10)	.	.	no
C18	C119B	2.903(13)	.	.	no
C18	C114A	3.498(11)	.	.	no
C18	C119A	2.710(16)	.	.	no
C119B	F212	3.204(8)	.	2_645	no
C119B	C18	2.903(13)	.	.	no
C19	F215	3.349(9)	.	2_545	no
C19	C121	3.532(11)	.	.	no
C19	Zr1	3.675(8)	.	.	no
C120A	Zr1	3.573(9)	.	.	no
C120B	F22	3.274(6)	.	.	no
C120B	C121	3.117(11)	.	.	no
C120B	F218	3.076(7)	.	.	no
C21	F224	2.859(6)	.	.	no
C21	F28	2.975(6)	.	.	no
C21	F214	3.123(6)	.	.	no
C22	C224	3.376(7)	.	.	no
C22	F224	2.793(6)	.	.	no
C25	C123	3.596(8)	.	3_565	no
C26	F28	3.022(6)	.	.	no
C26	F214	3.203(6)	.	.	no
C26	C28	3.378(7)	.	.	no
C27	F26	2.840(6)	.	.	no
C27	F214	2.984(6)	.	.	no
C27	F220	3.060(6)	.	.	no
C28	F26	2.794(6)	.	.	no
C28	C26	3.378(7)	.	.	no
C110	F222	3.245(8)	.	1_455	no
C110	C124	3.585(9)	.	.	no
C110	C121	3.539(9)	.	.	no

C110	F221	3.297(8)	.	1_455	no
C110	F216	3.231(8)	.	2_545	no
C110	O1	3.126(7)	.	.	no
C116A	H1201	2.7800	.	.	no
C116A	H1171'	2.7900	.	.	no
C116A	H121	2.5100	.	.	no
C12	H1191	3.0600	.	.	no
C116B	H124'	2.8000	.	.	no
C116B	H1202	2.7600	.	.	no
C116B	H1172'	2.9700	.	.	no
C13	H1191	2.6600	.	.	no
C13	H1192'	2.5900	.	.	no
C117A	H1161'	3.1000	.	.	no
C117A	H1181"	2.9200	.	.	no
C14	H121'	3.0300	.	.	no
C117B	H1162'	2.8900	.	.	no
C117B	H126"	2.7900	.	.	no
C117B	H1182	3.0600	.	.	no
C118A	H1191	3.0800	.	.	no
C118A	H19	3.0100	.	2_545	no
C118A	H1171	2.9500	.	.	no
C118A	H126"	3.0900	.	.	no
C118A	H126'	2.6100	.	.	no
C16	H128	3.0600	.	.	no
C16	H110	2.9500	.	.	no
C16	H17"	2.8500	.	.	no
C118B	H1172	2.7900	.	.	no
C118B	H1192	2.7900	.	.	no
C118B	H17'	2.9200	.	.	no
C17	H126'	3.0700	.	.	no
C17	H18'	2.8900	.	.	no
C17	H1191	3.0600	.	.	no
C17	H16'	2.8300	.	.	no
C119A	H1181'	2.8000	.	.	no
C119A	H18	2.6900	.	.	no
C119A	H1201'	2.9100	.	.	no
C119A	H18'	2.1100	.	.	no
C18	H1192'	2.0700	.	.	no
C18	H1191	2.2100	.	.	no
C18	H1192	3.0000	.	.	no
C18	H17'	2.9800	.	.	no
C18	H1191'	2.4200	.	.	no
C18	H19	2.8900	.	.	no
C119B	H18'	2.6500	.	.	no
C119B	H18	2.4900	.	.	no
C119B	H1202'	3.0200	.	.	no
C119B	H1182'	2.7600	.	.	no
C19	H121'	2.6300	.	.	no
C19	H110'	2.8500	.	.	no
C19	H18	2.7700	.	.	no
C19	H1201"	2.7800	.	.	no
C120A	H1191'	2.7400	.	.	no
C120A	H1161	2.7400	.	.	no
C120A	H19"	2.8600	.	.	no
C120B	H121'	3.1000	.	.	no
C120B	H121	2.5000	.	.	no
C120B	H1192"	2.9600	.	.	no
C120B	H1162	2.8400	.	.	no
C121	C110	3.539(9)	.	.	no
C121	C116A	3.148(13)	.	.	no
C121	F22	3.298(7)	.	.	no
C121	C19	3.532(11)	.	.	no
C121	C120B	3.117(11)	.	.	no
C122	F224	3.365(6)	.	.	no
C122	F224	3.306(6)	.	3_565	no
C123	F224	3.185(6)	.	3_565	no

C23	H18'	2.9400	.	2_555	no
C123	C25	3.596(8)	.	3_565	no
C124	C127	3.286(9)	.	.	no
C124	C116B	3.365(9)	.	.	no
C124	C116A	3.565(12)	.	.	no
C124	C110	3.585(9)	.	.	no
C125	C16	3.114(9)	.	.	no
C125	C117B	2.803(11)	.	.	no
C125	C118B	3.505(11)	.	.	no
C125	C11	2.937(8)	.	.	no
C125	C12	3.065(8)	.	.	no
C125	C118A	2.924(13)	.	.	no
C125	C17	3.415(10)	.	.	no
C125	C127	2.418(8)	.	.	no
C25	H123	3.0400	.	3_565	no
C125	C113B	3.249(8)	.	.	no
C125	C113A	2.966(10)	.	.	no
C125	C117A	3.160(12)	.	.	no
C125	C112B	2.930(8)	.	.	no
C125	C112A	3.072(11)	.	.	no
C126	C117B	3.209(12)	.	.	no
C26	H123	3.0500	.	3_565	no
C126	C17	3.599(11)	.	.	no
C126	C118A	3.020(14)	.	.	no
C127	C124	3.286(9)	.	.	no
C127	C117A	3.500(13)	.	.	no
C128	C16	3.569(12)	.	.	no
C128	F25	3.314(10)	.	1_545	no
C110	H19'	2.7800	.	.	no
C110	H16"	2.9400	.	.	no
C110	H122'	3.0800	.	.	no
C211	F24	3.253(7)	.	1_655	no
C212	F220	3.080(7)	.	.	no
C212	F24	3.351(6)	.	1_655	no
C212	C214	3.346(8)	.	.	no
C212	F214	3.022(7)	.	.	no
C213	F212	2.845(6)	.	.	no
C213	F220	2.957(5)	.	.	no
C213	F22	3.068(6)	.	.	no
C214	C212	3.346(8)	.	.	no
C214	F212	2.748(6)	.	.	no
C216	C11	3.519(8)	.	2_555	no
C216	C114B	3.537(8)	.	2_655	no
C217	C113B	3.452(8)	.	2_655	no
C217	C113A	3.562(10)	.	2_655	no
C218	F220	3.028(6)	.	.	no
C218	F22	3.092(6)	.	.	no
C218	C220	3.345(7)	.	.	no
C219	F218	2.808(6)	.	.	no
C219	F28	3.094(6)	.	.	no
C219	F22	2.986(6)	.	.	no
C220	F218	2.802(6)	.	.	no
C220	C218	3.345(7)	.	.	no
C121	H1161'	2.7800	.	.	no
C121	H1202"	2.5600	.	.	no
C121	H1161	2.7900	.	.	no
C121	H1162	2.9100	.	.	no
C221	F223	3.267(6)	.	3_665	no
C121	H110'	2.8700	.	.	no
C121	H1202	2.9700	.	.	no
C122	H110'	2.9400	.	.	no
C222	C222	3.438(8)	.	3_665	no
C222	F223	3.329(6)	.	3_665	no
C222	C223	3.300(8)	.	3_665	no
C223	F222	3.213(6)	.	3_665	no
C223	C116A	3.488(11)	.	.	no

C223	C222	3.300(8)	.	3_665	no
C124	H110	3.0600	.	.	no
C124	H1162'	3.0200	.	.	no
C224	C22	3.376(7)	.	.	no
C124	H1161'	2.6900	.	.	no
C124	H1162	2.9400	.	.	no
C124	H128"	3.0900	.	.	no
C224	F28	3.175(6)	.	.	no
C224	F222	3.304(6)	.	3_665	no
C124	H127'	2.8400	.	.	no
C224	F22	3.042(6)	.	.	no
C125	H1181	2.2100	.	.	no
C125	H1171"	2.5100	.	.	no
C125	H17"	3.0200	.	.	no
C125	H1172	3.0600	.	.	no
C125	H1182	2.8500	.	.	no
C125	H1172"	2.1500	.	.	no
C125	H16"	3.0800	.	.	no
C125	H16'	2.8200	.	.	no
C126	H1172"	2.5800	.	.	no
C126	H1172	3.0700	.	.	no
C126	H127	2.6300	.	.	no
C126	H1182	2.8900	.	.	no
C126	H17"	2.8900	.	.	no
C126	H16'	2.9300	.	.	no
C126	H1181	2.1300	.	.	no
C127	H124	2.9400	.	.	no
C127	H1171"	2.5300	.	.	no
C127	H126"	2.9700	.	.	no
C127	H1172"	2.6600	.	.	no
C127	H124'	2.8400	.	.	no
C127	H126	3.0100	.	.	no
C127	H128'	2.8100	.	3_555	no
C128	H124	2.9400	.	.	no
C128	H16"	2.7000	.	.	no
C214	H18"	2.8800	.	2_555	no
C215	H18"	3.0600	.	2_555	no
C217	H17	2.9700	.	2_555	no
C217	H1182"	3.0400	.	2_655	no
C218	H17	3.0500	.	2_555	no
C223	H1161	3.0500	.	.	no
H110'	F221	2.5200	.	1_455	no
H110'	O1	2.8500	.	.	no
H110'	H122'	2.2800	.	.	no
H110'	H19'	2.2100	.	.	no
H110'	C121	2.8700	.	.	no
H110'	C122	2.9400	.	.	no
H110'	C19	2.8500	.	.	no
H110'	H121'	2.5200	.	.	no
H110"	F216	2.5400	.	2_545	no
H121'	F23	2.8200	.	.	no
H121'	C19	2.6300	.	.	no
H121'	C120B	3.1000	.	.	no
H121'	H110'	2.5200	.	.	no
H121'	H19'	2.2800	.	.	no
H121'	H19"	2.3800	.	.	no
H121'	H1202"	2.3000	.	.	no
H121'	C14	3.0300	.	.	no
H122'	C110	3.0800	.	.	no
H122'	H110'	2.2800	.	.	no
H122'	F221	2.7200	.	1_455	no
H123'	F223	2.5000	.	.	no
H124'	H1162	2.5700	.	.	no
H124'	H1162'	2.2400	.	.	no
H124'	H127'	2.1800	.	.	no
H124'	N1	2.8300	.	.	no

H124'	C116B	2.8000	.	.	no
H124'	H1161'	2.3200	.	.	no
H124'	C127	2.8400	.	.	no
H126'	C118A	2.6100	.	.	no
H126'	C17	3.0700	.	.	no
H126'	H1182	2.3000	.	.	no
H126'	H18	2.5600	.	2_545	no
H126'	H1181	1.6600	.	.	no
H126'	H17"	2.3700	.	.	no
H126"	H1172	2.5800	.	.	no
H126"	F26	2.7700	.	1_545	no
H126"	C127	2.9700	.	.	no
H126"	C118A	3.0900	.	.	no
H126"	H1172"	2.1600	.	.	no
H126"	H127	2.3400	.	.	no
H126"	H1181	2.3900	.	.	no
H126"	F214	2.7800	.	1_545	no
H126"	C117B	2.7900	.	.	no
H127'	H128'	2.5900	.	3_555	no
H127'	H1171"	2.4500	.	.	no
H127'	H124'	2.1800	.	.	no
H127'	C124	2.8400	.	.	no
H128'	C127	2.8100	.	3_555	no
H128'	H127	2.3200	.	3_555	no
H128'	F26	2.8100	.	3_565	no
H128'	H127'	2.5900	.	3_555	no
H128"	H124	2.2200	.	.	no
H128"	H16"	2.4000	.	.	no
H128"	C124	3.0900	.	.	no
H1161	H1201	2.1300	.	.	no
H1161	C121	2.7900	.	.	no
H1161	C120A	2.7400	.	.	no
H1161	H121	1.9600	.	.	no
H1161	C223	3.0500	.	.	no
H1161'	C124	2.6900	.	.	no
H1161'	C121	2.7800	.	.	no
H1161'	H121	2.3100	.	.	no
H1161'	C117A	3.1000	.	.	no
H1161'	H124'	2.3200	.	.	no
H1161'	O1	2.3700	.	.	no
H1161'	Zr1	3.4300	.	.	no
H1161"	H1171'	2.5900	.	.	no
H1162	O1	2.6400	.	.	no
H1162	C120B	2.8400	.	.	no
H1162	H121	2.3400	.	.	no
H1162	H124'	2.5700	.	.	no
H1162	H1202	2.2400	.	.	no
H1162	C121	2.9100	.	.	no
H1162	C124	2.9400	.	.	no
H16	F216	2.7400	.	2_545	no
H16	F217	2.7100	.	2_545	no
H16'	H126	2.4400	.	.	no
H16'	C125	2.8200	.	.	no
H16'	H17"	2.2200	.	.	no
H16'	C17	2.8300	.	.	no
H16'	C126	2.9300	.	.	no
H16'	F211	2.8400	.	1_445	no
H16"	C110	2.9400	.	.	no
H16"	N1	2.9000	.	.	no
H16"	C125	3.0800	.	.	no
H16"	C128	2.7000	.	.	no
H16"	F29	2.8600	.	3_565	no
H16"	H110	2.4600	.	.	no
H16"	H128	2.2900	.	.	no
H16"	H128"	2.4000	.	.	no
H1162'	C117B	2.8900	.	.	no

H1162'	H124'	2.2400	.	.	no
H1162'	C124	3.0200	.	.	no
H17	C218	3.0500	.	2_545	no
H17	C217	2.9700	.	2_545	no
H17	F22	2.8600	.	2_545	no
H17'	H1191	2.3200	.	.	no
H17'	C118B	2.9200	.	.	no
H17'	C18	2.9800	.	.	no
H17'	H18'	2.4400	.	.	no
H17'	H1182	2.4700	.	.	no
H17'	H1182'	2.5600	.	.	no
H17"	C126	2.8900	.	.	no
H17"	C16	2.8500	.	.	no
H17"	H126'	2.3700	.	.	no
H17"	H16'	2.2200	.	.	no
H17"	C125	3.0200	.	.	no
H18	C119A	2.6900	.	.	no
H18	H1191	2.5400	.	.	no
H18	H1192'	1.5500	.	.	no
H18	H126'	2.5600	.	2_555	no
H18	C19	2.7700	.	.	no
H18	H1191'	2.0800	.	.	no
H18	C119B	2.4900	.	.	no
H18	H19	2.5700	.	.	no
H18'	C17	2.8900	.	.	no
H18'	H1192	2.4500	.	.	no
H18'	C119A	2.1100	.	.	no
H18'	H1191	1.4400	.	.	no
H18'	H1192'	2.0900	.	.	no
H18'	C119B	2.6500	.	.	no
H18'	H17'	2.4400	.	.	no
H18'	C23	2.9400	.	2_545	no
H18'	H1191'	2.0600	.	.	no
H18"	C214	2.8800	.	2_545	no
H18"	C215	3.0600	.	2_545	no
H1171	H1181"	2.4200	.	.	no
H1171	C118A	2.9500	.	.	no
H19	F215	2.6400	.	2_545	no
H19	H1182	2.5200	.	2_555	no
H19	H18	2.5700	.	.	no
H19	C18	2.8900	.	.	no
H19	C118A	3.0100	.	2_555	no
H19'	H121'	2.2800	.	.	no
H19'	C110	2.7800	.	.	no
H19'	H110'	2.2100	.	.	no
H19"	Zr1	3.6400	.	.	no
H19"	H121'	2.3800	.	.	no
H19"	C120A	2.8600	.	.	no
H19"	H1201"	1.8800	.	.	no
H19"	H1202"	2.4700	.	.	no
H1171'	C116A	2.7900	.	.	no
H1171'	H1161"	2.5900	.	.	no
H1171"	N1	2.2000	.	.	no
H1171"	Zr1	3.2600	.	.	no
H1171"	C127	2.5300	.	.	no
H1171"	H127'	2.4500	.	.	no
H1171"	C125	2.5100	.	.	no
H1171"	H127	2.4800	.	.	no
H1172	H126"	2.5800	.	.	no
H1172	C118B	2.7900	.	.	no
H1172	F214	2.5900	.	1_545	no
H1172	C125	3.0600	.	.	no
H1172	C126	3.0700	.	.	no
H1172'	C116B	2.9700	.	.	no
H1172"	H127	2.4200	.	.	no
H1172"	C125	2.1500	.	.	no

H1172"	N1	2.2200	.	.	no
H1172"	C127	2.6600	.	.	no
H1172"	H126"	2.1600	.	.	no
H1172"	C126	2.5800	.	.	no
H1181	C126	2.1300	.	.	no
H1181	C125	2.2100	.	.	no
H1181	Zr1	3.2300	.	.	no
H1181	H126"	2.3900	.	.	no
H1181	H126'	1.6600	.	.	no
H1181'	C119A	2.8000	.	.	no
H1181"	C117A	2.9200	.	.	no
H1181"	H1171	2.4200	.	.	no
H1181"	F214	2.8100	.	1_545	no
H1181"	F215	2.5700	.	1_545	no
H1181"	F217	2.8200	.	2_645	no
H1182	C117B	3.0600	.	.	no
H1182	H126'	2.3000	.	.	no
H1182	H17'	2.4700	.	.	no
H1182	C125	2.8500	.	.	no
H1182	C126	2.8900	.	.	no
H1182	H19	2.5200	.	2_545	no
H1182'	H1192	2.1600	.	.	no
H1182'	H17'	2.5600	.	.	no
H1182'	C119B	2.7600	.	.	no
H1182"	F215	2.8500	.	1_545	no
H1182"	F217	2.6300	.	2_645	no
H1182"	C217	3.0400	.	2_645	no
H1191	H18	2.5400	.	.	no
H1191	H18'	1.4400	.	.	no
H1191	C17	3.0600	.	.	no
H1191	C18	2.2100	.	.	no
H1191	H17'	2.3200	.	.	no
H1191	Zr1	3.4900	.	.	no
H1191	C118A	3.0800	.	.	no
H1191	C13	2.6600	.	.	no
H1191	C12	3.0600	.	.	no
H1191'	H1201'	2.3200	.	.	no
H1191'	C18	2.4200	.	.	no
H1191'	C120A	2.7400	.	.	no
H1191'	H18	2.0800	.	.	no
H1191'	H18'	2.0600	.	.	no
H1191"	F220	2.5300	.	2_645	no
H1192	F212	2.7700	.	2_645	no
H1192	H18'	2.4500	.	.	no
H1192	H1182'	2.1600	.	.	no
H1192	C118B	2.7900	.	.	no
H1192	C18	3.0000	.	.	no
H1192'	H18'	2.0900	.	.	no
H1192'	C13	2.5900	.	.	no
H1192'	H18	1.5500	.	.	no
H1192'	C18	2.0700	.	.	no
H1192"	C120B	2.9600	.	.	no
H1192"	H1202'	2.5100	.	.	no
H1192"	F212	2.7400	.	2_645	no
H1201	C116A	2.7800	.	.	no
H1201	H1161	2.1300	.	.	no
H1201	F218	2.6600	.	.	no
H1201'	C119A	2.9100	.	.	no
H1201'	H1191'	2.3200	.	.	no
H1201"	C19	2.7800	.	.	no
H1201"	Zr1	3.4000	.	.	no
H1201"	H19"	1.8800	.	.	no
H1202	C121	2.9700	.	.	no
H1202	H1162	2.2400	.	.	no
H1202	C116B	2.7600	.	.	no
H1202	H121	2.1400	.	.	no

H1202'	F218	2.5100	.	.	no
H1202'	C119B	3.0200	.	.	no
H1202'	H1192"	2.5100	.	.	no
H1202"	F22	2.7700	.	.	no
H1202"	C121	2.5600	.	.	no
H1202"	H121'	2.3000	.	.	no
H1202"	H121	2.1500	.	.	no
H1202"	H19"	2.4700	.	.	no
H110	C16	2.9500	.	.	no
H110	C124	3.0600	.	.	no
H110	Zr1	3.6700	.	.	no
H110	H124	2.3900	.	.	no
H110	F29	2.8400	.	3_565	no
H110	H16"	2.4600	.	.	no
H121	H1161'	2.3100	.	.	no
H121	F22	2.7900	.	.	no
H121	C120B	2.5000	.	.	no
H121	H1162	2.3400	.	.	no
H121	H1202	2.1400	.	.	no
H121	H1202"	2.1500	.	.	no
H121	C116A	2.5100	.	.	no
H121	H1161	1.9600	.	.	no
H122	F224	2.5700	.	.	no
H123	C25	3.0400	.	3_565	no
H123	C26	3.0500	.	3_565	no
H123	F224	2.4000	.	3_565	no
H124	N1	2.8900	.	.	no
H124	C128	2.9400	.	.	no
H124	H128"	2.2200	.	.	no
H124	C127	2.9400	.	.	no
H124	H110	2.3900	.	.	no
H126	F25	2.8400	.	1_545	no
H126	C127	3.0100	.	.	no
H126	H16'	2.4400	.	.	no
H127	F25	2.7500	.	1_545	no
H127	F26	2.8400	.	1_545	no
H127	C126	2.6300	.	.	no
H127	H1172"	2.4200	.	.	no
H127	H1171"	2.4800	.	.	no
H127	H128'	2.3200	.	3_555	no
H127	H126"	2.3400	.	.	no
H128	F25	2.8300	.	1_545	no
H128	C16	3.0600	.	.	no
H128	H16"	2.2900	.	.	no
H128	F211	2.5700	.	1_445	no

loop_

_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
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#	#D	H	A	D - H	H...A	D...A	D - H...A	symm(A)		
#										
	C110		H110'		F221	0.9800	2.5200	3.297(8)	136.00	1_455 yes
	C110		H110"		F216	0.9800	2.5400	3.231(8)	127.00	2_545 yes
	C123		H123'		F223	0.9900	2.5000	3.450(6)	160.00	. yes
	C117B		H1172"		N1	0.9800	2.2200	3.029(10)	139.00	. yes
	C120B		H1202'		F218	0.9800	2.5100	3.076(7)	116.00	. yes
	C123		H123		F224	0.9900	2.4000	3.185(6)	136.00	3_565 yes

```

#===END of Crystallographic Information File

# CIF-file generated for C25H43NZr                      P21/c                      q1547
#=====
data_global
#=====

# 0. AUDIT DETAILS

_audit_creation_date                '2009-03-11  09:11:10'
_audit_creation_method
;
  PLATON <TABLE ACC> option      (version :: 170209)
  SHELXL97-2 & Manual Editing
;
_audit_update_record
;
?

2010-06-04 # Formatted by publCIF
;

#=====

# 1. SUBMISSION DETAILS

_publ_contact_author_name          # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email          A.Meetsma@rug.nl
_publ_contact_author_fax            '+31 50 3634441'
_publ_contact_author_phone          '+31 50 3634368'

_publ_requested_journal              'J. Am. Chem. Soc'
# Publication choose FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                 # Include date of submission
;
  Date of submission :  2010-06-04  14:11:10

  Consider this CIF submission for deposition of the second
  X-ray structure of a manuscript to be submitted to : J. Am. Chem. Soc
  (Our Compound_Identification_Code : q1547)
;

#=====

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?
_journal_date_to_coeditor             ?
_journal_date_from_coeditor           ?

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_journal_date_accepted          ?
_journal_date_printers_first    ?
_journal_date_printers_final    ?
_journal_date_proofs_out        ?
_journal_date_proofs_in         ?

_journal_coeditor_name          ?
_journal_coeditor_code          ?
_journal_coeditor_notes
;
;

_journal_techeditor_code        ?
_journal_techeditor_notes
;
;

_journal_coden_ASTM             ?
_journal_name_full              ?
_journal_year                   ?
_journal_volume                 ?
_journal_issue                  ?
_journal_page_first             ?
_journal_page_last              ?

_journal_suppl_publ_number      ?
_journal_suppl_publ_pages       ?

```

```
#=====
```

3. TITLE AND AUTHOR LIST

```

_publ_section_title
;
Title (type here to add)?
;
_publ_section_title_footnote
.

```

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_footnote
_publ_author_address
'?' # author name
; # author related footnote
;
; # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote
;
;
Crystal Structure Center, Chemical Physics,
Zernike Institute for Advanced Materials,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen, The Netherlands.
;

```

```

#=====

# 4. TEXT

_publ_section_synopsis
.
_publ_section_abstract
;
?(type here to add abstract)
;

# Insert blank lines between paragraphs

_publ_section_comment
;
?(type here to add)
;
_publ_section_exptl_prep
;
?
;
_publ_section_exptl_refinement
;
?The hydrogen atoms were generated by geometrical considerations, constrained to
idealized geometries, and allowed to ride on the carrier atom with an
isotropic displacement parameter related to the equivalent displacement
parameter of their carrier atoms, with  $U_{iso}(H) = 1.2 U_{eq}(C)$ 
or  $1.5 U_{eq}(\text{methyl C})$ . The methyl-groups were refined as rigid groups,
which were allowed to rotate freely. Assigned values of bond distances:
secondary C---H2 = 0.99 Å, methyl C---H3 = 0.98 Å and aromatic C---H =
0.95 Å.
;

_publ_section_related_literature
;
;

# Insert blank lines between references

_publ_section_references
;
Beurskens, P. T., Beurskens, G., de Gelder, R., Smits, J. M. M.,
Garc'ia-Granda, S. & Gould, R. O. (2008). The DIRDIF08 program system,
Technical Report of the Crystallography Laboratory, University of Nijmegen,
The Netherlands.

Bruker, (2007). SMART (Version 5.632), SAINT-Plus (Version
7.46a) and SADABS (Version 2.10). Bruker AXS Inc., Madison, Wisconsin,
USA.

Meetsma, A. (2008). Extended version of the program PLUTO. University of
Groningen, The Netherlands. (unpublished).

Sheldrick, G. M. (2008). Acta Cryst. 64, 112--122.

van der Sluis, P. & Spek, A. L. (1990). Acta Cryst. 46,
194--201.

Spek, A. L. (1988). J. Appl. Cryst. 21, 578--579.

Spek, A. L. (2003). J. Appl. Cryst. 36, 7--13.
;

```

```
_publ_section_figure_captions
;
?
```

Fig. 1. Perspective *PLUTO* drawings of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective *ORTEP* drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

```
;
```

```
_publ_section_acknowledgements
;
??
;
```

```
#=====
```

5. CHEMICAL DATA

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_chemical_name_systematic
;
;
_chemical_name_common          ?
_chemical_melting_point        ?
_chemical_formula_moiety
'C25 H43 N Zr'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural    ?
_chemical_formula_sum
'C25 H43 N Zr'
_chemical_formula_iupac         ?
_chemical_formula_weight        448.85
_chemical_compound_source       'see text'
```

```
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
Zr  Zr  -2.9673  0.5597
'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'
H   H   0.0000  0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C   C   0.0033  0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
```

```
#=====
```

6. CRYSTAL DATA

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_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_Hall '-P 2ybc'
_symmetry_space_group_name_H-M  'P 21/c'
_symmetry_Int_Tables_number     14
```

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
```

```

2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z

```

```

_cell_length_a          10.0380(16)
_cell_length_b          14.222(2)
_cell_length_c          16.969(3)
_cell_angle_alpha       90
_cell_angle_beta        106.879(2)
_cell_angle_gamma       90
_cell_volume            2318.1(6)
_cell_formula_units_Z   4

```

```

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 6518
_cell_measurement_theta_min 2.51
_cell_measurement_theta_max 29.50
_cell_special_details

```

```
;
```

The final unit cell was obtained from the xyz centroids of 6518 reflections after integration using the SAINTPLUS software package (Bruker, 2007).

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 'needle'
_exptl_crystal_colour      'yellow'
_exptl_crystal_size_max    0.48
_exptl_crystal_size_mid    0.44
_exptl_crystal_size_min    0.38
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.286
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       960
_exptl_absorpt_coefficient_mu 0.484
_exptl_absorpt_correction_type 'multi-scan'
_exptl_absorpt_process_details '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min 0.7828
_exptl_absorpt_correction_T_max 0.8321

```

```
#=====
```

7. EXPERIMENTAL DATA

```

_exptl_special_details
;
;
_diffn_ambient_temperature 100(1)
_diffn_radiation_wavelength 0.71073
_diffn_radiation_type      'MoK\alpha'
_diffn_radiation_source     'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator 'parallel mounted graphite'
_diffn_radiation_detector
;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method '\f and \w scans'
_diffn_special_details

```



```

;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2007)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              0
_diffrn_standards_interval_count      .
_diffrn_standards_interval_time       .
_diffrn_standards_decay_%             0

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                 18072
_diffrn_reflns_av_R_equivalents       0.0471
_diffrn_reflns_av_sigmaI/netI         0.0432
_diffrn_reflns_limit_h_min            -12
_diffrn_reflns_limit_h_max            12
_diffrn_reflns_limit_k_min            -17
_diffrn_reflns_limit_k_max            17
_diffrn_reflns_limit_l_min            -21
_diffrn_reflns_limit_l_max            21
_diffrn_reflns_theta_min               2.56
_diffrn_reflns_theta_max               26.37
_diffrn_measured_fraction_theta_max   0.993
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full  0.997

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
_reflns_number_total                  4705
_reflns_number_gt                     3963
_reflns_threshold_expression           I>2\sigma(I)

_computing_data_collection             'SMART (Bruker, 2007)'
_computing_cell_refinement             'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction              'SAINT-Plus'
_computing_structure_solution
;
DIRDIF-08 (Beurskens et al., 2008)
;
_computing_structure_refinement         'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
;
PLATON (Spek, 2003)
PLUTO (Meetsma, 2008)
;
_computing_publication_material        'PLATON (Spek, 2003)'

#=====

# 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
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0513P)^2^+0.4038P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration '.'

_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 4705
_refine_ls_number_parameters 257
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0456
_refine_ls_R_factor_gt 0.0364
_refine_ls_wR_factor_ref 0.0948
_refine_ls_wR_factor_gt 0.0901
_refine_ls_goodness_of_fit_ref 1.074
_refine_ls_restrained_S_all 1.074
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000

_refine_diff_density_max 1.086
_refine_diff_density_min -0.553
_refine_diff_density_rms 0.086

_vrn_publ_code_number_frames 1800
_vrn_publ_code_frame_time_sec 10.0
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#=====

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Zr Zr Uani 0.25748(2) 0.23759(1) 0.14095(1) 1.000 0.0147(1) . .
N N Uani 0.0488(2) 0.24035(13) 0.14175(13) 1.000 0.0196(6) . .
Cl C Uani 0.2830(3) 0.41441(15) 0.10206(15) 1.000 0.0181(7) . .

```

C2	C	Uani	0.2494(3)	0.41473(15)	0.17738(15)	1.000	0.0196(7)	. .
C3	C	Uani	0.3620(3)	0.37227(16)	0.23820(15)	1.000	0.0213(7)	. .
C4	C	Uani	0.4692(2)	0.35205(15)	0.20061(15)	1.000	0.0208(7)	. .
C5	C	Uani	0.4181(2)	0.37406(15)	0.11635(15)	1.000	0.0193(7)	. .
C6	C	Uani	0.2051(3)	0.46557(17)	0.02455(16)	1.000	0.0259(8)	. .
C7	C	Uani	0.1292(3)	0.46521(17)	0.19452(17)	1.000	0.0282(8)	. .
C8	C	Uani	0.3732(3)	0.36624(18)	0.32873(15)	1.000	0.0307(8)	. .
C9	C	Uani	0.6193(3)	0.33508(18)	0.24642(18)	1.000	0.0301(8)	. .
C10	C	Uani	0.4994(3)	0.37043(18)	0.05446(17)	1.000	0.0291(8)	. .
C11	C	Uani	0.2923(2)	0.09006(15)	0.23599(14)	1.000	0.0182(7)	. .
C12	C	Uani	0.4278(2)	0.12098(15)	0.23810(15)	1.000	0.0195(7)	. .
C13	C	Uani	0.4445(2)	0.10845(15)	0.15834(15)	1.000	0.0186(7)	. .
C14	C	Uani	0.3196(3)	0.06860(15)	0.10745(14)	1.000	0.0190(7)	. .
C15	C	Uani	0.2257(3)	0.05703(15)	0.15498(15)	1.000	0.0188(7)	. .
C16	C	Uani	0.2478(3)	0.07596(17)	0.31267(15)	1.000	0.0257(8)	. .
C17	C	Uani	0.5425(3)	0.13450(17)	0.31744(15)	1.000	0.0257(8)	. .
C18	C	Uani	0.5746(3)	0.12245(18)	0.13261(17)	1.000	0.0271(8)	. .
C19	C	Uani	0.3035(3)	0.02622(17)	0.02415(15)	1.000	0.0252(8)	. .
C20	C	Uani	0.0874(3)	0.00728(17)	0.12400(16)	1.000	0.0244(8)	. .
C21	C	Uani	-0.0233(3)	0.19609(18)	0.19582(16)	1.000	0.0251(8)	. .
C22	C	Uani	-0.0277(3)	0.25680(19)	0.26988(19)	1.000	0.0309(9)	. .
C23	C	Uani	-0.0488(3)	0.30088(18)	0.08097(16)	1.000	0.0250(8)	. .
C24	C	Uani	-0.1474(3)	0.24585(18)	0.01013(19)	1.000	0.0315(9)	. .
C25	C	Uani	0.2032(3)	0.23083(17)	0.00000(16)	1.000	0.0251(8)	. .
H6	H	Uiso	0.10574	0.46740	0.02051	1.000	0.0388	. .
H6'	H	Uiso	0.21815	0.43266	-0.02340	1.000	0.0388	. .
H6''	H	Uiso	0.24077	0.52990	0.02617	1.000	0.0388	. .
H7	H	Uiso	0.16307	0.52225	0.22647	1.000	0.0423	. .
H7'	H	Uiso	0.08520	0.42396	0.22594	1.000	0.0423	. .
H7''	H	Uiso	0.06098	0.48233	0.14233	1.000	0.0423	. .
H8	H	Uiso	0.29537	0.40029	0.33946	1.000	0.0461	. .
H8'	H	Uiso	0.46129	0.39436	0.36098	1.000	0.0461	. .
H8''	H	Uiso	0.37015	0.30016	0.34450	1.000	0.0461	. .
H9	H	Uiso	0.66010	0.29194	0.21477	1.000	0.0451	. .
H9'	H	Uiso	0.62584	0.30732	0.30028	1.000	0.0451	. .
H9''	H	Uiso	0.66993	0.39488	0.25413	1.000	0.0451	. .
H10	H	Uiso	0.52812	0.43414	0.04458	1.000	0.0436	. .
H10'	H	Uiso	0.44090	0.34380	0.00269	1.000	0.0436	. .
H10''	H	Uiso	0.58207	0.33097	0.07586	1.000	0.0436	. .
H16	H	Uiso	0.32003	0.04093	0.35341	1.000	0.0385	. .
H16'	H	Uiso	0.16040	0.04048	0.29899	1.000	0.0385	. .
H16''	H	Uiso	0.23417	0.13728	0.33550	1.000	0.0385	. .
H17	H	Uiso	0.51561	0.18370	0.35028	1.000	0.0385	. .
H17'	H	Uiso	0.62828	0.15312	0.30505	1.000	0.0385	. .
H17''	H	Uiso	0.55823	0.07545	0.34856	1.000	0.0385	. .
H18	H	Uiso	0.60249	0.06246	0.11374	1.000	0.0406	. .
H18'	H	Uiso	0.64951	0.14554	0.17959	1.000	0.0406	. .
H18''	H	Uiso	0.55660	0.16845	0.08774	1.000	0.0406	. .
H19	H	Uiso	0.33369	-0.03959	0.03058	1.000	0.0378	. .
H19'	H	Uiso	0.36074	0.06123	-0.00377	1.000	0.0378	. .
H19''	H	Uiso	0.20562	0.02937	-0.00871	1.000	0.0378	. .
H20	H	Uiso	0.02090	0.04818	0.08528	1.000	0.0366	. .
H20'	H	Uiso	0.05186	-0.00763	0.17059	1.000	0.0366	. .
H20''	H	Uiso	0.09952	-0.05097	0.09603	1.000	0.0366	. .
H21	H	Uiso	0.02358	0.13592	0.21638	1.000	0.0300	. .
H21'	H	Uiso	-0.11994	0.18139	0.16311	1.000	0.0300	. .
H22	H	Uiso	0.06750	0.27034	0.30360	1.000	0.0463	. .
H22'	H	Uiso	-0.07730	0.22286	0.30306	1.000	0.0463	. .
H22''	H	Uiso	-0.07615	0.31592	0.25024	1.000	0.0463	. .
H23	H	Uiso	0.00527	0.34586	0.05794	1.000	0.0300	. .
H23'	H	Uiso	-0.10482	0.33771	0.10939	1.000	0.0300	. .
H24	H	Uiso	-0.09296	0.21058	-0.01939	1.000	0.0472	. .
H24'	H	Uiso	-0.20960	0.28973	-0.02783	1.000	0.0472	. .
H24''	H	Uiso	-0.20282	0.20201	0.03228	1.000	0.0472	. .
H25	H	Uiso	0.14173	0.17707	-0.02028	1.000	0.0376	. .
H25'	H	Uiso	0.28879	0.22357	-0.01613	1.000	0.0376	. .

H25" H Uiso 0.15590 0.28896 -0.02375 1.000 0.0376 . .

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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
Zr 0.0151(1) 0.0135(1) 0.0154(1) -0.0003(1) 0.0046(1) -0.0002(1)
N 0.0181(10) 0.0179(10) 0.0226(11) 0.0003(8) 0.0057(9) 0.0012(8)
C1 0.0200(12) 0.0095(10) 0.0246(13) -0.0005(9) 0.0064(10) -0.0012(9)
C2 0.0244(13) 0.0109(10) 0.0245(13) -0.0026(9) 0.0087(11) -0.0020(9)
C3 0.0287(14) 0.0139(11) 0.0208(12) -0.0039(9) 0.0063(11) -0.0058(10)
C4 0.0197(12) 0.0128(11) 0.0276(13) -0.0027(9) 0.0035(10) -0.0046(9)
C5 0.0207(12) 0.0132(11) 0.0250(13) 0.0018(9) 0.0081(10) -0.0029(9)
C6 0.0284(14) 0.0202(12) 0.0281(14) 0.0069(10) 0.0067(12) 0.0013(10)
C7 0.0306(14) 0.0200(12) 0.0373(15) -0.0078(11) 0.0149(12) 0.0024(10)
C8 0.0467(17) 0.0229(13) 0.0211(13) -0.0033(10) 0.0075(12) -0.0008(12)
C9 0.0237(14) 0.0193(12) 0.0425(16) 0.0039(11) 0.0022(12) -0.0038(10)
C10 0.0308(15) 0.0257(13) 0.0358(15) 0.0039(11) 0.0176(13) -0.0024(11)
C11 0.0227(12) 0.0110(10) 0.0204(12) 0.0023(9) 0.0056(10) 0.0010(9)
C12 0.0209(12) 0.0133(11) 0.0229(13) 0.0016(9) 0.0040(10) 0.0015(9)
C13 0.0196(12) 0.0119(10) 0.0256(13) 0.0009(9) 0.0084(10) 0.0030(9)
C14 0.0237(13) 0.0120(10) 0.0200(12) -0.0004(9) 0.0045(10) 0.0033(9)
C15 0.0231(12) 0.0127(11) 0.0214(12) 0.0004(9) 0.0076(10) -0.0008(9)
C16 0.0303(14) 0.0238(13) 0.0233(13) 0.0024(10) 0.0084(11) 0.0004(11)
C17 0.0267(14) 0.0203(12) 0.0250(13) 0.0010(10) -0.0004(11) 0.0003(10)
C18 0.0229(13) 0.0236(13) 0.0365(15) -0.0042(11) 0.0113(12) 0.0008(10)
C19 0.0321(14) 0.0201(12) 0.0244(13) -0.0067(10) 0.0099(11) 0.0013(10)
C20 0.0258(14) 0.0193(12) 0.0287(14) -0.0027(10) 0.0089(11) -0.0041(10)
C21 0.0187(13) 0.0274(13) 0.0302(14) 0.0022(11) 0.0088(11) -0.0011(10)
C22 0.0263(15) 0.0386(16) 0.0323(16) -0.0008(12) 0.0158(13) -0.0002(11)
C23 0.0191(13) 0.0226(12) 0.0315(14) 0.0008(10) 0.0044(11) 0.0012(10)
C24 0.0236(14) 0.0308(14) 0.0339(17) -0.0004(11) -0.0012(13) 0.0016(11)
C25 0.0321(15) 0.0213(12) 0.0204(13) -0.0007(10) 0.0055(12) -0.0006(10)
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10. MOLECULAR GEOMETRY

_geom_special_details

;
Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's 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
;

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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
Zr      N      2.099(2)      .      .      yes
Zr      C1     2.631(2)      .      .      yes
Zr      C2     2.601(2)      .      .      yes
Zr      C3     2.547(2)      .      .      yes
Zr      C4     2.635(2)      .      .      yes
Zr      C5     2.633(2)      .      .      yes
Zr      C11    2.607(2)      .      .      yes
Zr      C12    2.599(2)      .      .      yes
```

Zr	C13	2.581(2)	.	.	yes
Zr	C14	2.587(2)	.	.	yes
Zr	C15	2.607(2)	.	.	yes
Zr	C25	2.296(3)	.	.	yes
N	C21	1.465(4)	.	.	yes
N	C23	1.476(3)	.	.	yes
C1	C2	1.413(4)	.	.	no
C1	C5	1.427(4)	.	.	no
C1	C6	1.508(4)	.	.	no
C2	C3	1.425(4)	.	.	no
C2	C7	1.503(4)	.	.	no
C3	C4	1.430(4)	.	.	no
C3	C8	1.510(4)	.	.	no
C4	C5	1.407(3)	.	.	no
C4	C9	1.501(4)	.	.	no
C5	C10	1.506(4)	.	.	no
C11	C12	1.420(3)	.	.	no
C11	C15	1.423(3)	.	.	no
C11	C16	1.507(3)	.	.	no
C12	C13	1.423(3)	.	.	no
C12	C17	1.508(4)	.	.	no
C13	C14	1.418(4)	.	.	no
C13	C18	1.506(4)	.	.	no
C14	C15	1.417(4)	.	.	no
C14	C19	1.502(3)	.	.	no
C15	C20	1.510(4)	.	.	no
C21	C22	1.536(4)	.	.	no
C23	C24	1.532(4)	.	.	no
C6	H6	0.9800	.	.	no
C6	H6'	0.9800	.	.	no
C6	H6''	0.9800	.	.	no
C7	H7	0.9800	.	.	no
C7	H7'	0.9800	.	.	no
C7	H7''	0.9800	.	.	no
C8	H8	0.9800	.	.	no
C8	H8'	0.9800	.	.	no
C8	H8''	0.9800	.	.	no
C9	H9	0.9800	.	.	no
C9	H9'	0.9800	.	.	no
C9	H9''	0.9800	.	.	no
C10	H10	0.9800	.	.	no
C10	H10'	0.9800	.	.	no
C10	H10''	0.9800	.	.	no
C16	H16	0.9800	.	.	no
C16	H16'	0.9800	.	.	no
C16	H16''	0.9800	.	.	no
C17	H17	0.9800	.	.	no
C17	H17'	0.9800	.	.	no
C17	H17''	0.9800	.	.	no
C18	H18	0.9800	.	.	no
C18	H18'	0.9800	.	.	no
C18	H18''	0.9800	.	.	no
C19	H19	0.9800	.	.	no
C19	H19'	0.9800	.	.	no
C19	H19''	0.9800	.	.	no
C20	H20	0.9800	.	.	no
C20	H20'	0.9800	.	.	no
C20	H20''	0.9800	.	.	no
C21	H21	0.9900	.	.	no
C21	H21'	0.9900	.	.	no
C22	H22	0.9800	.	.	no
C22	H22'	0.9800	.	.	no
C22	H22''	0.9800	.	.	no
C23	H23	0.9900	.	.	no
C23	H23'	0.9900	.	.	no
C24	H24	0.9800	.	.	no

C24	H24'	0.9800	.	.	no
C24	H24''	0.9800	.	.	no
C25	H25	0.9800	.	.	no
C25	H25'	0.9800	.	.	no
C25	H25''	0.9800	.	.	no
loop_					
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_geom_angle_atom_site_label_3					
_geom_angle					
_geom_angle_site_symmetry_1					
_geom_angle_site_symmetry_2					
_geom_angle_site_symmetry_3					
_geom_angle_publ_flag					
N	Zr	C1	98.85(8)	.	yes
N	Zr	C2	83.13(9)	.	yes
N	Zr	C3	101.88(9)	.	yes
N	Zr	C4	132.93(7)	.	yes
N	Zr	C5	130.20(7)	.	yes
N	Zr	C11	88.04(7)	.	yes
N	Zr	C12	118.80(7)	.	yes
N	Zr	C13	134.96(7)	.	yes
N	Zr	C14	108.87(8)	.	yes
N	Zr	C15	82.47(8)	.	yes
N	Zr	C25	94.14(10)	.	yes
C1	Zr	C2	31.34(8)	.	yes
C1	Zr	C3	52.55(8)	.	yes
C1	Zr	C4	51.65(8)	.	yes
C1	Zr	C5	31.46(8)	.	yes
C1	Zr	C11	156.77(7)	.	yes
C1	Zr	C12	132.45(8)	.	yes
C1	Zr	C13	126.03(8)	.	yes
C1	Zr	C14	141.76(8)	.	yes
C1	Zr	C15	171.00(8)	.	yes
C1	Zr	C25	77.86(8)	.	yes
C2	Zr	C3	32.11(8)	.	yes
C2	Zr	C4	52.23(8)	.	yes
C2	Zr	C5	52.15(8)	.	yes
C2	Zr	C11	129.81(7)	.	yes
C2	Zr	C12	121.84(8)	.	yes
C2	Zr	C13	137.21(8)	.	yes
C2	Zr	C14	168.00(10)	.	yes
C2	Zr	C15	156.82(8)	.	yes
C2	Zr	C25	105.89(8)	.	yes
C3	Zr	C4	31.99(8)	.	yes
C3	Zr	C5	52.58(8)	.	yes
C3	Zr	C11	104.38(7)	.	yes
C3	Zr	C12	89.86(8)	.	yes
C3	Zr	C13	108.18(8)	.	yes
C3	Zr	C14	139.53(9)	.	yes
C3	Zr	C15	136.04(8)	.	yes
C3	Zr	C25	129.42(8)	.	yes
C4	Zr	C5	30.98(7)	.	yes
C4	Zr	C11	108.13(7)	.	yes
C4	Zr	C12	80.90(7)	.	yes
C4	Zr	C13	85.24(7)	.	yes
C4	Zr	C14	116.06(8)	.	yes
C4	Zr	C15	132.84(8)	.	yes
C4	Zr	C25	110.31(9)	.	yes
C5	Zr	C11	135.48(7)	.	yes
C5	Zr	C12	104.52(7)	.	yes
C5	Zr	C13	94.83(7)	.	yes
C5	Zr	C14	116.89(8)	.	yes
C5	Zr	C15	146.87(8)	.	yes
C5	Zr	C25	80.60(9)	.	yes

C11	Zr	C12	31.66(7)	.	.	.	yes
C11	Zr	C13	52.72(7)	.	.	.	yes
C11	Zr	C14	52.47(7)	.	.	.	yes
C11	Zr	C15	31.66(7)	.	.	.	yes
C11	Zr	C25	124.01(8)	.	.	.	yes
C12	Zr	C13	31.87(7)	.	.	.	yes
C12	Zr	C14	52.45(7)	.	.	.	yes
C12	Zr	C15	52.33(8)	.	.	.	yes
C12	Zr	C25	123.20(8)	.	.	.	yes
C13	Zr	C14	31.84(8)	.	.	.	yes
C13	Zr	C15	52.62(8)	.	.	.	yes
C13	Zr	C25	91.95(9)	.	.	.	yes
C14	Zr	C15	31.66(9)	.	.	.	yes
C14	Zr	C25	74.43(8)	.	.	.	yes
C15	Zr	C25	93.19(8)	.	.	.	yes
Zr	N	C21	132.16(17)	.	.	.	yes
Zr	N	C23	117.88(17)	.	.	.	yes
C21	N	C23	109.9(2)	.	.	.	yes
Zr	C1	C2	73.15(13)	.	.	.	yes
Zr	C1	C5	74.33(12)	.	.	.	yes
Zr	C1	C6	128.05(17)	.	.	.	yes
C2	C1	C5	108.2(2)	.	.	.	no
C2	C1	C6	126.0(3)	.	.	.	no
C5	C1	C6	124.7(2)	.	.	.	no
Zr	C2	C1	75.51(13)	.	.	.	yes
Zr	C2	C3	71.86(13)	.	.	.	yes
Zr	C2	C7	126.21(18)	.	.	.	yes
C1	C2	C3	107.8(3)	.	.	.	no
C1	C2	C7	126.3(2)	.	.	.	no
C3	C2	C7	125.1(2)	.	.	.	no
Zr	C3	C2	76.03(14)	.	.	.	yes
Zr	C3	C4	77.38(13)	.	.	.	yes
Zr	C3	C8	120.76(17)	.	.	.	yes
C2	C3	C4	107.7(2)	.	.	.	no
C2	C3	C8	124.8(3)	.	.	.	no
C4	C3	C8	126.8(2)	.	.	.	no
Zr	C4	C3	70.62(13)	.	.	.	yes
Zr	C4	C5	74.43(13)	.	.	.	yes
Zr	C4	C9	132.54(15)	.	.	.	yes
C3	C4	C5	108.0(2)	.	.	.	no
C3	C4	C9	125.0(2)	.	.	.	no
C5	C4	C9	125.3(2)	.	.	.	no
Zr	C5	C1	74.21(13)	.	.	.	yes
Zr	C5	C4	74.59(12)	.	.	.	yes
Zr	C5	C10	124.47(15)	.	.	.	yes
C1	C5	C4	108.1(2)	.	.	.	no
C1	C5	C10	125.2(2)	.	.	.	no
C4	C5	C10	126.1(2)	.	.	.	no
Zr	C11	C12	73.85(13)	.	.	.	yes
Zr	C11	C15	74.16(13)	.	.	.	yes
Zr	C11	C16	128.40(15)	.	.	.	yes
C12	C11	C15	107.7(2)	.	.	.	no
C12	C11	C16	122.8(2)	.	.	.	no
C15	C11	C16	128.1(2)	.	.	.	no
Zr	C12	C11	74.50(13)	.	.	.	yes
Zr	C12	C13	73.38(13)	.	.	.	yes
Zr	C12	C17	132.53(15)	.	.	.	yes
C11	C12	C13	108.3(2)	.	.	.	no
C11	C12	C17	122.6(2)	.	.	.	no
C13	C12	C17	126.5(2)	.	.	.	no
Zr	C13	C12	74.75(12)	.	.	.	yes
Zr	C13	C14	74.31(13)	.	.	.	yes
Zr	C13	C18	122.41(15)	.	.	.	yes
C12	C13	C14	107.6(2)	.	.	.	no
C12	C13	C18	127.7(2)	.	.	.	no
C14	C13	C18	124.4(2)	.	.	.	no

Zr	C14	C13	73.85(12)	.	.	.	yes
Zr	C14	C15	74.94(13)	.	.	.	yes
Zr	C14	C19	127.79(15)	.	.	.	yes
C13	C14	C15	108.5(2)	.	.	.	no
C13	C14	C19	124.6(3)	.	.	.	no
C15	C14	C19	125.6(2)	.	.	.	no
Zr	C15	C11	74.18(12)	.	.	.	yes
Zr	C15	C14	73.40(13)	.	.	.	yes
Zr	C15	C20	123.66(17)	.	.	.	yes
C11	C15	C14	107.9(2)	.	.	.	no
C11	C15	C20	128.2(2)	.	.	.	no
C14	C15	C20	123.5(2)	.	.	.	no
N	C21	C22	114.1(2)	.	.	.	yes
N	C23	C24	113.4(2)	.	.	.	yes
C1	C6	H6	109.00	.	.	.	no
C1	C6	H6'	109.00	.	.	.	no
C1	C6	H6"	109.00	.	.	.	no
H6	C6	H6'	109.00	.	.	.	no
H6	C6	H6"	109.00	.	.	.	no
H6'	C6	H6"	109.00	.	.	.	no
C2	C7	H7	109.00	.	.	.	no
C2	C7	H7'	109.00	.	.	.	no
C2	C7	H7"	109.00	.	.	.	no
H7	C7	H7'	109.00	.	.	.	no
H7	C7	H7"	109.00	.	.	.	no
H7'	C7	H7"	109.00	.	.	.	no
C3	C8	H8	109.00	.	.	.	no
C3	C8	H8'	109.00	.	.	.	no
C3	C8	H8"	109.00	.	.	.	no
H8	C8	H8'	109.00	.	.	.	no
H8	C8	H8"	109.00	.	.	.	no
H8'	C8	H8"	109.00	.	.	.	no
C4	C9	H9	109.00	.	.	.	no
C4	C9	H9'	109.00	.	.	.	no
C4	C9	H9"	109.00	.	.	.	no
H9	C9	H9'	109.00	.	.	.	no
H9	C9	H9"	109.00	.	.	.	no
H9'	C9	H9"	109.00	.	.	.	no
C5	C10	H10	109.00	.	.	.	no
C5	C10	H10'	109.00	.	.	.	no
C5	C10	H10"	109.00	.	.	.	no
H10	C10	H10'	109.00	.	.	.	no
H10	C10	H10"	109.00	.	.	.	no
H10'	C10	H10"	109.00	.	.	.	no
C11	C16	H16	109.00	.	.	.	no
C11	C16	H16'	109.00	.	.	.	no
C11	C16	H16"	109.00	.	.	.	no
H16	C16	H16'	109.00	.	.	.	no
H16	C16	H16"	109.00	.	.	.	no
H16'	C16	H16"	110.00	.	.	.	no
C12	C17	H17	109.00	.	.	.	no
C12	C17	H17'	109.00	.	.	.	no
C12	C17	H17"	109.00	.	.	.	no
H17	C17	H17'	109.00	.	.	.	no
H17	C17	H17"	109.00	.	.	.	no
H17'	C17	H17"	109.00	.	.	.	no
C13	C18	H18	109.00	.	.	.	no
C13	C18	H18'	109.00	.	.	.	no
C13	C18	H18"	109.00	.	.	.	no
H18	C18	H18'	109.00	.	.	.	no
H18	C18	H18"	109.00	.	.	.	no
H18'	C18	H18"	109.00	.	.	.	no
C14	C19	H19	109.00	.	.	.	no
C14	C19	H19'	109.00	.	.	.	no
C14	C19	H19"	109.00	.	.	.	no
H19	C19	H19'	109.00	.	.	.	no

H19	C19	H19"	109.00	.	.	.	no
H19'	C19	H19"	109.00	.	.	.	no
C15	C20	H20	109.00	.	.	.	no
C15	C20	H20'	109.00	.	.	.	no
C15	C20	H20"	110.00	.	.	.	no
H20	C20	H20'	109.00	.	.	.	no
H20	C20	H20"	109.00	.	.	.	no
H20'	C20	H20"	109.00	.	.	.	no
N	C21	H21	109.00	.	.	.	no
N	C21	H21'	109.00	.	.	.	no
C22	C21	H21	109.00	.	.	.	no
C22	C21	H21'	109.00	.	.	.	no
H21	C21	H21'	108.00	.	.	.	no
C21	C22	H22	109.00	.	.	.	no
C21	C22	H22'	109.00	.	.	.	no
C21	C22	H22"	109.00	.	.	.	no
H22	C22	H22'	109.00	.	.	.	no
H22	C22	H22"	109.00	.	.	.	no
H22'	C22	H22"	109.00	.	.	.	no
N	C23	H23	109.00	.	.	.	no
N	C23	H23'	109.00	.	.	.	no
C24	C23	H23	109.00	.	.	.	no
C24	C23	H23'	109.00	.	.	.	no
H23	C23	H23'	108.00	.	.	.	no
C23	C24	H24	109.00	.	.	.	no
C23	C24	H24'	109.00	.	.	.	no
C23	C24	H24"	109.00	.	.	.	no
H24	C24	H24'	109.00	.	.	.	no
H24	C24	H24"	109.00	.	.	.	no
H24'	C24	H24"	109.00	.	.	.	no
Zr	C25	H25	109.00	.	.	.	no
Zr	C25	H25'	109.00	.	.	.	no
Zr	C25	H25"	109.00	.	.	.	no
H25	C25	H25'	109.00	.	.	.	no
H25	C25	H25"	109.00	.	.	.	no
H25'	C25	H25"	109.00	.	.	.	no

loop_

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_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag

C1	Zr	N	C21	-140.6(2)	.	.	.	.	no
C1	Zr	N	C23	35.45(17)	.	.	.	.	no
C2	Zr	N	C21	-113.4(2)	.	.	.	.	no
C2	Zr	N	C23	62.65(17)	.	.	.	.	no
C3	Zr	N	C21	-87.2(2)	.	.	.	.	no
C3	Zr	N	C23	88.86(17)	.	.	.	.	no
C4	Zr	N	C21	-96.1(2)	.	.	.	.	no
C4	Zr	N	C23	79.98(19)	.	.	.	.	no
C5	Zr	N	C21	-137.77(19)	.	.	.	.	no
C5	Zr	N	C23	38.3(2)	.	.	.	.	no
C11	Zr	N	C21	17.1(2)	.	.	.	.	no
C11	Zr	N	C23	-166.85(17)	.	.	.	.	no
C12	Zr	N	C21	9.3(2)	.	.	.	.	no
C12	Zr	N	C23	-174.66(15)	.	.	.	.	no
C13	Zr	N	C21	44.1(3)	.	.	.	.	no
C13	Zr	N	C23	-139.80(16)	.	.	.	.	no
C14	Zr	N	C21	66.1(2)	.	.	.	.	no
C14	Zr	N	C23	-117.83(16)	.	.	.	.	no

C15	Zr	N	C21	48.4(2)	.	.	.	.	no
C15	Zr	N	C23	-135.56(17)	.	.	.	.	no
C25	Zr	N	C21	141.1(2)	.	.	.	.	no
C25	Zr	N	C23	-42.88(17)	.	.	.	.	no
N	Zr	C1	C2	60.76(18)	.	.	.	.	no
N	Zr	C1	C5	175.83(14)	.	.	.	.	no
N	Zr	C1	C6	-62.1(2)	.	.	.	.	no
C2	Zr	C1	C5	115.1(2)	.	.	.	.	no
C2	Zr	C1	C6	-122.9(3)	.	.	.	.	no
C3	Zr	C1	C2	-37.48(17)	.	.	.	.	no
C3	Zr	C1	C5	77.59(16)	.	.	.	.	no
C3	Zr	C1	C6	-160.4(3)	.	.	.	.	no
C4	Zr	C1	C2	-78.34(17)	.	.	.	.	no
C4	Zr	C1	C5	36.73(13)	.	.	.	.	no
C4	Zr	C1	C6	158.8(3)	.	.	.	.	no
C5	Zr	C1	C2	-115.1(2)	.	.	.	.	no
C5	Zr	C1	C6	122.1(3)	.	.	.	.	no
C11	Zr	C1	C2	-45.2(3)	.	.	.	.	no
C11	Zr	C1	C5	69.9(3)	.	.	.	.	no
C11	Zr	C1	C6	-168.07(19)	.	.	.	.	no
C12	Zr	C1	C2	-82.7(2)	.	.	.	.	no
C12	Zr	C1	C5	32.40(18)	.	.	.	.	no
C12	Zr	C1	C6	154.5(2)	.	.	.	.	no
C13	Zr	C1	C2	-123.39(17)	.	.	.	.	no
C13	Zr	C1	C5	-8.33(17)	.	.	.	.	no
C13	Zr	C1	C6	113.7(2)	.	.	.	.	no
C14	Zr	C1	C2	-162.66(16)	.	.	.	.	no
C14	Zr	C1	C5	-47.6(2)	.	.	.	.	no
C14	Zr	C1	C6	74.5(3)	.	.	.	.	no
C25	Zr	C1	C2	153.12(19)	.	.	.	.	no
C25	Zr	C1	C5	-91.81(16)	.	.	.	.	no
C25	Zr	C1	C6	30.2(2)	.	.	.	.	no
N	Zr	C2	C1	-119.72(17)	.	.	.	.	no
N	Zr	C2	C3	125.60(17)	.	.	.	.	no
N	Zr	C2	C7	5.0(2)	.	.	.	.	no
C1	Zr	C2	C3	-114.7(3)	.	.	.	.	no
C1	Zr	C2	C7	124.7(3)	.	.	.	.	no
C3	Zr	C2	C1	114.7(3)	.	.	.	.	no
C3	Zr	C2	C7	-120.7(3)	.	.	.	.	no
C4	Zr	C2	C1	76.29(18)	.	.	.	.	no
C4	Zr	C2	C3	-38.39(16)	.	.	.	.	no
C4	Zr	C2	C7	-159.0(2)	.	.	.	.	no
C5	Zr	C2	C1	36.77(16)	.	.	.	.	no
C5	Zr	C2	C3	-77.90(18)	.	.	.	.	no
C5	Zr	C2	C7	161.5(2)	.	.	.	.	no
C11	Zr	C2	C1	158.63(15)	.	.	.	.	no
C11	Zr	C2	C3	44.0(2)	.	.	.	.	no
C11	Zr	C2	C7	-76.7(2)	.	.	.	.	no
C12	Zr	C2	C1	120.52(16)	.	.	.	.	no
C12	Zr	C2	C3	5.9(2)	.	.	.	.	no
C12	Zr	C2	C7	-114.8(2)	.	.	.	.	no
C13	Zr	C2	C1	83.72(19)	.	.	.	.	no
C13	Zr	C2	C3	-31.0(2)	.	.	.	.	no
C13	Zr	C2	C7	-151.60(19)	.	.	.	.	no
C15	Zr	C2	C1	-171.6(2)	.	.	.	.	no
C15	Zr	C2	C3	73.7(3)	.	.	.	.	no
C15	Zr	C2	C7	-47.0(3)	.	.	.	.	no
C25	Zr	C2	C1	-27.36(19)	.	.	.	.	no
C25	Zr	C2	C3	-142.04(17)	.	.	.	.	no
C25	Zr	C2	C7	97.3(2)	.	.	.	.	no
N	Zr	C3	C2	-55.58(17)	.	.	.	.	no
N	Zr	C3	C4	-167.68(13)	.	.	.	.	no
N	Zr	C3	C8	66.8(2)	.	.	.	.	no
C1	Zr	C3	C2	36.53(16)	.	.	.	.	no
C1	Zr	C3	C4	-75.57(15)	.	.	.	.	no
C1	Zr	C3	C8	158.9(3)	.	.	.	.	no

C2	Zr	C3	C4	-112.1(2)	.	.	.	.	no
C2	Zr	C3	C8	122.4(3)	.	.	.	.	no
C4	Zr	C3	C2	112.1(2)	.	.	.	.	no
C4	Zr	C3	C8	-125.5(3)	.	.	.	.	no
C5	Zr	C3	C2	76.45(16)	.	.	.	.	no
C5	Zr	C3	C4	-35.64(13)	.	.	.	.	no
C5	Zr	C3	C8	-161.2(3)	.	.	.	.	no
C11	Zr	C3	C2	-146.61(16)	.	.	.	.	no
C11	Zr	C3	C4	101.30(14)	.	.	.	.	no
C11	Zr	C3	C8	-24.2(2)	.	.	.	.	no
C12	Zr	C3	C2	-175.04(17)	.	.	.	.	no
C12	Zr	C3	C4	72.87(14)	.	.	.	.	no
C12	Zr	C3	C8	-52.7(2)	.	.	.	.	no
C13	Zr	C3	C2	158.42(16)	.	.	.	.	no
C13	Zr	C3	C4	46.33(15)	.	.	.	.	no
C13	Zr	C3	C8	-79.2(2)	.	.	.	.	no
C14	Zr	C3	C2	165.34(15)	.	.	.	.	no
C14	Zr	C3	C4	53.24(19)	.	.	.	.	no
C14	Zr	C3	C8	-72.3(3)	.	.	.	.	no
C15	Zr	C3	C2	-147.03(16)	.	.	.	.	no
C15	Zr	C3	C4	100.87(17)	.	.	.	.	no
C15	Zr	C3	C8	-24.7(3)	.	.	.	.	no
C25	Zr	C3	C2	50.0(2)	.	.	.	.	no
C25	Zr	C3	C4	-62.11(18)	.	.	.	.	no
C25	Zr	C3	C8	172.4(2)	.	.	.	.	no
N	Zr	C4	C3	16.58(18)	.	.	.	.	no
N	Zr	C4	C5	-99.40(15)	.	.	.	.	no
N	Zr	C4	C9	136.7(2)	.	.	.	.	no
C1	Zr	C4	C3	78.65(15)	.	.	.	.	no
C1	Zr	C4	C5	-37.32(13)	.	.	.	.	no
C1	Zr	C4	C9	-161.2(3)	.	.	.	.	no
C2	Zr	C4	C3	38.54(13)	.	.	.	.	no
C2	Zr	C4	C5	-77.44(14)	.	.	.	.	no
C2	Zr	C4	C9	158.7(3)	.	.	.	.	no
C3	Zr	C4	C5	-115.97(19)	.	.	.	.	no
C3	Zr	C4	C9	120.2(3)	.	.	.	.	no
C5	Zr	C4	C3	115.97(19)	.	.	.	.	no
C5	Zr	C4	C9	-123.9(3)	.	.	.	.	no
C11	Zr	C4	C3	-88.23(14)	.	.	.	.	no
C11	Zr	C4	C5	155.80(12)	.	.	.	.	no
C11	Zr	C4	C9	31.9(2)	.	.	.	.	no
C12	Zr	C4	C3	-104.58(14)	.	.	.	.	no
C12	Zr	C4	C5	139.45(13)	.	.	.	.	no
C12	Zr	C4	C9	15.6(2)	.	.	.	.	no
C13	Zr	C4	C3	-136.40(14)	.	.	.	.	no
C13	Zr	C4	C5	107.62(13)	.	.	.	.	no
C13	Zr	C4	C9	-16.3(2)	.	.	.	.	no
C14	Zr	C4	C3	-144.63(13)	.	.	.	.	no
C14	Zr	C4	C5	99.40(13)	.	.	.	.	no
C14	Zr	C4	C9	-24.5(3)	.	.	.	.	no
C15	Zr	C4	C3	-111.63(15)	.	.	.	.	no
C15	Zr	C4	C5	132.39(13)	.	.	.	.	no
C15	Zr	C4	C9	8.5(3)	.	.	.	.	no
C25	Zr	C4	C3	133.28(14)	.	.	.	.	no
C25	Zr	C4	C5	17.30(15)	.	.	.	.	no
C25	Zr	C4	C9	-106.6(2)	.	.	.	.	no
N	Zr	C5	C1	-5.40(18)	.	.	.	.	no
N	Zr	C5	C4	108.96(14)	.	.	.	.	no
N	Zr	C5	C10	-127.52(19)	.	.	.	.	no
C1	Zr	C5	C4	114.36(19)	.	.	.	.	no
C1	Zr	C5	C10	-122.1(3)	.	.	.	.	no
C2	Zr	C5	C1	-36.63(14)	.	.	.	.	no
C2	Zr	C5	C4	77.73(14)	.	.	.	.	no
C2	Zr	C5	C10	-158.8(2)	.	.	.	.	no
C3	Zr	C5	C1	-77.51(15)	.	.	.	.	no
C3	Zr	C5	C4	36.85(13)	.	.	.	.	no

C3	Zr	C5	C10	160.4(2)	.	.	.	.	no
C4	Zr	C5	C1	-114.36(19)	.	.	.	.	no
C4	Zr	C5	C10	123.5(2)	.	.	.	.	no
C11	Zr	C5	C1	-148.11(13)	.	.	.	.	no
C11	Zr	C5	C4	-33.76(17)	.	.	.	.	no
C11	Zr	C5	C10	89.8(2)	.	.	.	.	no
C12	Zr	C5	C1	-155.89(14)	.	.	.	.	no
C12	Zr	C5	C4	-41.54(14)	.	.	.	.	no
C12	Zr	C5	C10	82.0(2)	.	.	.	.	no
C13	Zr	C5	C1	173.25(14)	.	.	.	.	no
C13	Zr	C5	C4	-72.39(13)	.	.	.	.	no
C13	Zr	C5	C10	51.1(2)	.	.	.	.	no
C14	Zr	C5	C1	149.18(13)	.	.	.	.	no
C14	Zr	C5	C4	-96.46(14)	.	.	.	.	no
C14	Zr	C5	C10	27.1(2)	.	.	.	.	no
C15	Zr	C5	C1	163.41(14)	.	.	.	.	no
C15	Zr	C5	C4	-82.23(18)	.	.	.	.	no
C15	Zr	C5	C10	41.3(3)	.	.	.	.	no
C25	Zr	C5	C1	82.07(15)	.	.	.	.	no
C25	Zr	C5	C4	-163.58(14)	.	.	.	.	no
C25	Zr	C5	C10	-40.1(2)	.	.	.	.	no
N	Zr	C11	C12	-166.88(14)	.	.	.	.	no
N	Zr	C11	C15	78.80(16)	.	.	.	.	no
N	Zr	C11	C16	-47.6(2)	.	.	.	.	no
C1	Zr	C11	C12	-58.8(3)	.	.	.	.	no
C1	Zr	C11	C15	-173.1(2)	.	.	.	.	no
C1	Zr	C11	C16	60.5(3)	.	.	.	.	no
C2	Zr	C11	C12	-87.51(16)	.	.	.	.	no
C2	Zr	C11	C15	158.17(16)	.	.	.	.	no
C2	Zr	C11	C16	31.8(2)	.	.	.	.	no
C3	Zr	C11	C12	-65.12(15)	.	.	.	.	no
C3	Zr	C11	C15	-179.44(16)	.	.	.	.	no
C3	Zr	C11	C16	54.2(2)	.	.	.	.	no
C4	Zr	C11	C12	-31.98(14)	.	.	.	.	no
C4	Zr	C11	C15	-146.30(15)	.	.	.	.	no
C4	Zr	C11	C16	87.3(2)	.	.	.	.	no
C5	Zr	C11	C12	-14.46(18)	.	.	.	.	no
C5	Zr	C11	C15	-128.78(16)	.	.	.	.	no
C5	Zr	C11	C16	104.9(2)	.	.	.	.	no
C12	Zr	C11	C15	-114.3(2)	.	.	.	.	no
C12	Zr	C11	C16	119.3(3)	.	.	.	.	no
C13	Zr	C11	C12	36.97(13)	.	.	.	.	no
C13	Zr	C11	C15	-77.35(16)	.	.	.	.	no
C13	Zr	C11	C16	156.3(2)	.	.	.	.	no
C14	Zr	C11	C12	77.38(15)	.	.	.	.	no
C14	Zr	C11	C15	-36.94(16)	.	.	.	.	no
C14	Zr	C11	C16	-163.3(2)	.	.	.	.	no
C15	Zr	C11	C12	114.3(2)	.	.	.	.	no
C15	Zr	C11	C16	-126.4(3)	.	.	.	.	no
C25	Zr	C11	C12	99.45(16)	.	.	.	.	no
C25	Zr	C11	C15	-14.87(19)	.	.	.	.	no
C25	Zr	C11	C16	-141.2(2)	.	.	.	.	no
N	Zr	C12	C11	15.00(16)	.	.	.	.	no
N	Zr	C12	C13	130.01(13)	.	.	.	.	no
N	Zr	C12	C17	-105.3(2)	.	.	.	.	no
C1	Zr	C12	C11	152.79(13)	.	.	.	.	no
C1	Zr	C12	C13	-92.21(15)	.	.	.	.	no
C1	Zr	C12	C17	32.5(3)	.	.	.	.	no
C2	Zr	C12	C11	115.40(14)	.	.	.	.	no
C2	Zr	C12	C13	-129.59(13)	.	.	.	.	no
C2	Zr	C12	C17	-4.9(3)	.	.	.	.	no
C3	Zr	C12	C11	118.51(14)	.	.	.	.	no
C3	Zr	C12	C13	-126.49(14)	.	.	.	.	no
C3	Zr	C12	C17	-1.8(2)	.	.	.	.	no
C4	Zr	C12	C11	149.35(14)	.	.	.	.	no
C4	Zr	C12	C13	-95.64(13)	.	.	.	.	no

C4	Zr	C12	C17	29.0(2)	.	.	.	.	no
C5	Zr	C12	C11	169.58(13)	.	.	.	.	no
C5	Zr	C12	C13	-75.42(13)	.	.	.	.	no
C5	Zr	C12	C17	49.3(2)	.	.	.	.	no
C11	Zr	C12	C13	115.01(19)	.	.	.	.	no
C11	Zr	C12	C17	-120.3(3)	.	.	.	.	no
C13	Zr	C12	C11	-115.01(19)	.	.	.	.	no
C13	Zr	C12	C17	124.7(3)	.	.	.	.	no
C14	Zr	C12	C11	-77.46(15)	.	.	.	.	no
C14	Zr	C12	C13	37.55(13)	.	.	.	.	no
C14	Zr	C12	C17	162.2(3)	.	.	.	.	no
C15	Zr	C12	C11	-37.18(13)	.	.	.	.	no
C15	Zr	C12	C13	77.83(14)	.	.	.	.	no
C15	Zr	C12	C17	-157.5(3)	.	.	.	.	no
C25	Zr	C12	C11	-102.26(15)	.	.	.	.	no
C25	Zr	C12	C13	12.74(16)	.	.	.	.	no
C25	Zr	C12	C17	137.4(2)	.	.	.	.	no
N	Zr	C13	C12	-71.55(16)	.	.	.	.	no
N	Zr	C13	C14	42.14(19)	.	.	.	.	no
N	Zr	C13	C18	163.20(17)	.	.	.	.	no
C1	Zr	C13	C12	114.26(13)	.	.	.	.	no
C1	Zr	C13	C14	-132.06(14)	.	.	.	.	no
C1	Zr	C13	C18	-11.0(2)	.	.	.	.	no
C2	Zr	C13	C12	74.53(16)	.	.	.	.	no
C2	Zr	C13	C14	-171.79(14)	.	.	.	.	no
C2	Zr	C13	C18	-50.7(2)	.	.	.	.	no
C3	Zr	C13	C12	57.80(14)	.	.	.	.	no
C3	Zr	C13	C14	171.48(14)	.	.	.	.	no
C3	Zr	C13	C18	-67.5(2)	.	.	.	.	no
C4	Zr	C13	C12	80.42(13)	.	.	.	.	no
C4	Zr	C13	C14	-165.90(15)	.	.	.	.	no
C4	Zr	C13	C18	-44.84(19)	.	.	.	.	no
C5	Zr	C13	C12	109.91(13)	.	.	.	.	no
C5	Zr	C13	C14	-136.41(14)	.	.	.	.	no
C5	Zr	C13	C18	-15.3(2)	.	.	.	.	no
C11	Zr	C13	C12	-36.71(12)	.	.	.	.	no
C11	Zr	C13	C14	76.97(14)	.	.	.	.	no
C11	Zr	C13	C18	-162.0(2)	.	.	.	.	no
C12	Zr	C13	C14	113.68(19)	.	.	.	.	no
C12	Zr	C13	C18	-125.3(2)	.	.	.	.	no
C14	Zr	C13	C12	-113.68(19)	.	.	.	.	no
C14	Zr	C13	C18	121.1(3)	.	.	.	.	no
C15	Zr	C13	C12	-76.84(14)	.	.	.	.	no
C15	Zr	C13	C14	36.84(13)	.	.	.	.	no
C15	Zr	C13	C18	157.9(2)	.	.	.	.	no
C25	Zr	C13	C12	-169.36(14)	.	.	.	.	no
C25	Zr	C13	C14	-55.68(15)	.	.	.	.	no
C25	Zr	C13	C18	65.4(2)	.	.	.	.	no
N	Zr	C14	C13	-149.89(14)	.	.	.	.	no
N	Zr	C14	C15	-35.11(16)	.	.	.	.	no
N	Zr	C14	C19	88.5(3)	.	.	.	.	no
C1	Zr	C14	C13	75.98(18)	.	.	.	.	no
C1	Zr	C14	C15	-169.24(15)	.	.	.	.	no
C1	Zr	C14	C19	-45.6(3)	.	.	.	.	no
C3	Zr	C14	C13	-12.5(2)	.	.	.	.	no
C3	Zr	C14	C15	102.26(19)	.	.	.	.	no
C3	Zr	C14	C19	-134.1(2)	.	.	.	.	no
C4	Zr	C14	C13	15.68(16)	.	.	.	.	no
C4	Zr	C14	C15	130.46(15)	.	.	.	.	no
C4	Zr	C14	C19	-105.9(2)	.	.	.	.	no
C5	Zr	C14	C13	50.39(15)	.	.	.	.	no
C5	Zr	C14	C15	165.17(14)	.	.	.	.	no
C5	Zr	C14	C19	-71.2(3)	.	.	.	.	no
C11	Zr	C14	C13	-77.83(14)	.	.	.	.	no
C11	Zr	C14	C15	36.95(14)	.	.	.	.	no
C11	Zr	C14	C19	160.6(3)	.	.	.	.	no

C12	Zr	C14	C13	-37.59(13)	.	.	.	.	no
C12	Zr	C14	C15	77.19(15)	.	.	.	.	no
C12	Zr	C14	C19	-159.2(3)	.	.	.	.	no
C13	Zr	C14	C15	114.8(2)	.	.	.	.	no
C13	Zr	C14	C19	-121.6(3)	.	.	.	.	no
C15	Zr	C14	C13	-114.8(2)	.	.	.	.	no
C15	Zr	C14	C19	123.6(3)	.	.	.	.	no
C25	Zr	C14	C13	121.04(16)	.	.	.	.	no
C25	Zr	C14	C15	-124.18(17)	.	.	.	.	no
C25	Zr	C14	C19	-0.6(2)	.	.	.	.	no
N	Zr	C15	C11	-98.55(15)	.	.	.	.	no
N	Zr	C15	C14	146.71(16)	.	.	.	.	no
N	Zr	C15	C20	27.1(2)	.	.	.	.	no
C2	Zr	C15	C11	-46.5(3)	.	.	.	.	no
C2	Zr	C15	C14	-161.3(2)	.	.	.	.	no
C2	Zr	C15	C20	79.1(3)	.	.	.	.	no
C3	Zr	C15	C11	0.8(2)	.	.	.	.	no
C3	Zr	C15	C14	-113.96(17)	.	.	.	.	no
C3	Zr	C15	C20	126.4(2)	.	.	.	.	no
C4	Zr	C15	C11	45.98(19)	.	.	.	.	no
C4	Zr	C15	C14	-68.77(17)	.	.	.	.	no
C4	Zr	C15	C20	171.62(17)	.	.	.	.	no
C5	Zr	C15	C11	90.05(19)	.	.	.	.	no
C5	Zr	C15	C14	-24.7(2)	.	.	.	.	no
C5	Zr	C15	C20	-144.31(19)	.	.	.	.	no
C11	Zr	C15	C14	-114.8(2)	.	.	.	.	no
C11	Zr	C15	C20	125.6(3)	.	.	.	.	no
C12	Zr	C15	C11	37.17(13)	.	.	.	.	no
C12	Zr	C15	C14	-77.58(16)	.	.	.	.	no
C12	Zr	C15	C20	162.8(2)	.	.	.	.	no
C13	Zr	C15	C11	77.68(16)	.	.	.	.	no
C13	Zr	C15	C14	-37.07(15)	.	.	.	.	no
C13	Zr	C15	C20	-156.7(2)	.	.	.	.	no
C14	Zr	C15	C11	114.8(2)	.	.	.	.	no
C14	Zr	C15	C20	-119.6(3)	.	.	.	.	no
C25	Zr	C15	C11	167.70(16)	.	.	.	.	no
C25	Zr	C15	C14	52.95(16)	.	.	.	.	no
C25	Zr	C15	C20	-66.7(2)	.	.	.	.	no
Zr	N	C21	C22	90.7(3)	.	.	.	.	no
C23	N	C21	C22	-85.6(3)	.	.	.	.	no
Zr	N	C23	C24	105.6(2)	.	.	.	.	no
C21	N	C23	C24	-77.5(3)	.	.	.	.	no
Zr	C1	C2	C3	65.11(16)	.	.	.	.	no
Zr	C1	C2	C7	-124.6(3)	.	.	.	.	no
C5	C1	C2	Zr	-66.64(16)	.	.	.	.	no
C5	C1	C2	C3	-1.5(3)	.	.	.	.	no
C5	C1	C2	C7	168.8(2)	.	.	.	.	no
C6	C1	C2	Zr	125.2(3)	.	.	.	.	no
C6	C1	C2	C3	-169.7(2)	.	.	.	.	no
C6	C1	C2	C7	0.6(4)	.	.	.	.	no
Zr	C1	C5	C4	-67.49(15)	.	.	.	.	no
Zr	C1	C5	C10	121.3(2)	.	.	.	.	no
C2	C1	C5	Zr	65.85(16)	.	.	.	.	no
C2	C1	C5	C4	-1.6(3)	.	.	.	.	no
C2	C1	C5	C10	-172.8(2)	.	.	.	.	no
C6	C1	C5	Zr	-125.8(2)	.	.	.	.	no
C6	C1	C5	C4	166.8(2)	.	.	.	.	no
C6	C1	C5	C10	-4.4(4)	.	.	.	.	no
Zr	C2	C3	C4	71.61(16)	.	.	.	.	no
Zr	C2	C3	C8	-118.0(2)	.	.	.	.	no
C1	C2	C3	Zr	-67.55(16)	.	.	.	.	no
C1	C2	C3	C4	4.1(3)	.	.	.	.	no
C1	C2	C3	C8	174.5(2)	.	.	.	.	no
C7	C2	C3	Zr	122.0(2)	.	.	.	.	no
C7	C2	C3	C4	-166.4(2)	.	.	.	.	no
C7	C2	C3	C8	4.0(4)	.	.	.	.	no

Zr	C3	C4	C5	65.58(16)	.	.	.	.	no
Zr	C3	C4	C9	-129.0(2)	.	.	.	.	no
C2	C3	C4	Zr	-70.67(17)	.	.	.	.	no
C2	C3	C4	C5	-5.1(3)	.	.	.	.	no
C2	C3	C4	C9	160.4(2)	.	.	.	.	no
C8	C3	C4	Zr	119.2(2)	.	.	.	.	no
C8	C3	C4	C5	-175.3(2)	.	.	.	.	no
C8	C3	C4	C9	-9.8(4)	.	.	.	.	no
Zr	C4	C5	C1	67.24(15)	.	.	.	.	no
Zr	C4	C5	C10	-121.7(2)	.	.	.	.	no
C3	C4	C5	Zr	-63.09(16)	.	.	.	.	no
C3	C4	C5	C1	4.2(3)	.	.	.	.	no
C3	C4	C5	C10	175.2(2)	.	.	.	.	no
C9	C4	C5	Zr	131.5(2)	.	.	.	.	no
C9	C4	C5	C1	-161.3(2)	.	.	.	.	no
C9	C4	C5	C10	9.8(4)	.	.	.	.	no
Zr	C11	C12	C13	-66.15(15)	.	.	.	.	no
Zr	C11	C12	C17	130.9(2)	.	.	.	.	no
C15	C11	C12	Zr	66.98(15)	.	.	.	.	no
C15	C11	C12	C13	0.8(2)	.	.	.	.	no
C15	C11	C12	C17	-162.1(2)	.	.	.	.	no
C16	C11	C12	Zr	-125.6(2)	.	.	.	.	no
C16	C11	C12	C13	168.2(2)	.	.	.	.	no
C16	C11	C12	C17	5.3(3)	.	.	.	.	no
Zr	C11	C15	C14	66.18(15)	.	.	.	.	no
Zr	C11	C15	C20	-120.7(3)	.	.	.	.	no
C12	C11	C15	Zr	-66.77(15)	.	.	.	.	no
C12	C11	C15	C14	-0.6(3)	.	.	.	.	no
C12	C11	C15	C20	172.6(2)	.	.	.	.	no
C16	C11	C15	Zr	126.7(2)	.	.	.	.	no
C16	C11	C15	C14	-167.1(2)	.	.	.	.	no
C16	C11	C15	C20	6.1(4)	.	.	.	.	no
Zr	C12	C13	C14	-67.65(15)	.	.	.	.	no
Zr	C12	C13	C18	119.4(2)	.	.	.	.	no
C11	C12	C13	Zr	66.89(15)	.	.	.	.	no
C11	C12	C13	C14	-0.8(2)	.	.	.	.	no
C11	C12	C13	C18	-173.7(2)	.	.	.	.	no
C17	C12	C13	Zr	-131.1(2)	.	.	.	.	no
C17	C12	C13	C14	161.3(2)	.	.	.	.	no
C17	C12	C13	C18	-11.6(4)	.	.	.	.	no
Zr	C13	C14	C15	-67.56(16)	.	.	.	.	no
Zr	C13	C14	C19	125.1(2)	.	.	.	.	no
C12	C13	C14	Zr	67.94(15)	.	.	.	.	no
C12	C13	C14	C15	0.4(3)	.	.	.	.	no
C12	C13	C14	C19	-166.9(2)	.	.	.	.	no
C18	C13	C14	Zr	-118.9(2)	.	.	.	.	no
C18	C13	C14	C15	173.6(2)	.	.	.	.	no
C18	C13	C14	C19	6.3(4)	.	.	.	.	no
Zr	C14	C15	C11	-66.70(15)	.	.	.	.	no
Zr	C14	C15	C20	119.8(2)	.	.	.	.	no
C13	C14	C15	Zr	66.83(16)	.	.	.	.	no
C13	C14	C15	C11	0.1(3)	.	.	.	.	no
C13	C14	C15	C20	-173.4(2)	.	.	.	.	no
C19	C14	C15	Zr	-126.0(2)	.	.	.	.	no
C19	C14	C15	C11	167.3(2)	.	.	.	.	no
C19	C14	C15	C20	-6.2(4)	.	.	.	.	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

Zr	H20	3.5300	.	.	.	.	.	no
Zr	H25	2.7800	.	.	.	.	.	no

Zr	H25'	2.7800	.	.	no
Zr	H25"	2.7800	.	.	no
N	C2	3.141(3)	.	.	no
N	C7	3.356(3)	.	.	no
N	C11	3.291(3)	.	.	no
N	C15	3.126(3)	.	.	no
N	C20	3.361(3)	.	.	no
N	C25	3.220(4)	.	.	no
N	H7'	2.9500	.	.	no
N	H20	2.8800	.	.	no
C1	C3	2.294(3)	.	.	no
C1	C4	2.294(4)	.	.	no
C1	C7	2.603(4)	.	.	no
C1	C10	2.604(4)	.	.	no
C1	C25	3.107(3)	.	.	no
C2	C8	2.601(4)	.	.	no
C2	C23	3.379(4)	.	.	no
C2	C5	2.301(4)	.	.	no
C2	N	3.141(3)	.	.	no
C2	C4	2.305(4)	.	.	no
C2	C6	2.603(4)	.	.	no
C3	C5	2.296(4)	.	.	no
C3	C1	2.294(3)	.	.	no
C3	C7	2.598(4)	.	.	no
C3	C9	2.600(4)	.	.	no
C4	C10	2.598(4)	.	.	no
C4	C8	2.629(4)	.	.	no
C4	C12	3.396(3)	.	.	no
C4	C2	2.305(4)	.	.	no
C4	C1	2.294(4)	.	.	no
C4	C13	3.532(3)	.	.	no
C5	C25	3.198(4)	.	.	no
C5	C2	2.301(4)	.	.	no
C5	C6	2.600(4)	.	.	no
C5	C9	2.583(4)	.	.	no
C5	C3	2.296(4)	.	.	no
C7	C23	3.220(4)	.	.	no
C9	C17	3.275(4)	.	.	no
C9	C18	3.546(4)	.	.	no
C11	C14	2.296(3)	.	.	no
C11	C21	3.394(4)	.	.	no
C11	C13	2.304(3)	.	.	no
C11	C20	2.638(4)	.	.	no
C11	N	3.291(3)	.	.	no
C11	C17	2.569(4)	.	.	no
C12	C4	3.396(3)	.	.	no
C12	C18	2.628(4)	.	.	no
C12	C15	2.296(4)	.	.	no
C12	C9	3.582(4)	.	.	no
C12	C16	2.570(4)	.	.	no
C12	C14	2.292(3)	.	.	no
C13	C11	2.304(3)	.	.	no
C13	C25	3.512(4)	.	.	no
C13	C4	3.532(3)	.	.	no
C13	C17	2.618(3)	.	.	no
C13	C19	2.585(3)	.	.	no
C13	C15	2.300(4)	.	.	no
C14	C18	2.586(4)	.	.	no
C14	C11	2.296(3)	.	.	no
C14	C12	2.292(3)	.	.	no
C14	C25	2.962(3)	.	.	no
C14	C20	2.579(4)	.	.	no
C15	C12	2.296(4)	.	.	no
C15	C13	2.300(4)	.	.	no
C15	C25	3.568(3)	.	.	no
C15	C16	2.634(4)	.	.	no

C15	C21	3.412(4)	.	.	no
C15	N	3.126(3)	.	.	no
C15	C19	2.596(4)	.	.	no
C16	C21	3.335(4)	.	.	no
C17	C9	3.275(4)	.	.	no
C18	C9	3.546(4)	.	.	no
C19	C25	3.068(4)	.	.	no
C20	C21	3.274(4)	.	.	no
C20	N	3.361(3)	.	.	no
C21	C20	3.274(4)	.	.	no
C21	C16	3.335(4)	.	.	no
C23	C7	3.220(4)	.	.	no
C24	C25	3.579(4)	.	.	no
C25	C13	3.512(4)	.	.	no
C25	C1	3.107(3)	.	.	no
C25	C5	3.198(4)	.	.	no
C25	C6	3.364(3)	.	.	no
C25	C19	3.068(4)	.	.	no
C25	C23	3.361(4)	.	.	no
C25	N	3.220(4)	.	.	no
C25	C15	3.568(3)	.	.	no
C25	C14	2.962(3)	.	.	no
C25	C10	3.470(4)	.	.	no
C25	C24	3.579(4)	.	.	no
C1	H25"	2.7900	.	.	no
C1	H17"	2.7800	.	2_655	no
C1	H23	2.8400	.	.	no
C2	H23	2.8600	.	.	no
C5	H17"	2.9200	.	2_655	no
C6	H7"	2.8000	.	.	no
C6	H10'	3.0400	.	.	no
C6	H25"	2.6400	.	.	no
C6	H23	2.8100	.	.	no
C7	H6	2.8900	.	.	no
C7	H8	2.7000	.	.	no
C7	H23	2.8500	.	.	no
C7	H23'	2.9900	.	.	no
C8	H17	2.9300	.	.	no
C8	H18	2.9400	.	2_655	no
C8	H7'	3.0200	.	.	no
C8	H19'	3.0600	.	4_555	no
C8	H9'	2.8400	.	.	no
C9	H10"	2.8100	.	.	no
C9	H22"	3.0500	.	1_655	no
C9	H17'	2.7600	.	.	no
C9	H18'	2.9700	.	.	no
C9	H8'	2.9700	.	.	no
C10	H25'	2.9700	.	.	no
C10	H18"	2.9500	.	.	no
C10	H9	2.9500	.	.	no
C10	H6'	2.8900	.	.	no
C11	H9"	2.8000	.	2_645	no
C11	H21	2.7000	.	.	no
C14	H25	2.8300	.	.	no
C14	H25'	3.0000	.	.	no
C15	H9"	2.8000	.	2_645	no
C15	H21	2.7700	.	.	no
C16	H9"	3.0200	.	2_645	no
C16	H6'	2.8800	.	4_555	no
C16	H17	3.0000	.	.	no
C16	H17"	3.0000	.	.	no
C16	H21	2.5200	.	.	no
C16	H20'	2.8900	.	.	no
C17	H18'	2.8500	.	.	no
C17	H16	2.8100	.	.	no
C17	H9'	2.6400	.	.	no

C17	H8"	3.0400	.	.	no
C18	H9	2.7900	.	.	no
C18	H17'	2.8500	.	.	no
C18	H19'	2.8000	.	.	no
C18	H21'	3.0700	.	1_655	no
C19	H20"	2.8900	.	.	no
C19	H18	3.0400	.	3_655	no
C19	H18	2.9900	.	.	no
C19	H25	2.6600	.	.	no
C19	H25'	2.8800	.	.	no
C20	H19"	3.0700	.	3_555	no
C20	H21	2.6100	.	.	no
C20	H19"	2.8500	.	.	no
C20	H16'	2.8800	.	.	no
C21	H24"	2.8400	.	.	no
C21	H16"	3.0700	.	.	no
C21	H20'	3.0600	.	.	no
C21	H16'	3.0800	.	.	no
C21	H20	2.9400	.	.	no
C22	H7'	2.8300	.	.	no
C22	H23'	2.8500	.	.	no
C22	H16"	3.0600	.	.	no
C22	H9	3.0400	.	1_455	no
C23	H22"	2.9700	.	.	no
C23	H7'	3.0000	.	.	no
C23	H25"	3.0900	.	.	no
C23	H7"	2.8800	.	.	no
C24	H21'	2.6900	.	.	no
C25	H6'	2.9100	.	.	no
C25	H10'	2.8700	.	.	no
C25	H19'	2.9000	.	.	no
C25	H19"	2.8700	.	.	no
C25	H23	2.9500	.	.	no
C25	H24	2.9100	.	.	no
H6	C7	2.8900	.	.	no
H6	H7"	2.2500	.	.	no
H6	H23	2.1900	.	.	no
H6	H6	2.2300	.	3_565	no
H6'	C10	2.8900	.	.	no
H6'	C25	2.9100	.	.	no
H6'	H10'	2.4900	.	.	no
H6'	H25"	2.1400	.	.	no
H6'	C16	2.8800	.	4_554	no
H6"	H17"	2.5500	.	2_655	no
H6"	H24'	2.5900	.	3_565	no
H7'	N	2.9500	.	.	no
H7'	C8	3.0200	.	.	no
H7'	C22	2.8300	.	.	no
H7'	C23	3.0000	.	.	no
H7'	H8	2.4300	.	.	no
H7'	H22	2.5800	.	.	no
H7'	H22"	2.3500	.	.	no
H7"	C6	2.8000	.	.	no
H7"	C23	2.8800	.	.	no
H7"	H6	2.2500	.	.	no
H7"	H23	2.3800	.	.	no
H8	C7	2.7000	.	.	no
H8	H7'	2.4300	.	.	no
H8	H18	2.5600	.	2_655	no
H8'	C9	2.9700	.	.	no
H8'	H9'	2.5100	.	.	no
H8'	H18	2.5400	.	2_655	no
H8'	H19	2.5100	.	2_655	no
H8"	C17	3.0400	.	.	no
H8"	H17	2.1900	.	.	no
H9	C10	2.9500	.	.	no

H9	C18	2.7900	.	.	no
H9	C22	3.0400	.	1_655	no
H9	H10"	2.3300	.	.	no
H9	H17'	2.5800	.	.	no
H9	H18'	2.1600	.	.	no
H9	H22"	2.5600	.	1_655	no
H9'	C8	2.8400	.	.	no
H9'	C17	2.6400	.	.	no
H9'	H8'	2.5100	.	.	no
H9'	H17	2.3600	.	.	no
H9'	H17'	2.1900	.	.	no
H9"	C11	2.8000	.	2_655	no
H9"	C15	2.8000	.	2_655	no
H9"	C16	3.0200	.	2_655	no
H10	H16	2.4700	.	2_655	no
H10	H10	2.3700	.	3_665	no
H10'	C6	3.0400	.	.	no
H10'	C25	2.8700	.	.	no
H10'	H6'	2.4900	.	.	no
H10'	H25'	2.2500	.	.	no
H10"	C9	2.8100	.	.	no
H10"	H9	2.3300	.	.	no
H10"	H18"	2.3400	.	.	no
H16	C17	2.8100	.	.	no
H16	H17"	2.4700	.	.	no
H16	H10	2.4700	.	2_645	no
H16'	C20	2.8800	.	.	no
H16'	C21	3.0800	.	.	no
H16'	H20'	2.2400	.	.	no
H16'	H21	2.1400	.	.	no
H16"	C21	3.0700	.	.	no
H16"	C22	3.0600	.	.	no
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H16"	H22	2.4800	.	.	no
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H17	C16	3.0000	.	.	no
H17	H8"	2.1900	.	.	no
H17	H9'	2.3600	.	.	no
H17'	C9	2.7600	.	.	no
H17'	C18	2.8500	.	.	no
H17'	H9	2.5800	.	.	no
H17'	H9'	2.1900	.	.	no
H17'	H18'	2.2000	.	.	no
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H18	C19	2.9900	.	.	no
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H18	H8	2.5600	.	2_645	no
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H18	C19	3.0400	.	3_655	no
H18'	C9	2.9700	.	.	no
H18'	C17	2.8500	.	.	no
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H18'	H17'	2.2000	.	.	no
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H19"	C20	2.8500	.	.	no

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H20"	H19"	2.5900	.	.	no
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H21	C16	2.5200	.	.	no
H21	C20	2.6100	.	.	no
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H21	H20	2.5400	.	.	no
H21	H20'	2.2300	.	.	no
H21'	C18	3.0700	.	1_455	no
H21'	C24	2.6900	.	.	no
H21'	H18'	2.4600	.	1_455	no
H21'	H23'	2.4200	.	.	no
H21'	H24"	2.1500	.	.	no
H22	H7'	2.5800	.	.	no
H22	H16"	2.4800	.	.	no
H22"	C9	3.0500	.	1_455	no
H22"	C23	2.9700	.	.	no
H22"	H7'	2.3500	.	.	no
H22"	H9	2.5600	.	1_455	no
H22"	H23'	2.3400	.	.	no
H23	C1	2.8400	.	.	no
H23	C2	2.8600	.	.	no
H23	C6	2.8100	.	.	no
H23	C7	2.8500	.	.	no
H23	C25	2.9500	.	.	no
H23	H6	2.1900	.	.	no
H23	H7"	2.3800	.	.	no
H23	H25"	2.4700	.	.	no
H23'	C7	2.9900	.	.	no
H23'	C22	2.8500	.	.	no
H23'	H21'	2.4200	.	.	no
H23'	H22"	2.3400	.	.	no
H24	C25	2.9100	.	.	no
H24	H25	2.4100	.	.	no
H24'	H6"	2.5900	.	3_565	no
H24"	C21	2.8400	.	.	no
H24"	H21'	2.1500	.	.	no
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H25	C19	2.6600	.	.	no
H25	H19"	2.1900	.	.	no
H25	H24	2.4100	.	.	no
H25'	Zr	2.7800	.	.	no
H25'	C10	2.9700	.	.	no
H25'	C14	3.0000	.	.	no
H25'	C19	2.8800	.	.	no
H25'	H10'	2.2500	.	.	no
H25'	H19'	2.4100	.	.	no
H25"	Zr	2.7800	.	.	no
H25"	C1	2.7900	.	.	no

H25"	C6	2.6400	.	.	no
H25"	C23	3.0900	.	.	no
H25"	H6'	2.1400	.	.	no
H25"	H23	2.4700	.	.	no

====END of Crystallographic Information File

CIF-file generated for C48H57BOZr P-1 q1560

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SHELXL97-2 & Manual Editing

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2010-06-04 # Formatted by publCIF

;

1. SUBMISSION DETAILS

_publ_contact_author_name # Name of author for correspondence

;

Drs. A. Meetsma

;

_publ_contact_author_address # Address of author for correspondence

;

Crystal Structure Center, Chemical Physics,
Zernike Institute for Advanced Materials,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen, The Netherlands.

;

_publ_contact_author_email A.Meetsma@rug.nl

_publ_contact_author_fax '+31 50 3634441'

_publ_contact_author_phone '+31 50 3634368'

_publ_requested_journal 'J. Am. Chem. Soc'

Publication choice FI, CI or EI for Inorganic

FM, CM or EM for Metal-organic

FO, CO or EO for Organic

_publ_requested_category ?

_publ_requested_coeditor_name ?

_publ_contact_letter # Include date of submission

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Date of submission : 2010-06-04 14:14:23

Consider this CIF submission for deposition of the third
X-ray structure of a manuscript to be submitted to : J. Am. Chem. Soc
(Our Compound_Identification_Code : q1560)

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2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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3. TITLE AND AUTHOR LIST

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Title (type here to add)?
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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_footnote
_publ_author_address
'?' # author name
;   # author related footnote
;
;   # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote
;
;
Crystal Structure Center, Chemical Physics,

```

Zernike Institute for Advanced Materials,
University of Groningen,
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_prep

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?

;

_publ_section_exptl_refinement

;

?

The final difference Fourier map was essentially featureless:

no significant peaks (0.56(10) e/ $\text{\AA}^3$) having chemical meaning above the
general background were observed, except one peak of 3.34 e/ $\text{\AA}^3$
located near the Zr position.

The hydrogen atoms were generated by geometrical considerations, constrained to
idealized geometries, and allowed to ride on the carrier atom with an
isotropic displacement parameter related to the equivalent displacement
parameter of their carrier atoms, with $U^{\text{iso}}(\text{H}) = 1.2 U^{\text{eq}}(\text{C})$
or $1.5 U^{\text{eq}}(\text{methyl C})$. The methyl-groups were refined as rigid groups,
which were allowed to rotate freely. Assigned values of bond distances for
secondary C---H₂ = 0.99 $\text{\AA}$ and methyl C---H₃ = 0.98 $\text{\AA}$

;

_publ_section_related_literature

;

;

Insert blank lines between references

_publ_section_references

;

?Beurskens, P. T., Beurskens, G., de Gelder, R., Smits, J. M. M.,
Garc'ia-Granda, S. & Gould, R. O. (2008). The *DIRDIF08* program system,
Technical Report of the Crystallography Laboratory, University of Nijmegen,
The Netherlands.

Bruker, (2007). *SMART* (Version 5.632), *SAINT-Plus* (Version 7.46a)
and *SADABS* (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Meetsma, A. (2009). Extended version of the program *PLUTO*. University of
Groningen, The Netherlands. (unpublished).

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112--122.

Spek, A. L. (2003). <i>J. Appl. Cryst.</i> **36**, 7--13.

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_publ_section_figure_captions

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Fig. 1. Perspective <i>PLUTO</i> drawings of the ions illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective <i>ORTEP</i> drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

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_publ_section_acknowledgements

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5. CHEMICAL DATA

_chemical_name_systematic

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;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C24 H37 O Zr, C24 H20 B'

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

_chemical_formula_structural ?

_chemical_formula_sum

' C48 H57 B O Zr'

_chemical_formula_iupac ?

_chemical_formula_weight 752.01

_chemical_compound_source 'see text'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

Zr Zr -2.9673 0.5597

'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'

B B 0.0013 0.0007

'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'

C C 0.0033 0.0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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6. CRYSTAL DATA

_symmetry_cell_setting triclinic

_symmetry_space_group_name_Hall '-P 1'


```

_symmetry_space_group_name_H-M      'P -1'
_symmetry_Int_Tables_number          2

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
  1  x,y,z
  2 -x,-y,-z

_cell_length_a                      10.4210(11)
_cell_length_b                      11.5754(12)
_cell_length_c                      16.7801(17)
_cell_angle_alpha                   94.799(1)
_cell_angle_beta                    104.394(1)
_cell_angle_gamma                   92.759(1)
_cell_volume                        1948.7(3)
_cell_formula_units_Z                2

_cell_measurement_temperature        100(1)
_cell_measurement_reflns_used        4125
_cell_measurement_theta_min          2.52
_cell_measurement_theta_max          26.93
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
4125 reflections after integration using the SAINTPLUS
software package (Bruker, 2007).

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)
;

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_exptl_crystal_size_min              0.21
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_exptl_crystal_density_meas          ?
_exptl_crystal_density_diffrn        1.283
_exptl_crystal_density_method        'not measured'
_exptl_crystal_F_000                 798
_exptl_absorpt_coefficient_mu         0.318
_exptl_absorpt_correction_type        'multi-scan'
_exptl_absorpt_process_details        '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min       0.8678
_exptl_absorpt_correction_T_max       0.9354

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# 7. EXPERIMENTAL DATA

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_diffrn_radiation_wavelength          0.71073
_diffrn_radiation_type                'MoK\alpha'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator        'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type

```

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;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method      '\f and \w scans'
_diffrn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2007)).
;
_diffrn_detector_area_resol_mean    66.06

_diffrn_standards_number           0
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_diffrn_standards_interval_time    .
_diffrn_standards_decay_%          0

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_av_R_equivalents    0.0354
_diffrn_reflns_av_sigmaI/netI     0.0641
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_diffrn_reflns_limit_k_max         14
_diffrn_reflns_limit_l_min         -21
_diffrn_reflns_limit_l_max         21
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_diffrn_reflns_theta_max           26.73
_diffrn_measured_fraction_theta_max 0.972
_diffrn_reflns_theta_full          25.00
_diffrn_measured_fraction_theta_full 0.982

_diffrn_reflns_reduction_process
;
  Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to  $F_o^2$ 
  using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
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_reflns_number_gt                 6341
_reflns_threshold_expression       I>2\sigma(I)

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_computing_cell_refinement         'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction          'SAINT-Plus'
_computing_structure_solution
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  DIRDIF-08 (Beurskens et al., 2008)
;
_computing_structure_refinement    'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
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  PLATON (Spek, 2003)
  PLUTO (Meetsma, 2009)
;
_computing_publication_material    'PLATON (Spek, 2003)'

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8. REFINEMENT DATA

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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 $F^2 > 2\sigma(F^2)$ 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

_refine_ls_weighting_details

'calc w=1/[\s^2(Fo^2)+(0.0684P)^2+2.1474P] where P=(Fo^2+2Fc^2)/3'

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_atom_sites_solution_secondary direct

_atom_sites_solution_hydrogens geom

_refine_ls_hydrogen_treatment constr

_refine_ls_extinction_method none

_refine_ls_extinction_coef ?

_refine_ls_abs_structure_details ?

_chemical_absolute_configuration '.'

_refine_ls_abs_structure_Flack ?

_refine_ls_number_reflns 8049

_refine_ls_number_parameters 469

_refine_ls_number_restraints 0

_refine_ls_number_constraints ?

_refine_ls_R_factor_all 0.0753

_refine_ls_R_factor_gt 0.0568

_refine_ls_wR_factor_ref 0.1416

_refine_ls_wR_factor_gt 0.1314

_refine_ls_goodness_of_fit_ref 1.043

_refine_ls_restrained_S_all 1.043

_refine_ls_shift/su_max 0.000

_refine_ls_shift/su_mean 0.000

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_refine_diff_density_rms 0.095

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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

_atom_site_U_iso_or_equiv

_atom_site_calc_flag

_atom_site_refinement_flags

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C11 C Uani 0.2986(4) 0.2276(3) 0.05567(19) 1.0 0.0219(10) . .
C12 C Uani 0.4183(3) 0.2119(3) 0.1153(2) 1.0 0.0211(10) . .
C13 C Uani 0.4479(3) 0.3123(3) 0.1738(2) 1.0 0.0214(10) . .
C14 C Uani 0.3447(3) 0.3884(3) 0.1522(2) 1.0 0.0201(10) . .
C15 C Uani 0.2538(4) 0.3378(3) 0.0773(2) 1.0 0.0222(10) . .
C16 C Uani 0.2431(4) 0.1471(3) -0.0220(2) 1.0 0.0291(11) . .
C17 C Uani 0.5054(4) 0.1127(3) 0.1104(2) 1.0 0.0271(11) . .
C18 C Uani 0.5735(4) 0.3398(3) 0.2417(2) 1.0 0.0284(12) . .
C19 C Uani 0.3390(4) 0.5052(3) 0.1967(2) 1.0 0.0314(11) . .
C110 C Uani 0.1501(4) 0.4036(3) 0.0236(2) 1.0 0.0281(11) . .
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C115 C Uani 0.0361(3) 0.1106(3) 0.1709(2) 1.0 0.0229(10) . .
C116 C Uani 0.1194(4) 0.0506(3) 0.3203(2) 1.0 0.0221(10) . .
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C119 C Uani -0.0839(4) 0.2218(3) 0.0475(2) 1.0 0.0323(12) . .
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C122 C Uani 0.4765(4) 0.0441(3) 0.3983(2) 1.0 0.0326(12) . .
C123 C Uani 0.5026(4) 0.1678(4) 0.4424(2) 1.0 0.0404(15) . .
C124 C Uani 0.4093(4) 0.2392(3) 0.3866(2) 1.0 0.0310(11) . .

H16 H Uiso 0.28833 0.16634 -0.06433 1.0 0.0435 . .
H16' H Uiso 0.14775 0.156 -0.04213 1.000 0.0435 . .
H16'' H Uiso 0.25701 0.06656 -0.00996 1.0 0.0435 . .
H17 H Uiso 0.45240 0.03876 0.10425 1.0 0.0404 . .
H17' H Uiso 0.57744 0.11751 0.16110 1.0 0.0404 . .
H17'' H Uiso 0.54318 0.11740 0.06269 1.0 0.0404 . .
H18 H Uiso 0.64648 0.36239 0.21769 1.0 0.0429 . .
H18' H Uiso 0.59513 0.27102 0.27137 1.0 0.0429 . .
H18'' H Uiso 0.56056 0.40394 0.28029 1.0 0.0429 . .
H19 H Uiso 0.35305 0.49778 0.25599 1.0 0.0470 . .
H19' H Uiso 0.25180 0.53472 0.17526 1.0 0.0470 . .
H19'' H Uiso 0.40841 0.55924 0.18807 1.0 0.0470 . .
H110 H Uiso 0.09818 0.44310 0.05757 1.0 0.0422 . .
H110' H Uiso 0.09093 0.34915 -0.01930 1.0 0.0422 . .
H110'' H Uiso 0.19356 0.46121 -0.00250 1.0 0.0422 . .
H116 H Uiso 0.17432 0.09032 0.37229 1.0 0.0333 . .
H116' H Uiso 0.17097 -0.00639 0.29769 1.0 0.0333 . .
H116'' H Uiso 0.04076 0.01074 0.33045 1.0 0.0333 . .
H117 H Uiso 0.11330 0.27320 0.40444 1.0 0.0386 . .
H117' H Uiso -0.00483 0.35088 0.36513 1.0 0.0386 . .
H117'' H Uiso 0.14524 0.39116 0.36746 1.0 0.0386 . .
H118 H Uiso -0.10540 0.43638 0.22014 1.0 0.0432 . .
H118' H Uiso -0.05119 0.44623 0.13953 1.0 0.0432 . .
H118'' H Uiso 0.04492 0.48374 0.22935 1.0 0.0432 . .
H119 H Uiso -0.17279 0.18316 0.03861 1.0 0.0485 . .
H119' H Uiso -0.03688 0.18219 0.01052 1.0 0.0485 . .
H119'' H Uiso -0.09158 0.30305 0.03587 1.0 0.0485 . .
H120 H Uiso 0.08534 0.02298 0.06910 1.0 0.0327 . .
H120' H Uiso 0.14354 -0.03530 0.15690 1.0 0.0327 . .
H121 H Uiso 0.52820 0.07474 0.28955 1.0 0.0296 . .
H121' H Uiso 0.38806 0.00002 0.27328 1.0 0.0296 . .
H122 H Uiso 0.55582 -0.00104 0.41362 1.0 0.0390 . .
H122' H Uiso 0.40038 0.00223 0.41140 1.0 0.0390 . .
H123 H Uiso 0.48365 0.16989 0.49742 1.0 0.0483 . .
H123' H Uiso 0.59606 0.19681 0.44942 1.0 0.0483 . .
H124 H Uiso 0.32819 0.24982 0.40617 1.0 0.0373 . .

H124' H Uiso 0.45266 0.31663 0.38481 1.0 0.0373 . .

C21 C Uani 0.2425(3) 0.3439(3) 0.63778(18) 1.0 0.0182(9) . .
C22 C Uani 0.1616(3) 0.4329(3) 0.60934(19) 1.0 0.0204(10) . .
C23 C Uani 0.1937(4) 0.5130(3) 0.5584(2) 1.0 0.0260(11) . .
C24 C Uani 0.3119(4) 0.5083(3) 0.5353(2) 1.0 0.0271(11) . .
C25 C Uani 0.3967(4) 0.4234(3) 0.5640(2) 1.0 0.0294(11) . .
C26 C Uani 0.3618(4) 0.3435(3) 0.6136(2) 1.0 0.0238(11) . .
C27 C Uani 0.2084(3) 0.1134(3) 0.65687(19) 1.0 0.0175(9) . .
C28 C Uani 0.1855(3) 0.0834(3) 0.5715(2) 1.0 0.0201(10) . .
C29 C Uani 0.1684(4) -0.0323(3) 0.5372(2) 1.0 0.0252(11) . .
C210 C Uani 0.1750(3) -0.1220(3) 0.5872(2) 1.0 0.0234(10) . .
C211 C Uani 0.1982(3) -0.0955(3) 0.6722(2) 1.0 0.0217(10) . .
C212 C Uani 0.2135(3) 0.0199(3) 0.7054(2) 1.0 0.0195(10) . .
C213 C Uani 0.3264(3) 0.2726(3) 0.78537(19) 1.0 0.0182(9) . .
C214 C Uani 0.4380(3) 0.2075(3) 0.8064(2) 1.0 0.0211(10) . .
C215 C Uani 0.5370(4) 0.2308(3) 0.8798(2) 1.0 0.0250(11) . .
C216 C Uani 0.5278(4) 0.3224(3) 0.9369(2) 1.0 0.0295(11) . .
C217 C Uani 0.4206(4) 0.3910(3) 0.9177(2) 1.0 0.0284(11) . .
C218 C Uani 0.3243(3) 0.3671(3) 0.8440(2) 1.0 0.0220(10) . .
C219 C Uani 0.0575(3) 0.2559(3) 0.71064(18) 1.0 0.0149(9) . .
C220 C Uani 0.0222(3) 0.2571(3) 0.78661(19) 1.0 0.0173(9) . .
C221 C Uani -0.1080(3) 0.2577(3) 0.7928(2) 1.0 0.0204(10) . .
C222 C Uani -0.2120(3) 0.2557(3) 0.7223(2) 1.0 0.0209(10) . .
C223 C Uani -0.1823(3) 0.2524(3) 0.6457(2) 1.0 0.0220(10) . .
C224 C Uani -0.0511(3) 0.2516(3) 0.64097(19) 1.0 0.0195(10) . .
B2 B Uani 0.2095(4) 0.2481(3) 0.6986(2) 1.0 0.0162(10) . .

H22 H Uiso 0.08089 0.43891 0.62556 1.0 0.0245 . .
H23 H Uiso 0.13445 0.57059 0.53971 1.0 0.0311 . .
H24 H Uiso 0.33462 0.56203 0.50040 1.0 0.0325 . .
H25 H Uiso 0.47921 0.42013 0.54969 1.0 0.0349 . .
H26 H Uiso 0.42139 0.28597 0.63182 1.0 0.0286 . .
H28 H Uiso 0.18155 0.14352 0.53593 1.0 0.0240 . .
H29 H Uiso 0.15197 -0.04941 0.47908 1.0 0.0302 . .
H210 H Uiso 0.16391 -0.20055 0.56382 1.0 0.0281 . .
H211 H Uiso 0.20346 -0.15610 0.70747 1.0 0.0260 . .
H212 H Uiso 0.22816 0.03618 0.76350 1.0 0.0234 . .
H214 H Uiso 0.44633 0.14413 0.76863 1.0 0.0253 . .
H215 H Uiso 0.61080 0.18415 0.89094 1.0 0.0301 . .
H216 H Uiso 0.59346 0.33770 0.98780 1.0 0.0353 . .
H217 H Uiso 0.41336 0.45465 0.95557 1.0 0.0340 . .
H218 H Uiso 0.25323 0.41659 0.83215 1.0 0.0264 . .
H220 H Uiso 0.09101 0.25758 0.83593 1.0 0.0208 . .
H221 H Uiso -0.12617 0.25939 0.84555 1.0 0.0243 . .
H222 H Uiso -0.30135 0.25652 0.72623 1.0 0.0251 . .
H223 H Uiso -0.25175 0.25077 0.59664 1.0 0.0263 . .
H224 H Uiso -0.03392 0.24788 0.58785 1.0 0.0234 . .

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

Zr1 0.0194(2) 0.0214(2) 0.0164(2) 0.0032(1) 0.0046(1) 0.0038(1)

O1 0.0200(13) 0.0222(12) 0.0183(11) 0.0026(9) 0.0022(9) 0.0039(10)

C11 0.030(2) 0.0227(18) 0.0166(15) 0.0046(13) 0.0112(14) 0.0065(15)

C12 0.024(2) 0.0212(18) 0.0233(16) 0.0048(13) 0.0141(14) 0.0060(14)

C13 0.025(2) 0.0169(17) 0.0248(16) 0.0016(13) 0.0115(14) 0.0000(14)

C14 0.0247(19) 0.0125(16) 0.0256(16) 0.0019(13) 0.0120(14) -0.0024(14)

C15 0.028(2) 0.0191(17) 0.0224(16) 0.0061(13) 0.0097(15) 0.0057(15)
 C16 0.039(2) 0.029(2) 0.0194(16) 0.0026(14) 0.0065(16) 0.0080(17)
 C17 0.034(2) 0.0221(19) 0.0292(18) 0.0046(14) 0.0135(16) 0.0107(16)
 C18 0.025(2) 0.025(2) 0.035(2) 0.0022(15) 0.0079(16) -0.0010(16)
 C19 0.035(2) 0.0213(19) 0.041(2) 0.0010(16) 0.0155(18) 0.0045(16)
 C110 0.033(2) 0.029(2) 0.0264(18) 0.0115(15) 0.0113(16) 0.0094(17)
 C111 0.0188(18) 0.0181(17) 0.0252(16) 0.0052(13) 0.0070(14) 0.0032(14)
 C112 0.0170(18) 0.0218(18) 0.0260(17) 0.0058(14) 0.0099(14) 0.0033(14)
 C113 0.0134(18) 0.0262(19) 0.0295(18) 0.0060(14) 0.0080(14) 0.0047(14)
 C114 0.0181(19) 0.0229(18) 0.0267(17) 0.0056(14) 0.0022(14) 0.0023(14)
 C115 0.0221(19) 0.0170(17) 0.0273(17) 0.0016(13) 0.0025(14) -0.0004(14)
 C116 0.023(2) 0.0180(17) 0.0288(17) 0.0089(14) 0.0106(15) 0.0033(14)
 C117 0.035(2) 0.0194(18) 0.0275(18) 0.0025(14) 0.0148(16) 0.0070(16)
 C118 0.031(2) 0.025(2) 0.0345(19) 0.0084(15) 0.0121(17) 0.0108(16)
 C119 0.027(2) 0.033(2) 0.032(2) 0.0056(16) -0.0026(16) 0.0016(17)
 C120 0.038(2) 0.0186(18) 0.0242(17) -0.0006(14) 0.0061(16) 0.0031(16)
 C121 0.0200(19) 0.0260(19) 0.0279(18) 0.0021(14) 0.0046(15) 0.0090(15)
 C122 0.026(2) 0.040(2) 0.035(2) 0.0170(17) 0.0073(16) 0.0143(17)
 C123 0.042(3) 0.056(3) 0.0209(18) 0.0000(18) 0.0015(17) 0.021(2)
 C124 0.043(2) 0.027(2) 0.0183(16) -0.0007(14) 0.0006(16) 0.0002(17)
 C21 0.0211(18) 0.0161(16) 0.0160(14) -0.0060(12) 0.0052(13) -0.0032(13)
 C22 0.0239(19) 0.0154(17) 0.0236(16) -0.0004(13) 0.0103(14) -0.0015(14)
 C23 0.036(2) 0.0201(18) 0.0240(17) 0.0019(14) 0.0119(16) -0.0003(16)
 C24 0.039(2) 0.0189(18) 0.0254(17) 0.0001(14) 0.0142(16) -0.0051(16)
 C25 0.027(2) 0.032(2) 0.0328(19) -0.0027(16) 0.0180(16) -0.0071(16)
 C26 0.022(2) 0.0226(18) 0.0267(17) -0.0019(14) 0.0074(14) 0.0011(15)
 C27 0.0119(17) 0.0191(17) 0.0207(15) -0.0035(12) 0.0047(13) 0.0000(13)
 C28 0.0203(19) 0.0165(17) 0.0227(16) 0.0018(13) 0.0042(14) 0.0015(14)
 C29 0.028(2) 0.0227(19) 0.0219(16) -0.0079(14) 0.0040(14) 0.0021(15)
 C210 0.0196(19) 0.0168(17) 0.0324(18) -0.0064(14) 0.0070(15) 0.0003(14)
 C211 0.0139(18) 0.0180(17) 0.0327(18) 0.0015(14) 0.0054(14) 0.0016(14)
 C212 0.0132(17) 0.0222(18) 0.0213(16) -0.0013(13) 0.0025(13) -0.0001(13)
 C213 0.0169(18) 0.0167(16) 0.0204(15) -0.0006(12) 0.0051(13) -0.0035(13)
 C214 0.0214(19) 0.0140(16) 0.0269(17) -0.0030(13) 0.0069(14) -0.0032(14)
 C215 0.0190(19) 0.0192(18) 0.0347(19) 0.0027(14) 0.0024(15) 0.0028(14)
 C216 0.027(2) 0.028(2) 0.0280(18) -0.0021(15) -0.0007(16) -0.0035(16)
 C217 0.026(2) 0.0242(19) 0.0286(18) -0.0098(15) -0.0002(15) -0.0024(16)
 C218 0.0179(18) 0.0189(18) 0.0272(17) -0.0016(14) 0.0031(14) 0.0032(14)
 C219 0.0196(18) 0.0058(14) 0.0191(15) -0.0001(11) 0.0050(13) -0.0005(12)
 C220 0.0205(18) 0.0124(16) 0.0186(15) 0.0021(12) 0.0039(13) 0.0020(13)
 C221 0.027(2) 0.0138(16) 0.0233(16) -0.0005(12) 0.0126(14) 0.0007(14)
 C222 0.0164(18) 0.0141(16) 0.0339(18) -0.0002(13) 0.0099(15) 0.0025(13)
 C223 0.0184(19) 0.0169(17) 0.0257(17) -0.0024(13) -0.0015(14) -0.0014(14)
 C224 0.0254(19) 0.0151(16) 0.0176(15) -0.0008(12) 0.0054(14) 0.0015(14)
 B2 0.018(2) 0.0132(18) 0.0162(16) -0.0037(13) 0.0036(14) 0.0011(14)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's 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

Zr1	O1	2.224(2)	.	.	yes
Zr1	C11	2.515(3)	.	.	yes
Zr1	C12	2.539(3)	.	.	yes
Zr1	C13	2.543(3)	.	.	yes
Zr1	C14	2.485(3)	.	.	yes
Zr1	C15	2.503(3)	.	.	yes
Zr1	C111	2.410(3)	.	.	yes
Zr1	C112	2.599(3)	.	.	yes
Zr1	C113	2.618(3)	.	.	yes
Zr1	C114	2.447(3)	.	.	yes
Zr1	C115	2.265(3)	.	.	yes
Zr1	C120	2.366(4)	.	.	yes
O1	C121	1.473(4)	.	.	yes
O1	C124	1.474(4)	.	.	yes
C11	C12	1.422(5)	.	.	no
C11	C15	1.429(5)	.	.	no
C11	C16	1.507(5)	.	.	no
C12	C13	1.426(5)	.	.	no
C12	C17	1.507(5)	.	.	no
C13	C14	1.419(5)	.	.	no
C13	C18	1.507(5)	.	.	no
C14	C15	1.432(5)	.	.	no
C14	C19	1.500(5)	.	.	no
C15	C110	1.507(5)	.	.	no
C111	C112	1.412(5)	.	.	no
C111	C115	1.446(5)	.	.	no
C111	C116	1.499(5)	.	.	no
C112	C113	1.427(5)	.	.	no
C112	C117	1.505(5)	.	.	no
C113	C114	1.421(5)	.	.	no
C113	C118	1.499(5)	.	.	no
C114	C115	1.448(5)	.	.	no
C114	C119	1.514(5)	.	.	no
C115	C120	1.457(5)	.	.	no
C16	H16	0.98	.	.	no
C16	H16'	0.98	.	.	no
C16	H16"	0.98	.	.	no
C17	H17'	0.98	.	.	no
C17	H17"	0.98	.	.	no
C17	H17	0.98	.	.	no
C18	H18	0.98	.	.	no
C18	H18'	0.98	.	.	no
C18	H18"	0.98	.	.	no
C19	H19	0.98	.	.	no
C19	H19"	0.98	.	.	no
C19	H19'	0.98	.	.	no
C121	C122	1.509(5)	.	.	no
C122	C123	1.535(6)	.	.	no
C123	C124	1.503(5)	.	.	no
C110	H110'	0.98	.	.	no
C110	H110"	0.98	.	.	no
C110	H110	0.98	.	.	no
C116	H116'	0.98	.	.	no
C116	H116"	0.98	.	.	no
C116	H116	0.98	.	.	no
C117	H117'	0.98	.	.	no
C117	H117"	0.98	.	.	no
C117	H117	0.98	.	.	no
C118	H118'	0.98	.	.	no
C118	H118"	0.98	.	.	no
C118	H118	0.98	.	.	no
C119	H119'	0.98	.	.	no
C119	H119"	0.98	.	.	no
C119	H119	0.98	.	.	no
C120	H120'	0.99	.	.	no
C120	H120	0.99	.	.	no

C121	H121'	0.99	.	.	no
C121	H121	0.99	.	.	no
C21	C26	1.401(5)	.	.	no
C21	B2	1.648(5)	.	.	yes
C21	C22	1.402(5)	.	.	no
C22	C23	1.395(5)	.	.	no
C122	H122'	0.99	.	.	no
C122	H122	0.99	.	.	no
C123	H123	0.99	.	.	no
C23	C24	1.382(6)	.	.	no
C123	H123'	0.99	.	.	no
C124	H124	0.99	.	.	no
C124	H124'	0.99	.	.	no
C24	C25	1.389(5)	.	.	no
C25	C26	1.388(5)	.	.	no
C27	C28	1.403(4)	.	.	no
C27	B2	1.653(5)	.	.	yes
C27	C212	1.403(5)	.	.	no
C28	C29	1.398(5)	.	.	no
C29	C210	1.382(5)	.	.	no
C22	H22	0.95	.	.	no
C23	H23	0.95	.	.	no
C24	H24	0.95	.	.	no
C25	H25	0.95	.	.	no
C26	H26	0.95	.	.	no
C28	H28	0.95	.	.	no
C29	H29	0.95	.	.	no
C210	C211	1.391(5)	.	.	no
C211	C212	1.390(5)	.	.	no
C213	C218	1.414(5)	.	.	no
C213	C214	1.404(5)	.	.	no
C213	B2	1.643(5)	.	.	yes
C214	C215	1.393(5)	.	.	no
C215	C216	1.392(5)	.	.	no
C216	C217	1.390(6)	.	.	no
C217	C218	1.383(5)	.	.	no
C219	C220	1.411(4)	.	.	no
C219	C224	1.406(4)	.	.	no
C219	B2	1.652(5)	.	.	yes
C220	C221	1.387(5)	.	.	no
C221	C222	1.389(5)	.	.	no
C222	C223	1.393(5)	.	.	no
C223	C224	1.390(5)	.	.	no
C210	H210	0.95	.	.	no
C211	H211	0.95	.	.	no
C212	H212	0.95	.	.	no
C214	H214	0.95	.	.	no
C215	H215	0.95	.	.	no
C216	H216	0.95	.	.	no
C217	H217	0.95	.	.	no
C218	H218	0.95	.	.	no
C220	H220	0.95	.	.	no
C221	H221	0.95	.	.	no
C222	H222	0.95	.	.	no
C223	H223	0.95	.	.	no
C224	H224	0.95	.	.	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

O1	Zr1	C11	122.37(11)	.	.	.	yes
O1	Zr1	C12	89.81(9)	.	.	.	yes
O1	Zr1	C13	78.86(9)	.	.	.	yes
O1	Zr1	C14	102.68(10)	.	.	.	yes
O1	Zr1	C15	132.89(11)	.	.	.	yes
O1	Zr1	C111	81.27(10)	.	.	.	yes
O1	Zr1	C112	87.96(9)	.	.	.	yes
O1	Zr1	C113	118.42(9)	.	.	.	yes
O1	Zr1	C114	137.85(10)	.	.	.	yes
O1	Zr1	C115	110.72(10)	.	.	.	yes
O1	Zr1	C120	105.76(10)	.	.	.	yes
C11	Zr1	C12	32.68(12)	.	.	.	yes
C11	Zr1	C13	54.19(11)	.	.	.	yes
C11	Zr1	C14	55.07(11)	.	.	.	yes
C11	Zr1	C15	33.08(12)	.	.	.	yes
C11	Zr1	C111	148.04(12)	.	.	.	yes
C11	Zr1	C112	148.59(12)	.	.	.	yes
C11	Zr1	C113	116.83(12)	.	.	.	yes
C11	Zr1	C114	98.58(12)	.	.	.	yes
C11	Zr1	C115	112.24(12)	.	.	.	yes
C11	Zr1	C120	87.92(12)	.	.	.	yes
C12	Zr1	C13	32.60(11)	.	.	.	yes
C12	Zr1	C14	54.66(11)	.	.	.	yes
C12	Zr1	C15	54.45(12)	.	.	.	yes
C12	Zr1	C111	157.86(11)	.	.	.	yes
C12	Zr1	C112	168.19(11)	.	.	.	yes
C12	Zr1	C113	145.38(11)	.	.	.	yes
C12	Zr1	C114	131.10(11)	.	.	.	yes
C12	Zr1	C115	134.88(11)	.	.	.	yes
C12	Zr1	C120	100.25(12)	.	.	.	yes
C13	Zr1	C14	32.78(11)	.	.	.	yes
C13	Zr1	C15	54.34(12)	.	.	.	yes
C13	Zr1	C111	157.52(11)	.	.	.	yes
C13	Zr1	C112	135.73(11)	.	.	.	yes
C13	Zr1	C113	128.69(11)	.	.	.	yes
C13	Zr1	C114	140.22(11)	.	.	.	yes
C13	Zr1	C115	166.28(11)	.	.	.	yes
C13	Zr1	C120	132.71(12)	.	.	.	yes
C14	Zr1	C15	33.37(11)	.	.	.	yes
C14	Zr1	C111	147.12(11)	.	.	.	yes
C14	Zr1	C112	114.65(11)	.	.	.	yes
C14	Zr1	C113	97.15(11)	.	.	.	yes
C14	Zr1	C114	109.37(11)	.	.	.	yes
C14	Zr1	C115	144.43(11)	.	.	.	yes
C14	Zr1	C120	141.78(11)	.	.	.	yes
C15	Zr1	C111	142.79(13)	.	.	.	yes
C15	Zr1	C112	120.45(12)	.	.	.	yes
C15	Zr1	C113	90.94(12)	.	.	.	yes
C15	Zr1	C114	86.71(12)	.	.	.	yes
C15	Zr1	C115	116.29(12)	.	.	.	yes
C15	Zr1	C120	109.72(11)	.	.	.	yes
C111	Zr1	C112	32.47(11)	.	.	.	yes
C111	Zr1	C113	54.48(11)	.	.	.	yes
C111	Zr1	C114	56.99(11)	.	.	.	yes
C111	Zr1	C115	35.85(11)	.	.	.	yes
C111	Zr1	C120	63.39(12)	.	.	.	yes
C112	Zr1	C113	31.76(10)	.	.	.	yes
C112	Zr1	C114	54.19(10)	.	.	.	yes
C112	Zr1	C115	56.40(11)	.	.	.	yes
C112	Zr1	C120	91.51(12)	.	.	.	yes
C113	Zr1	C114	32.37(11)	.	.	.	yes
C113	Zr1	C115	56.39(11)	.	.	.	yes
C113	Zr1	C120	91.30(13)	.	.	.	yes
C114	Zr1	C115	35.52(12)	.	.	.	yes
C114	Zr1	C120	62.87(13)	.	.	.	yes
C115	Zr1	C120	36.59(13)	.	.	.	yes

Zr1	O1	C121	121.82(18)	.	.	.	yes
Zr1	O1	C124	128.3(2)	.	.	.	yes
C121	O1	C124	109.8(2)	.	.	.	yes
Zr1	C11	C12	74.58(18)	.	.	.	yes
Zr1	C11	C15	73.0(2)	.	.	.	yes
Zr1	C11	C16	124.6(3)	.	.	.	yes
C12	C11	C15	108.1(3)	.	.	.	no
C12	C11	C16	124.0(3)	.	.	.	no
C15	C11	C16	127.4(3)	.	.	.	no
Zr1	C12	C11	72.7(2)	.	.	.	yes
Zr1	C12	C13	73.84(19)	.	.	.	yes
Zr1	C12	C17	124.8(2)	.	.	.	yes
C11	C12	C13	108.0(3)	.	.	.	no
C11	C12	C17	125.0(3)	.	.	.	no
C13	C12	C17	126.6(3)	.	.	.	no
Zr1	C13	C12	73.56(19)	.	.	.	yes
Zr1	C13	C14	71.36(19)	.	.	.	yes
Zr1	C13	C18	125.7(2)	.	.	.	yes
C12	C13	C14	108.3(3)	.	.	.	no
C12	C13	C18	126.3(3)	.	.	.	no
C14	C13	C18	125.1(3)	.	.	.	no
Zr1	C14	C13	75.9(2)	.	.	.	yes
Zr1	C14	C15	74.0(2)	.	.	.	yes
Zr1	C14	C19	119.8(2)	.	.	.	yes
C13	C14	C15	107.8(3)	.	.	.	no
C13	C14	C19	125.5(3)	.	.	.	no
C15	C14	C19	126.5(3)	.	.	.	no
Zr1	C15	C11	73.91(19)	.	.	.	yes
Zr1	C15	C14	72.59(19)	.	.	.	yes
Zr1	C15	C110	129.5(3)	.	.	.	yes
C11	C15	C14	107.8(3)	.	.	.	no
C11	C15	C110	127.1(3)	.	.	.	no
C14	C15	C110	123.8(3)	.	.	.	no
Zr1	C111	C112	81.1(2)	.	.	.	yes
Zr1	C111	C115	66.58(18)	.	.	.	yes
Zr1	C111	C116	119.2(2)	.	.	.	yes
C112	C111	C115	108.3(3)	.	.	.	no
C112	C111	C116	127.2(3)	.	.	.	no
C115	C111	C116	124.5(3)	.	.	.	no
Zr1	C112	C111	66.41(18)	.	.	.	yes
Zr1	C112	C113	74.87(19)	.	.	.	yes
Zr1	C112	C117	132.4(2)	.	.	.	yes
C111	C112	C113	108.8(3)	.	.	.	no
C111	C112	C117	128.0(3)	.	.	.	no
C113	C112	C117	122.5(3)	.	.	.	no
Zr1	C113	C112	73.37(19)	.	.	.	yes
Zr1	C113	C114	67.19(18)	.	.	.	yes
Zr1	C113	C118	132.8(2)	.	.	.	yes
C112	C113	C114	107.8(3)	.	.	.	no
C112	C113	C118	123.9(3)	.	.	.	no
C114	C113	C118	127.5(3)	.	.	.	no
Zr1	C114	C113	80.45(19)	.	.	.	yes
Zr1	C114	C115	65.35(18)	.	.	.	yes
Zr1	C114	C119	127.2(2)	.	.	.	yes
C113	C114	C115	108.5(3)	.	.	.	no
C113	C114	C119	127.1(3)	.	.	.	no
C115	C114	C119	123.7(3)	.	.	.	no
Zr1	C115	C111	77.57(19)	.	.	.	yes
Zr1	C115	C114	79.12(19)	.	.	.	yes
Zr1	C115	C120	75.5(2)	.	.	.	yes
C111	C115	C114	106.5(3)	.	.	.	no
C111	C115	C120	119.7(3)	.	.	.	no
C114	C115	C120	119.6(3)	.	.	.	no
C11	C16	H16"	109	.	.	.	no
H16	C16	H16'	110	.	.	.	no
H16	C16	H16"	109	.	.	.	no

H16'	C16	H16"	109	.	.	.	no
C11	C16	H16	109	.	.	.	no
C11	C16	H16'	109	.	.	.	no
C12	C17	H17	110	.	.	.	no
H17	C17	H17"	109	.	.	.	no
H17'	C17	H17"	109	.	.	.	no
C12	C17	H17'	109	.	.	.	no
C12	C17	H17"	109	.	.	.	no
H17	C17	H17'	109	.	.	.	no
C13	C18	H18	110	.	.	.	no
C13	C18	H18'	109	.	.	.	no
C13	C18	H18"	109	.	.	.	no
H18'	C18	H18"	109	.	.	.	no
H18	C18	H18'	109	.	.	.	no
H18	C18	H18"	109	.	.	.	no
C14	C19	H19	109	.	.	.	no
H19	C19	H19'	109	.	.	.	no
C14	C19	H19'	109	.	.	.	no
C14	C19	H19"	109	.	.	.	no
H19'	C19	H19"	110	.	.	.	no
H19	C19	H19"	109	.	.	.	no
Zr1	C120	C115	67.92(19)	.	.	.	yes
O1	C121	C122	104.3(3)	.	.	.	yes
C121	C122	C123	102.7(3)	.	.	.	no
C122	C123	C124	104.7(3)	.	.	.	no
O1	C124	C123	105.7(3)	.	.	.	yes
C15	C110	H110'	109	.	.	.	no
C15	C110	H110"	110	.	.	.	no
C15	C110	H110	110	.	.	.	no
H110'	C110	H110"	109	.	.	.	no
H110'	C110	H110	109	.	.	.	no
H110"	C110	H110	110	.	.	.	no
C111	C116	H116'	109	.	.	.	no
C111	C116	H116"	109	.	.	.	no
C111	C116	H116	109	.	.	.	no
H116'	C116	H116"	109	.	.	.	no
H116'	C116	H116	109	.	.	.	no
H116"	C116	H116	110	.	.	.	no
C112	C117	H117'	109	.	.	.	no
C112	C117	H117"	109	.	.	.	no
C112	C117	H117	110	.	.	.	no
H117'	C117	H117"	109	.	.	.	no
H117'	C117	H117	109	.	.	.	no
H117"	C117	H117	109	.	.	.	no
C113	C118	H118'	109	.	.	.	no
C113	C118	H118"	109	.	.	.	no
C113	C118	H118	109	.	.	.	no
H118'	C118	H118"	109	.	.	.	no
H118'	C118	H118	109	.	.	.	no
H118"	C118	H118	110	.	.	.	no
C114	C119	H119'	109	.	.	.	no
C114	C119	H119"	109	.	.	.	no
C114	C119	H119	109	.	.	.	no
H119'	C119	H119"	110	.	.	.	no
H119'	C119	H119	109	.	.	.	no
H119"	C119	H119	110	.	.	.	no
Zr1	C120	H120'	117	.	.	.	no
Zr1	C120	H120	117	.	.	.	no
C115	C120	H120'	117	.	.	.	no
C115	C120	H120	117	.	.	.	no
H120'	C120	H120	114	.	.	.	no
O1	C121	H121'	111	.	.	.	no
O1	C121	H121	111	.	.	.	no
C122	C121	H121'	111	.	.	.	no
C122	C121	H121	111	.	.	.	no
H121'	C121	H121	109	.	.	.	no

C22	C21	C26	114.8(3)	.	.	.	no
C22	C21	B2	125.0(3)	.	.	.	yes
C26	C21	B2	120.1(3)	.	.	.	yes
C123	C122	H122	111	.	.	.	no
H122'	C122	H122	109	.	.	.	no
C121	C122	H122'	111	.	.	.	no
C121	C122	H122	111	.	.	.	no
C123	C122	H122'	111	.	.	.	no
C21	C22	C23	123.3(3)	.	.	.	no
C122	C123	H123	111	.	.	.	no
C124	C123	H123'	111	.	.	.	no
C122	C123	H123'	111	.	.	.	no
C22	C23	C24	119.8(3)	.	.	.	no
H123'	C123	H123	109	.	.	.	no
C124	C123	H123	111	.	.	.	no
H124'	C124	H124	109	.	.	.	no
C123	C124	H124	111	.	.	.	no
O1	C124	H124'	111	.	.	.	no
O1	C124	H124	111	.	.	.	no
C123	C124	H124'	111	.	.	.	no
C23	C24	C25	118.8(3)	.	.	.	no
C24	C25	C26	120.4(4)	.	.	.	no
C21	C26	C25	122.9(3)	.	.	.	no
C28	C27	C212	115.7(3)	.	.	.	no
C28	C27	B2	123.4(3)	.	.	.	yes
C212	C27	B2	120.4(3)	.	.	.	yes
C27	C28	C29	122.0(3)	.	.	.	no
C28	C29	C210	120.6(3)	.	.	.	no
C21	C22	H22	118	.	.	.	no
C23	C22	H22	118	.	.	.	no
C22	C23	H23	120	.	.	.	no
C24	C23	H23	120	.	.	.	no
C23	C24	H24	121	.	.	.	no
C25	C24	H24	121	.	.	.	no
C24	C25	H25	120	.	.	.	no
C26	C25	H25	120	.	.	.	no
C21	C26	H26	119	.	.	.	no
C25	C26	H26	119	.	.	.	no
C29	C28	H28	119	.	.	.	no
C27	C28	H28	119	.	.	.	no
C28	C29	H29	120	.	.	.	no
C210	C29	H29	120	.	.	.	no
C29	C210	C211	119.0(3)	.	.	.	no
C210	C211	C212	119.8(3)	.	.	.	no
C27	C212	C211	122.9(3)	.	.	.	no
C214	C213	C218	114.3(3)	.	.	.	no
C218	C213	B2	121.3(3)	.	.	.	yes
C214	C213	B2	124.3(3)	.	.	.	yes
C213	C214	C215	123.4(3)	.	.	.	no
C214	C215	C216	120.0(4)	.	.	.	no
C215	C216	C217	118.6(3)	.	.	.	no
C216	C217	C218	120.5(3)	.	.	.	no
C213	C218	C217	123.2(3)	.	.	.	no
C220	C219	B2	125.5(3)	.	.	.	yes
C220	C219	C224	114.3(3)	.	.	.	no
C224	C219	B2	120.0(3)	.	.	.	yes
C219	C220	C221	123.2(3)	.	.	.	no
C220	C221	C222	120.5(3)	.	.	.	no
C221	C222	C223	118.5(3)	.	.	.	no
C222	C223	C224	120.1(3)	.	.	.	no
C219	C224	C223	123.5(3)	.	.	.	no
C29	C210	H210	120	.	.	.	no
C211	C210	H210	121	.	.	.	no
C212	C211	H211	120	.	.	.	no
C210	C211	H211	120	.	.	.	no
C27	C212	H212	119	.	.	.	no

C211	C212	H212	119	.	.	.	no
C213	C214	H214	118	.	.	.	no
C215	C214	H214	118	.	.	.	no
C216	C215	H215	120	.	.	.	no
C214	C215	H215	120	.	.	.	no
C215	C216	H216	121	.	.	.	no
C217	C216	H216	121	.	.	.	no
C218	C217	H217	120	.	.	.	no
C216	C217	H217	120	.	.	.	no
C213	C218	H218	118	.	.	.	no
C217	C218	H218	118	.	.	.	no
C219	C220	H220	118	.	.	.	no
C221	C220	H220	118	.	.	.	no
C222	C221	H221	120	.	.	.	no
C220	C221	H221	120	.	.	.	no
C221	C222	H222	121	.	.	.	no
C223	C222	H222	121	.	.	.	no
C222	C223	H223	120	.	.	.	no
C224	C223	H223	120	.	.	.	no
C223	C224	H224	118	.	.	.	no
C219	C224	H224	118	.	.	.	no
C21	B2	C213	106.0(3)	.	.	.	yes
C21	B2	C219	111.5(3)	.	.	.	yes
C27	B2	C219	103.3(3)	.	.	.	yes
C213	B2	C219	113.9(3)	.	.	.	yes
C27	B2	C213	110.7(3)	.	.	.	yes
C21	B2	C27	111.6(3)	.	.	.	yes

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C11	Zr1	O1	C121	-58.8(3)	.	.	.	.	no
C11	Zr1	O1	C124	126.4(3)	.	.	.	.	no
C12	Zr1	O1	C121	-61.7(2)	.	.	.	.	no
C12	Zr1	O1	C124	123.5(3)	.	.	.	.	no
C13	Zr1	O1	C121	-92.6(2)	.	.	.	.	no
C13	Zr1	O1	C124	92.6(3)	.	.	.	.	no
C14	Zr1	O1	C121	-115.3(2)	.	.	.	.	no
C14	Zr1	O1	C124	69.9(3)	.	.	.	.	no
C15	Zr1	O1	C121	-98.9(3)	.	.	.	.	no
C15	Zr1	O1	C124	86.3(3)	.	.	.	.	no
C111	Zr1	O1	C121	98.0(2)	.	.	.	.	no
C111	Zr1	O1	C124	-76.9(3)	.	.	.	.	no
C112	Zr1	O1	C121	129.9(2)	.	.	.	.	no
C112	Zr1	O1	C124	-44.9(3)	.	.	.	.	no
C113	Zr1	O1	C121	139.3(2)	.	.	.	.	no
C113	Zr1	O1	C124	-35.6(3)	.	.	.	.	no
C114	Zr1	O1	C121	105.7(3)	.	.	.	.	no
C114	Zr1	O1	C124	-69.2(3)	.	.	.	.	no
C115	Zr1	O1	C121	77.2(2)	.	.	.	.	no
C115	Zr1	O1	C124	-97.7(3)	.	.	.	.	no
C120	Zr1	O1	C121	38.9(3)	.	.	.	.	no
C120	Zr1	O1	C124	-135.9(3)	.	.	.	.	no
O1	Zr1	C11	C12	-5.4(2)	.	.	.	.	no
O1	Zr1	C11	C15	-120.2(2)	.	.	.	.	no
O1	Zr1	C11	C16	115.6(3)	.	.	.	.	no
C12	Zr1	C11	C15	-114.9(3)	.	.	.	.	no
C12	Zr1	C11	C16	121.0(4)	.	.	.	.	no

C13	Zr1	C11	C12	36.94(19)	.	.	.	.	no
C13	Zr1	C11	C15	-77.9(2)	.	.	.	.	no
C13	Zr1	C11	C16	157.9(4)	.	.	.	.	no
C14	Zr1	C11	C12	77.4(2)	.	.	.	.	no
C14	Zr1	C11	C15	-37.4(2)	.	.	.	.	no
C14	Zr1	C11	C16	-161.6(4)	.	.	.	.	no
C15	Zr1	C11	C12	114.9(3)	.	.	.	.	no
C15	Zr1	C11	C16	-124.2(4)	.	.	.	.	no
C111	Zr1	C11	C12	-137.9(2)	.	.	.	.	no
C111	Zr1	C11	C15	107.2(3)	.	.	.	.	no
C111	Zr1	C11	C16	-16.9(4)	.	.	.	.	no
C112	Zr1	C11	C12	157.8(2)	.	.	.	.	no
C112	Zr1	C11	C15	42.9(3)	.	.	.	.	no
C112	Zr1	C11	C16	-81.2(4)	.	.	.	.	no
C113	Zr1	C11	C12	156.86(19)	.	.	.	.	no
C113	Zr1	C11	C15	42.0(3)	.	.	.	.	no
C113	Zr1	C11	C16	-82.2(3)	.	.	.	.	no
C114	Zr1	C11	C12	-174.9(2)	.	.	.	.	no
C114	Zr1	C11	C15	70.3(2)	.	.	.	.	no
C114	Zr1	C11	C16	-53.9(3)	.	.	.	.	no
C115	Zr1	C11	C12	-140.8(2)	.	.	.	.	no
C115	Zr1	C11	C15	104.4(2)	.	.	.	.	no
C115	Zr1	C11	C16	-19.8(3)	.	.	.	.	no
C120	Zr1	C11	C12	-112.7(2)	.	.	.	.	no
C120	Zr1	C11	C15	132.4(2)	.	.	.	.	no
C120	Zr1	C11	C16	8.3(3)	.	.	.	.	no
O1	Zr1	C12	C11	175.5(2)	.	.	.	.	no
O1	Zr1	C12	C13	-69.29(19)	.	.	.	.	no
O1	Zr1	C12	C17	54.4(3)	.	.	.	.	no
C11	Zr1	C12	C13	115.2(3)	.	.	.	.	no
C11	Zr1	C12	C17	-121.1(4)	.	.	.	.	no
C13	Zr1	C12	C11	-115.2(3)	.	.	.	.	no
C13	Zr1	C12	C17	123.7(4)	.	.	.	.	no
C14	Zr1	C12	C11	-78.8(2)	.	.	.	.	no
C14	Zr1	C12	C13	36.45(19)	.	.	.	.	no
C14	Zr1	C12	C17	160.2(3)	.	.	.	.	no
C15	Zr1	C12	C11	-37.5(2)	.	.	.	.	no
C15	Zr1	C12	C13	77.7(2)	.	.	.	.	no
C15	Zr1	C12	C17	-158.6(3)	.	.	.	.	no
C111	Zr1	C12	C11	109.8(3)	.	.	.	.	no
C111	Zr1	C12	C13	-135.0(3)	.	.	.	.	no
C111	Zr1	C12	C17	-11.3(5)	.	.	.	.	no
C113	Zr1	C12	C11	-38.1(3)	.	.	.	.	no
C113	Zr1	C12	C13	77.1(3)	.	.	.	.	no
C113	Zr1	C12	C17	-159.2(2)	.	.	.	.	no
C114	Zr1	C12	C11	6.7(3)	.	.	.	.	no
C114	Zr1	C12	C13	121.9(2)	.	.	.	.	no
C114	Zr1	C12	C17	-114.4(3)	.	.	.	.	no
C115	Zr1	C12	C11	55.7(3)	.	.	.	.	no
C115	Zr1	C12	C13	170.97(19)	.	.	.	.	no
C115	Zr1	C12	C17	-65.3(3)	.	.	.	.	no
C120	Zr1	C12	C11	69.5(2)	.	.	.	.	no
C120	Zr1	C12	C13	-175.28(19)	.	.	.	.	no
C120	Zr1	C12	C17	-51.6(3)	.	.	.	.	no
O1	Zr1	C13	C12	107.6(2)	.	.	.	.	no
O1	Zr1	C13	C14	-136.0(2)	.	.	.	.	no
O1	Zr1	C13	C18	-15.6(3)	.	.	.	.	no
C11	Zr1	C13	C12	-37.04(19)	.	.	.	.	no
C11	Zr1	C13	C14	79.4(2)	.	.	.	.	no
C11	Zr1	C13	C18	-160.2(3)	.	.	.	.	no
C12	Zr1	C13	C14	116.5(3)	.	.	.	.	no
C12	Zr1	C13	C18	-123.2(4)	.	.	.	.	no
C14	Zr1	C13	C12	-116.5(3)	.	.	.	.	no
C14	Zr1	C13	C18	120.4(4)	.	.	.	.	no
C15	Zr1	C13	C12	-78.1(2)	.	.	.	.	no
C15	Zr1	C13	C14	38.36(19)	.	.	.	.	no

C15	Zr1	C13	C18	158.7(3)	.	.	.	.	no
C111	Zr1	C13	C12	135.9(3)	.	.	.	.	no
C111	Zr1	C13	C14	-107.7(3)	.	.	.	.	no
C111	Zr1	C13	C18	12.7(5)	.	.	.	.	no
C112	Zr1	C13	C12	-177.16(18)	.	.	.	.	no
C112	Zr1	C13	C14	-60.7(2)	.	.	.	.	no
C112	Zr1	C13	C18	59.7(3)	.	.	.	.	no
C113	Zr1	C13	C12	-134.81(19)	.	.	.	.	no
C113	Zr1	C13	C14	-18.4(2)	.	.	.	.	no
C113	Zr1	C13	C18	102.0(3)	.	.	.	.	no
C114	Zr1	C13	C12	-91.6(2)	.	.	.	.	no
C114	Zr1	C13	C14	24.8(3)	.	.	.	.	no
C114	Zr1	C13	C18	145.2(3)	.	.	.	.	no
C120	Zr1	C13	C12	6.3(3)	.	.	.	.	no
C120	Zr1	C13	C14	122.8(2)	.	.	.	.	no
C120	Zr1	C13	C18	-116.9(3)	.	.	.	.	no
O1	Zr1	C14	C13	44.3(2)	.	.	.	.	no
O1	Zr1	C14	C15	157.9(2)	.	.	.	.	no
O1	Zr1	C14	C19	-78.8(3)	.	.	.	.	no
C11	Zr1	C14	C13	-76.5(2)	.	.	.	.	no
C11	Zr1	C14	C15	37.1(2)	.	.	.	.	no
C11	Zr1	C14	C19	160.4(3)	.	.	.	.	no
C12	Zr1	C14	C13	-36.25(18)	.	.	.	.	no
C12	Zr1	C14	C15	77.3(2)	.	.	.	.	no
C12	Zr1	C14	C19	-159.4(3)	.	.	.	.	no
C13	Zr1	C14	C15	113.6(3)	.	.	.	.	no
C13	Zr1	C14	C19	-123.1(3)	.	.	.	.	no
C15	Zr1	C14	C13	-113.6(3)	.	.	.	.	no
C15	Zr1	C14	C19	123.3(4)	.	.	.	.	no
C111	Zr1	C14	C13	137.9(2)	.	.	.	.	no
C111	Zr1	C14	C15	-108.6(3)	.	.	.	.	no
C111	Zr1	C14	C19	14.8(4)	.	.	.	.	no
C112	Zr1	C14	C13	137.94(18)	.	.	.	.	no
C112	Zr1	C14	C15	-108.5(2)	.	.	.	.	no
C112	Zr1	C14	C19	14.8(3)	.	.	.	.	no
C113	Zr1	C14	C13	165.65(19)	.	.	.	.	no
C113	Zr1	C14	C15	-80.8(2)	.	.	.	.	no
C113	Zr1	C14	C19	42.6(3)	.	.	.	.	no
C114	Zr1	C14	C13	-163.46(18)	.	.	.	.	no
C114	Zr1	C14	C15	-49.9(2)	.	.	.	.	no
C114	Zr1	C14	C19	73.4(3)	.	.	.	.	no
C115	Zr1	C14	C13	-156.0(2)	.	.	.	.	no
C115	Zr1	C14	C15	-42.4(3)	.	.	.	.	no
C115	Zr1	C14	C19	81.0(3)	.	.	.	.	no
C120	Zr1	C14	C13	-93.0(3)	.	.	.	.	no
C120	Zr1	C14	C15	20.6(3)	.	.	.	.	no
C120	Zr1	C14	C19	143.9(3)	.	.	.	.	no
O1	Zr1	C15	C11	85.0(2)	.	.	.	.	no
O1	Zr1	C15	C14	-30.1(3)	.	.	.	.	no
O1	Zr1	C15	C110	-149.9(3)	.	.	.	.	no
C11	Zr1	C15	C14	-115.1(3)	.	.	.	.	no
C11	Zr1	C15	C110	125.2(4)	.	.	.	.	no
C12	Zr1	C15	C11	37.0(2)	.	.	.	.	no
C12	Zr1	C15	C14	-78.0(2)	.	.	.	.	no
C12	Zr1	C15	C110	162.2(3)	.	.	.	.	no
C13	Zr1	C15	C11	77.4(2)	.	.	.	.	no
C13	Zr1	C15	C14	-37.6(2)	.	.	.	.	no
C13	Zr1	C15	C110	-157.4(3)	.	.	.	.	no
C14	Zr1	C15	C11	115.1(3)	.	.	.	.	no
C14	Zr1	C15	C110	-119.8(4)	.	.	.	.	no
C111	Zr1	C15	C11	-123.3(2)	.	.	.	.	no
C111	Zr1	C15	C14	121.7(2)	.	.	.	.	no
C111	Zr1	C15	C110	1.9(4)	.	.	.	.	no
C112	Zr1	C15	C11	-155.7(2)	.	.	.	.	no
C112	Zr1	C15	C14	89.3(2)	.	.	.	.	no
C112	Zr1	C15	C110	-30.5(3)	.	.	.	.	no

C113	Zr1	C15	C11	-143.3(2)	.	.	.	.	no
C113	Zr1	C15	C14	101.6(2)	.	.	.	.	no
C113	Zr1	C15	C110	-18.2(3)	.	.	.	.	no
C114	Zr1	C15	C11	-111.2(2)	.	.	.	.	no
C114	Zr1	C15	C14	133.7(2)	.	.	.	.	no
C114	Zr1	C15	C110	13.9(3)	.	.	.	.	no
C115	Zr1	C15	C11	-90.9(2)	.	.	.	.	no
C115	Zr1	C15	C14	154.1(2)	.	.	.	.	no
C115	Zr1	C15	C110	34.3(3)	.	.	.	.	no
C120	Zr1	C15	C11	-51.6(3)	.	.	.	.	no
C120	Zr1	C15	C14	-166.7(2)	.	.	.	.	no
C120	Zr1	C15	C110	73.5(3)	.	.	.	.	no
O1	Zr1	C111	C112	100.03(19)	.	.	.	.	no
O1	Zr1	C111	C115	-145.5(2)	.	.	.	.	no
O1	Zr1	C111	C116	-27.8(2)	.	.	.	.	no
C11	Zr1	C111	C112	-119.0(2)	.	.	.	.	no
C11	Zr1	C111	C115	-4.5(3)	.	.	.	.	no
C11	Zr1	C111	C116	113.2(3)	.	.	.	.	no
C12	Zr1	C111	C112	167.3(3)	.	.	.	.	no
C12	Zr1	C111	C115	-78.2(3)	.	.	.	.	no
C12	Zr1	C111	C116	39.5(4)	.	.	.	.	no
C13	Zr1	C111	C112	72.0(4)	.	.	.	.	no
C13	Zr1	C111	C115	-173.5(3)	.	.	.	.	no
C13	Zr1	C111	C116	-55.8(4)	.	.	.	.	no
C14	Zr1	C111	C112	0.2(3)	.	.	.	.	no
C14	Zr1	C111	C115	114.7(2)	.	.	.	.	no
C14	Zr1	C111	C116	-127.7(3)	.	.	.	.	no
C15	Zr1	C111	C112	-59.4(3)	.	.	.	.	no
C15	Zr1	C111	C115	55.1(3)	.	.	.	.	no
C15	Zr1	C111	C116	172.8(2)	.	.	.	.	no
C112	Zr1	C111	C115	114.5(3)	.	.	.	.	no
C112	Zr1	C111	C116	-127.8(3)	.	.	.	.	no
C113	Zr1	C111	C112	-34.50(18)	.	.	.	.	no
C113	Zr1	C111	C115	80.0(2)	.	.	.	.	no
C113	Zr1	C111	C116	-162.3(3)	.	.	.	.	no
C114	Zr1	C111	C112	-73.8(2)	.	.	.	.	no
C114	Zr1	C111	C115	40.71(19)	.	.	.	.	no
C114	Zr1	C111	C116	158.4(3)	.	.	.	.	no
C115	Zr1	C111	C112	-114.5(3)	.	.	.	.	no
C115	Zr1	C111	C116	117.7(3)	.	.	.	.	no
C120	Zr1	C111	C112	-147.4(2)	.	.	.	.	no
C120	Zr1	C111	C115	-32.9(2)	.	.	.	.	no
C120	Zr1	C111	C116	84.8(3)	.	.	.	.	no
O1	Zr1	C112	C111	-76.89(19)	.	.	.	.	no
O1	Zr1	C112	C113	164.3(2)	.	.	.	.	no
O1	Zr1	C112	C117	43.8(3)	.	.	.	.	no
C11	Zr1	C112	C111	117.3(2)	.	.	.	.	no
C11	Zr1	C112	C113	-1.6(3)	.	.	.	.	no
C11	Zr1	C112	C117	-122.0(3)	.	.	.	.	no
C13	Zr1	C112	C111	-148.61(19)	.	.	.	.	no
C13	Zr1	C112	C113	92.5(2)	.	.	.	.	no
C13	Zr1	C112	C117	-27.9(4)	.	.	.	.	no
C14	Zr1	C112	C111	-179.91(18)	.	.	.	.	no
C14	Zr1	C112	C113	61.2(2)	.	.	.	.	no
C14	Zr1	C112	C117	-59.2(3)	.	.	.	.	no
C15	Zr1	C112	C111	142.85(19)	.	.	.	.	no
C15	Zr1	C112	C113	24.0(2)	.	.	.	.	no
C15	Zr1	C112	C117	-96.5(3)	.	.	.	.	no
C111	Zr1	C112	C113	-118.9(3)	.	.	.	.	no
C111	Zr1	C112	C117	120.7(4)	.	.	.	.	no
C113	Zr1	C112	C111	118.9(3)	.	.	.	.	no
C113	Zr1	C112	C117	-120.5(4)	.	.	.	.	no
C114	Zr1	C112	C111	83.3(2)	.	.	.	.	no
C114	Zr1	C112	C113	-35.59(19)	.	.	.	.	no
C114	Zr1	C112	C117	-156.0(4)	.	.	.	.	no
C115	Zr1	C112	C111	39.78(19)	.	.	.	.	no

C115	Zr1	C112	C113	-79.1(2)	.	.	.	.	no
C115	Zr1	C112	C117	160.5(4)	.	.	.	.	no
C120	Zr1	C112	C111	28.8(2)	.	.	.	.	no
C120	Zr1	C112	C113	-90.0(2)	.	.	.	.	no
C120	Zr1	C112	C117	149.5(3)	.	.	.	.	no
O1	Zr1	C113	C112	-18.0(2)	.	.	.	.	no
O1	Zr1	C113	C114	-136.13(19)	.	.	.	.	no
O1	Zr1	C113	C118	103.2(3)	.	.	.	.	no
C11	Zr1	C113	C112	179.10(19)	.	.	.	.	no
C11	Zr1	C113	C114	60.9(2)	.	.	.	.	no
C11	Zr1	C113	C118	-59.8(3)	.	.	.	.	no
C12	Zr1	C113	C112	-159.0(2)	.	.	.	.	no
C12	Zr1	C113	C114	82.9(3)	.	.	.	.	no
C12	Zr1	C113	C118	-37.9(4)	.	.	.	.	no
C13	Zr1	C113	C112	-116.7(2)	.	.	.	.	no
C13	Zr1	C113	C114	125.1(2)	.	.	.	.	no
C13	Zr1	C113	C118	4.4(3)	.	.	.	.	no
C14	Zr1	C113	C112	-126.6(2)	.	.	.	.	no
C14	Zr1	C113	C114	115.3(2)	.	.	.	.	no
C14	Zr1	C113	C118	-5.5(3)	.	.	.	.	no
C15	Zr1	C113	C112	-159.5(2)	.	.	.	.	no
C15	Zr1	C113	C114	82.4(2)	.	.	.	.	no
C15	Zr1	C113	C118	-38.4(3)	.	.	.	.	no
C111	Zr1	C113	C112	35.29(19)	.	.	.	.	no
C111	Zr1	C113	C114	-82.9(2)	.	.	.	.	no
C111	Zr1	C113	C118	156.4(3)	.	.	.	.	no
C112	Zr1	C113	C114	-118.2(3)	.	.	.	.	no
C112	Zr1	C113	C118	121.1(4)	.	.	.	.	no
C114	Zr1	C113	C112	118.2(3)	.	.	.	.	no
C114	Zr1	C113	C118	-120.7(4)	.	.	.	.	no
C115	Zr1	C113	C112	79.1(2)	.	.	.	.	no
C115	Zr1	C113	C114	-39.0(2)	.	.	.	.	no
C115	Zr1	C113	C118	-159.8(3)	.	.	.	.	no
C120	Zr1	C113	C112	90.8(2)	.	.	.	.	no
C120	Zr1	C113	C114	-27.4(2)	.	.	.	.	no
C120	Zr1	C113	C118	-148.1(3)	.	.	.	.	no
O1	Zr1	C114	C113	65.3(2)	.	.	.	.	no
O1	Zr1	C114	C115	-50.2(2)	.	.	.	.	no
O1	Zr1	C114	C119	-164.9(2)	.	.	.	.	no
C11	Zr1	C114	C113	-127.9(2)	.	.	.	.	no
C11	Zr1	C114	C115	116.59(19)	.	.	.	.	no
C11	Zr1	C114	C119	1.9(3)	.	.	.	.	no
C12	Zr1	C114	C113	-131.6(2)	.	.	.	.	no
C12	Zr1	C114	C115	112.9(2)	.	.	.	.	no
C12	Zr1	C114	C119	-1.8(4)	.	.	.	.	no
C13	Zr1	C114	C113	-86.0(2)	.	.	.	.	no
C13	Zr1	C114	C115	158.54(19)	.	.	.	.	no
C13	Zr1	C114	C119	43.8(4)	.	.	.	.	no
C14	Zr1	C114	C113	-72.0(2)	.	.	.	.	no
C14	Zr1	C114	C115	172.47(18)	.	.	.	.	no
C14	Zr1	C114	C119	57.7(3)	.	.	.	.	no
C15	Zr1	C114	C113	-97.0(2)	.	.	.	.	no
C15	Zr1	C114	C115	147.6(2)	.	.	.	.	no
C15	Zr1	C114	C119	32.8(3)	.	.	.	.	no
C111	Zr1	C114	C113	74.4(2)	.	.	.	.	no
C111	Zr1	C114	C115	-41.10(19)	.	.	.	.	no
C111	Zr1	C114	C119	-155.8(3)	.	.	.	.	no
C112	Zr1	C114	C113	34.91(19)	.	.	.	.	no
C112	Zr1	C114	C115	-80.6(2)	.	.	.	.	no
C112	Zr1	C114	C119	164.7(3)	.	.	.	.	no
C113	Zr1	C114	C115	-115.5(3)	.	.	.	.	no
C113	Zr1	C114	C119	129.8(4)	.	.	.	.	no
C115	Zr1	C114	C113	115.5(3)	.	.	.	.	no
C115	Zr1	C114	C119	-114.7(4)	.	.	.	.	no
C120	Zr1	C114	C113	148.9(2)	.	.	.	.	no
C120	Zr1	C114	C115	33.40(19)	.	.	.	.	no

C120	Zr1	C114	C119	-81.3(3)	.	.	.	.	no
O1	Zr1	C115	C111	36.8(2)	.	.	.	.	no
O1	Zr1	C115	C114	146.54(17)	.	.	.	.	no
O1	Zr1	C115	C120	-88.72(19)	.	.	.	.	no
C11	Zr1	C115	C111	177.45(19)	.	.	.	.	no
C11	Zr1	C115	C114	-72.8(2)	.	.	.	.	no
C11	Zr1	C115	C120	51.9(2)	.	.	.	.	no
C12	Zr1	C115	C111	148.63(19)	.	.	.	.	no
C12	Zr1	C115	C114	-101.6(2)	.	.	.	.	no
C12	Zr1	C115	C120	23.1(3)	.	.	.	.	no
C14	Zr1	C115	C111	-122.0(2)	.	.	.	.	no
C14	Zr1	C115	C114	-12.3(3)	.	.	.	.	no
C14	Zr1	C115	C120	112.5(2)	.	.	.	.	no
C15	Zr1	C115	C111	-146.42(19)	.	.	.	.	no
C15	Zr1	C115	C114	-36.7(2)	.	.	.	.	no
C15	Zr1	C115	C120	88.1(2)	.	.	.	.	no
C111	Zr1	C115	C114	109.7(3)	.	.	.	.	no
C111	Zr1	C115	C120	-125.5(3)	.	.	.	.	no
C112	Zr1	C115	C111	-35.91(18)	.	.	.	.	no
C112	Zr1	C115	C114	73.8(2)	.	.	.	.	no
C112	Zr1	C115	C120	-161.4(2)	.	.	.	.	no
C113	Zr1	C115	C111	-74.3(2)	.	.	.	.	no
C113	Zr1	C115	C114	35.47(18)	.	.	.	.	no
C113	Zr1	C115	C120	160.2(2)	.	.	.	.	no
C114	Zr1	C115	C111	-109.7(3)	.	.	.	.	no
C114	Zr1	C115	C120	124.7(3)	.	.	.	.	no
C120	Zr1	C115	C111	125.5(3)	.	.	.	.	no
C120	Zr1	C115	C114	-124.7(3)	.	.	.	.	no
O1	Zr1	C120	C115	103.69(19)	.	.	.	.	no
C11	Zr1	C120	C115	-133.2(2)	.	.	.	.	no
C12	Zr1	C120	C115	-163.59(19)	.	.	.	.	no
C13	Zr1	C120	C115	-167.04(18)	.	.	.	.	no
C14	Zr1	C120	C115	-119.7(2)	.	.	.	.	no
C15	Zr1	C120	C115	-107.8(2)	.	.	.	.	no
C111	Zr1	C120	C115	32.22(18)	.	.	.	.	no
C112	Zr1	C120	C115	15.39(19)	.	.	.	.	no
C113	Zr1	C120	C115	-16.38(19)	.	.	.	.	no
C114	Zr1	C120	C115	-32.45(18)	.	.	.	.	no
Zr1	O1	C121	C122	-153.9(2)	.	.	.	.	no
C124	O1	C121	C122	21.8(4)	.	.	.	.	no
Zr1	O1	C124	C123	175.4(2)	.	.	.	.	no
C121	O1	C124	C123	0.1(4)	.	.	.	.	no
Zr1	C11	C12	C13	-66.0(2)	.	.	.	.	no
Zr1	C11	C12	C17	120.8(3)	.	.	.	.	no
C15	C11	C12	Zr1	65.9(3)	.	.	.	.	no
C15	C11	C12	C13	-0.1(4)	.	.	.	.	no
C15	C11	C12	C17	-173.4(3)	.	.	.	.	no
C16	C11	C12	Zr1	-121.7(4)	.	.	.	.	no
C16	C11	C12	C13	172.4(3)	.	.	.	.	no
C16	C11	C12	C17	-0.9(6)	.	.	.	.	no
Zr1	C11	C15	C14	65.2(2)	.	.	.	.	no
Zr1	C11	C15	C110	-127.7(4)	.	.	.	.	no
C12	C11	C15	Zr1	-66.9(2)	.	.	.	.	no
C12	C11	C15	C14	-1.7(4)	.	.	.	.	no
C12	C11	C15	C110	165.4(4)	.	.	.	.	no
C16	C11	C15	Zr1	121.0(4)	.	.	.	.	no
C16	C11	C15	C14	-173.8(4)	.	.	.	.	no
C16	C11	C15	C110	-6.7(7)	.	.	.	.	no
Zr1	C12	C13	C14	-63.3(2)	.	.	.	.	no
Zr1	C12	C13	C18	122.6(3)	.	.	.	.	no
C11	C12	C13	Zr1	65.3(2)	.	.	.	.	no
C11	C12	C13	C14	1.9(4)	.	.	.	.	no
C11	C12	C13	C18	-172.2(3)	.	.	.	.	no
C17	C12	C13	Zr1	-121.6(3)	.	.	.	.	no
C17	C12	C13	C14	175.1(3)	.	.	.	.	no
C17	C12	C13	C18	1.0(6)	.	.	.	.	no

Zr1	C13	C14	C15	-67.7(2)	.	.	.	.	no
Zr1	C13	C14	C19	116.7(3)	.	.	.	.	no
C12	C13	C14	Zr1	64.8(2)	.	.	.	.	no
C12	C13	C14	C15	-3.0(4)	.	.	.	.	no
C12	C13	C14	C19	-178.5(3)	.	.	.	.	no
C18	C13	C14	Zr1	-121.1(3)	.	.	.	.	no
C18	C13	C14	C15	171.2(3)	.	.	.	.	no
C18	C13	C14	C19	-4.3(5)	.	.	.	.	no
Zr1	C14	C15	C11	-66.1(3)	.	.	.	.	no
Zr1	C14	C15	C110	126.3(4)	.	.	.	.	no
C13	C14	C15	Zr1	69.0(2)	.	.	.	.	no
C13	C14	C15	C11	2.9(4)	.	.	.	.	no
C13	C14	C15	C110	-164.8(3)	.	.	.	.	no
C19	C14	C15	Zr1	-115.6(3)	.	.	.	.	no
C19	C14	C15	C11	178.4(3)	.	.	.	.	no
C19	C14	C15	C110	10.7(6)	.	.	.	.	no
Zr1	C111	C112	C113	63.3(2)	.	.	.	.	no
Zr1	C111	C112	C117	-126.3(4)	.	.	.	.	no
C115	C111	C112	Zr1	-61.6(2)	.	.	.	.	no
C115	C111	C112	C113	1.7(4)	.	.	.	.	no
C115	C111	C112	C117	172.1(3)	.	.	.	.	no
C116	C111	C112	Zr1	120.1(4)	.	.	.	.	no
C116	C111	C112	C113	-176.7(3)	.	.	.	.	no
C116	C111	C112	C117	-6.3(6)	.	.	.	.	no
Zr1	C111	C115	C114	-74.5(2)	.	.	.	.	no
Zr1	C111	C115	C120	65.1(3)	.	.	.	.	no
C112	C111	C115	Zr1	71.3(2)	.	.	.	.	no
C112	C111	C115	C114	-3.3(4)	.	.	.	.	no
C112	C111	C115	C120	136.4(3)	.	.	.	.	no
C116	C111	C115	Zr1	-110.3(3)	.	.	.	.	no
C116	C111	C115	C114	175.2(3)	.	.	.	.	no
C116	C111	C115	C120	-45.2(5)	.	.	.	.	no
Zr1	C112	C113	C114	58.6(2)	.	.	.	.	no
Zr1	C112	C113	C118	-130.8(3)	.	.	.	.	no
C111	C112	C113	Zr1	-58.0(2)	.	.	.	.	no
C111	C112	C113	C114	0.6(4)	.	.	.	.	no
C111	C112	C113	C118	171.2(3)	.	.	.	.	no
C117	C112	C113	Zr1	131.0(3)	.	.	.	.	no
C117	C112	C113	C114	-170.4(3)	.	.	.	.	no
C117	C112	C113	C118	0.2(5)	.	.	.	.	no
Zr1	C113	C114	C115	59.9(2)	.	.	.	.	no
Zr1	C113	C114	C119	-129.9(4)	.	.	.	.	no
C112	C113	C114	Zr1	-62.5(2)	.	.	.	.	no
C112	C113	C114	C115	-2.7(4)	.	.	.	.	no
C112	C113	C114	C119	167.6(3)	.	.	.	.	no
C118	C113	C114	Zr1	127.3(3)	.	.	.	.	no
C118	C113	C114	C115	-172.8(3)	.	.	.	.	no
C118	C113	C114	C119	-2.6(6)	.	.	.	.	no
Zr1	C114	C115	C111	73.4(2)	.	.	.	.	no
Zr1	C114	C115	C120	-66.2(3)	.	.	.	.	no
C113	C114	C115	Zr1	-69.8(2)	.	.	.	.	no
C113	C114	C115	C111	3.6(4)	.	.	.	.	no
C113	C114	C115	C120	-136.0(3)	.	.	.	.	no
C119	C114	C115	Zr1	119.6(3)	.	.	.	.	no
C119	C114	C115	C111	-167.0(3)	.	.	.	.	no
C119	C114	C115	C120	53.3(5)	.	.	.	.	no
C111	C115	C120	Zr1	-66.2(3)	.	.	.	.	no
C114	C115	C120	Zr1	68.2(3)	.	.	.	.	no
O1	C121	C122	C123	-34.1(4)	.	.	.	.	no
C121	C122	C123	C124	34.5(4)	.	.	.	.	no
C122	C123	C124	O1	-21.6(4)	.	.	.	.	no
C26	C21	C22	C23	2.2(5)	.	.	.	.	no
B2	C21	C22	C23	179.4(3)	.	.	.	.	no
C22	C21	C26	C25	-1.2(5)	.	.	.	.	no
B2	C21	C26	C25	-178.6(3)	.	.	.	.	no
C22	C21	B2	C27	123.9(3)	.	.	.	.	no

C22	C21	B2	C213	-115.4(3)	.	.	.	.	no
C22	C21	B2	C219	9.0(4)	.	.	.	.	no
C26	C21	B2	C27	-59.0(4)	.	.	.	.	no
C26	C21	B2	C213	61.7(4)	.	.	.	.	no
C26	C21	B2	C219	-173.9(3)	.	.	.	.	no
C21	C22	C23	C24	-1.6(5)	.	.	.	.	no
C22	C23	C24	C25	-0.3(5)	.	.	.	.	no
C23	C24	C25	C26	1.3(5)	.	.	.	.	no
C24	C25	C26	C21	-0.5(5)	.	.	.	.	no
C212	C27	C28	C29	0.2(5)	.	.	.	.	no
B2	C27	C28	C29	-171.7(3)	.	.	.	.	no
C28	C27	B2	C21	-23.5(5)	.	.	.	.	no
C28	C27	B2	C213	-141.3(3)	.	.	.	.	no
C28	C27	B2	C219	96.4(3)	.	.	.	.	no
C212	C27	B2	C21	165.0(3)	.	.	.	.	no
C212	C27	B2	C213	47.1(4)	.	.	.	.	no
C212	C27	B2	C219	-75.1(3)	.	.	.	.	no
C28	C27	C212	C211	0.5(5)	.	.	.	.	no
B2	C27	C212	C211	172.7(3)	.	.	.	.	no
C27	C28	C29	C210	-0.7(6)	.	.	.	.	no
C28	C29	C210	C211	0.4(6)	.	.	.	.	no
C29	C210	C211	C212	0.4(5)	.	.	.	.	no
C210	C211	C212	C27	-0.9(5)	.	.	.	.	no
C218	C213	C214	C215	1.9(5)	.	.	.	.	no
B2	C213	C214	C215	179.0(3)	.	.	.	.	no
C214	C213	C218	C217	-2.7(5)	.	.	.	.	no
B2	C213	C218	C217	-179.9(3)	.	.	.	.	no
C214	C213	B2	C21	-100.0(4)	.	.	.	.	no
C214	C213	B2	C27	21.3(4)	.	.	.	.	no
C214	C213	B2	C219	137.1(3)	.	.	.	.	no
C218	C213	B2	C21	77.0(4)	.	.	.	.	no
C218	C213	B2	C27	-161.8(3)	.	.	.	.	no
C218	C213	B2	C219	-46.0(4)	.	.	.	.	no
C213	C214	C215	C216	0.3(6)	.	.	.	.	no
C214	C215	C216	C217	-1.9(5)	.	.	.	.	no
C215	C216	C217	C218	1.1(6)	.	.	.	.	no
C216	C217	C218	C213	1.3(6)	.	.	.	.	no
C224	C219	C220	C221	-1.9(5)	.	.	.	.	no
B2	C219	C220	C221	-176.6(3)	.	.	.	.	no
C220	C219	C224	C223	2.1(5)	.	.	.	.	no
B2	C219	C224	C223	177.0(3)	.	.	.	.	no
C220	C219	B2	C21	-133.7(3)	.	.	.	.	no
C220	C219	B2	C27	106.3(4)	.	.	.	.	no
C220	C219	B2	C213	-13.8(5)	.	.	.	.	no
C224	C219	B2	C21	52.0(4)	.	.	.	.	no
C224	C219	B2	C27	-68.0(4)	.	.	.	.	no
C224	C219	B2	C213	171.9(3)	.	.	.	.	no
C219	C220	C221	C222	0.8(5)	.	.	.	.	no
C220	C221	C222	C223	0.4(5)	.	.	.	.	no
C221	C222	C223	C224	-0.2(5)	.	.	.	.	no
C222	C223	C224	C219	-1.1(5)	.	.	.	.	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

Zr1	H119'	3.55	.	.	.	no
Zr1	H120'	2.95	.	.	.	no
Zr1	H120	2.95	.	.	.	no
O1	C12	3.369(4)	.	.	.	no
O1	C13	3.037(4)	.	.	.	no
O1	C18	3.173(4)	.	.	.	no
O1	C111	3.021(4)	.	.	.	no

O1	C112	3.359(4)	.	.	no
O1	C116	3.052(5)	.	.	no
O1	H116'	2.89	.	.	no
O1	H18'	2.70	.	.	no
O1	H116	2.80	.	.	no
C11	C13	2.303(5)	.	.	no
C11	C14	2.311(5)	.	.	no
C11	C17	2.599(6)	.	.	no
C11	C110	2.628(5)	.	.	no
C11	C120	3.390(5)	.	.	no
C11	C217	3.538(5)	.	1_554	no
C12	O1	3.369(4)	.	.	no
C12	C14	2.307(5)	.	.	no
C12	C15	2.307(5)	.	.	no
C12	C16	2.587(5)	.	.	no
C12	C18	2.616(5)	.	.	no
C13	O1	3.037(4)	.	.	no
C13	C11	2.303(5)	.	.	no
C13	C15	2.304(5)	.	.	no
C13	C17	2.621(5)	.	.	no
C13	C19	2.596(5)	.	.	no
C14	C11	2.311(5)	.	.	no
C14	C12	2.307(5)	.	.	no
C14	C18	2.598(5)	.	.	no
C14	C110	2.593(5)	.	.	no
C15	C12	2.307(5)	.	.	no
C15	C13	2.304(5)	.	.	no
C15	C16	2.633(5)	.	.	no
C15	C19	2.619(5)	.	.	no
C15	C114	3.399(5)	.	.	no
C18	C124	3.542(5)	.	.	no
C19	C222	3.446(5)	.	2_566	no
C22	C224	3.150(5)	.	.	no
C25	C124	3.547(5)	.	.	no
C26	C28	3.377(5)	.	.	no
C28	C224	3.569(5)	.	.	no
C28	C26	3.377(5)	.	.	no
C29	C29	3.559(6)	.	2_556	no
C110	C119	3.266(6)	.	.	no
C111	C113	2.309(5)	.	.	no
C111	O1	3.021(4)	.	.	no
C111	C211	3.370(5)	.	2_556	no
C111	C117	2.622(5)	.	.	no
C111	C114	2.318(5)	.	.	no
C111	C120	2.510(5)	.	.	no
C112	C116	2.607(5)	.	.	no
C112	C114	2.302(5)	.	.	no
C112	C120	3.560(5)	.	.	no
C112	C115	2.317(5)	.	.	no
C112	C211	3.568(5)	.	2_556	no
C112	C118	2.583(5)	.	.	no
C112	O1	3.359(4)	.	.	no
C113	C119	2.628(5)	.	.	no
C113	C115	2.328(5)	.	.	no
C113	C120	3.568(5)	.	.	no
C113	C117	2.571(5)	.	.	no
C113	C111	2.309(5)	.	.	no
C114	C112	2.302(5)	.	.	no
C114	C110	3.582(5)	.	.	no
C114	C120	2.511(5)	.	.	no
C114	C15	3.399(5)	.	.	no
C114	C111	2.318(5)	.	.	no
C114	C118	2.619(5)	.	.	no
C115	C112	2.317(5)	.	.	no
C115	C113	2.328(5)	.	.	no
C115	C119	2.612(5)	.	.	no

C115	C116	2.605(5)	.	.	no
C16	H220	2.94	.	1_554	no
C116	C124	3.524(6)	.	.	no
C16	H17	3.04	.	.	no
C116	C121	3.453(6)	.	.	no
C16	H120	2.91	.	.	no
C116	C211	3.406(5)	.	2_556	no
C116	C212	3.437(5)	.	2_556	no
C16	H110'	2.89	.	.	no
C117	C124	3.536(6)	.	.	no
C17	H18'	3.05	.	.	no
C17	H121	3.03	.	.	no
C17	H16"	2.86	.	.	no
C18	H19	3.05	.	.	no
C18	H124'	3.00	.	.	no
C18	H17'	2.81	.	.	no
C19	H110	2.98	.	.	no
C119	C110	3.266(6)	.	.	no
C19	H18"	2.76	.	.	no
C19	H222	3.03	.	2_566	no
C120	C116	3.165(5)	.	.	no
C120	C113	3.568(5)	.	.	no
C120	C11	3.390(5)	.	.	no
C120	C114	2.511(5)	.	.	no
C120	C119	3.215(5)	.	.	no
C120	C16	3.481(5)	.	.	no
C120	C111	2.510(5)	.	.	no
C120	C112	3.560(5)	.	.	no
C21	H28	2.71	.	.	no
C121	C116	3.453(6)	.	.	no
C21	H224	2.93	.	.	no
C22	H224	2.82	.	.	no
C122	C122	3.568(5)	.	2_656	no
C123	C210	3.574(5)	.	2_656	no
C23	H117'	3.04	.	2_566	no
C124	C25	3.547(5)	.	.	no
C24	H25	3.00	.	2_666	no
C124	C116	3.524(6)	.	.	no
C24	H124'	3.06	.	2_666	no
C124	C117	3.536(6)	.	.	no
C124	C18	3.542(5)	.	.	no
C24	H117"	3.08	.	.	no
C25	H124	3.10	.	.	no
C25	H18"	3.08	.	2_666	no
C26	H28	2.91	.	.	no
C27	H224	3.06	.	.	no
C27	H116"	2.97	.	2_556	no
C27	H214	2.70	.	.	no
C27	H26	3.04	.	.	no
C28	H122	2.86	.	2_656	no
C28	H224	3.09	.	.	no
C29	H122	2.78	.	2_656	no
C210	C123	3.574(5)	.	2_656	no
C110	H16'	2.98	.	.	no
C110	H19'	2.79	.	.	no
C110	H119"	2.78	.	.	no
C211	C116	3.406(5)	.	2_556	no
C211	C111	3.370(5)	.	2_556	no
C111	H120'	2.76	.	.	no
C211	C112	3.568(5)	.	2_556	no
C212	C116	3.437(5)	.	2_556	no
C112	H211	3.07	.	2_556	no
C112	H124	3.04	.	.	no
C212	C214	3.160(5)	.	.	no
C214	C212	3.160(5)	.	.	no
C114	H120	2.75	.	.	no

C115	H120'	2.10	.	.	no
C115	H120	2.10	.	.	no
C116	H124	3.09	.	.	no
C116	H120'	2.91	.	.	no
C116	H117	2.84	.	.	no
C116	H29	2.94	.	.	no
C116	H122'	3.05	.	.	no
C117	H124	2.70	.	.	no
C217	C217	3.591(5)	.	2_667	no
C217	C11	3.538(5)	.	1_556	no
C117	H118"	2.96	.	.	no
C117	H118	3.09	.	.	no
C117	H116	2.92	.	.	no
C118	H117"	3.05	.	.	no
C118	H119"	2.87	.	.	no
C118	H218	2.99	.	2_566	no
C118	H110	2.97	.	.	no
C218	C220	3.219(5)	.	.	no
C118	H117'	2.98	.	.	no
C119	H110'	2.79	.	.	no
C119	H110	3.08	.	.	no
C119	H120	2.96	.	.	no
C119	H118'	2.87	.	.	no
C220	C218	3.219(5)	.	.	no
C120	H119'	2.94	.	.	no
C120	H116'	2.81	.	.	no
C121	H18'	2.97	.	.	no
C121	H214	3.04	.	2_656	no
C121	H116'	2.90	.	.	no
C222	C19	3.446(5)	.	2_566	no
C124	H116	2.87	.	.	no
C224	C22	3.150(5)	.	.	no
C124	H18'	3.09	.	.	no
C224	C28	3.569(5)	.	.	no
C210	H122	3.09	.	2_656	no
C210	H123'	2.77	.	2_656	no
C211	H18'	3.06	.	2_656	no
C211	H116"	2.71	.	2_556	no
C211	H121	2.76	.	2_656	no
C212	H116"	2.57	.	2_556	no
C212	H121	2.94	.	2_656	no
C212	H214	2.69	.	.	no
C213	H26	2.99	.	.	no
C213	H220	2.79	.	.	no
C213	H16	3.00	.	1_556	no
C213	H212	2.84	.	.	no
C214	H212	2.79	.	.	no
C214	H16	3.02	.	1_556	no
C214	H19"	3.05	.	2_666	no
C215	H19"	2.86	.	2_666	no
C215	H16	3.05	.	1_556	no
C216	H217	2.97	.	2_667	no
C216	H16	3.00	.	1_556	no
C216	H19"	2.79	.	2_666	no
C217	H19"	2.88	.	2_666	no
C217	H16	2.96	.	1_556	no
C217	H217	2.82	.	2_667	no
C218	H16	2.95	.	1_556	no
C218	H19"	3.06	.	2_666	no
C218	H220	2.65	.	.	no
C219	H218	2.95	.	.	no
C219	H22	2.69	.	.	no
C220	H218	2.87	.	.	no
C221	H19'	2.97	.	2_566	no
C221	H120'	2.81	.	2_556	no
C222	H116'	2.94	.	2_556	no

C222	H19'	2.96	.	2_566	no
C223	H116'	3.07	.	2_556	no
C223	H29	3.10	.	2_556	no
C224	H29	2.93	.	2_556	no
C224	H22	2.58	.	.	no
H110'	C16	2.89	.	.	no
H110'	H220	2.57	.	1_554	no
H110'	C119	2.79	.	.	no
H110'	H119'	2.45	.	.	no
H110'	H119"	2.37	.	.	no
H110'	H16'	2.36	.	.	no
H110"	H217	2.56	.	1_554	no
H116'	O1	2.89	.	.	no
H116'	C120	2.81	.	.	no
H116'	C121	2.90	.	.	no
H116'	H120'	2.30	.	.	no
H116'	H121'	2.40	.	.	no
H116'	C222	2.94	.	2_556	no
H116'	C223	3.07	.	2_556	no
H116"	C27	2.97	.	2_556	no
H116"	C211	2.71	.	2_556	no
H116"	C212	2.57	.	2_556	no
H117'	H23	2.48	.	2_566	no
H117'	C23	3.04	.	2_566	no
H117'	H22	2.60	.	2_566	no
H117'	C118	2.98	.	.	no
H117"	C118	3.05	.	.	no
H117"	C24	3.08	.	.	no
H117"	H124	2.57	.	.	no
H118'	C119	2.87	.	.	no
H118'	H119"	2.24	.	.	no
H118'	H110	2.32	.	.	no
H118"	H19'	2.60	.	.	no
H118"	C117	2.96	.	.	no
H119'	Zr1	3.55	.	.	no
H119'	H16'	2.33	.	.	no
H119'	C120	2.94	.	.	no
H119'	H110'	2.45	.	.	no
H119'	H120	2.59	.	2_555	no
H119'	H120	2.43	.	.	no
H119"	H110'	2.37	.	.	no
H119"	C118	2.87	.	.	no
H119"	C110	2.78	.	.	no
H119"	H118'	2.24	.	.	no
H119"	H110	2.43	.	.	no
H120'	Zr1	2.95	.	.	no
H120'	H116'	2.30	.	.	no
H120'	C221	2.81	.	2_556	no
H120'	H221	2.59	.	2_556	no
H120'	C116	2.91	.	.	no
H121'	H116'	2.40	.	.	no
H122'	C116	3.05	.	.	no
H122'	H116	2.57	.	.	no
H123'	H210	2.56	.	2_656	no
H123'	C210	2.77	.	2_656	no
H123'	H223	2.59	.	1_655	no
H124'	C24	3.06	.	2_666	no
H124'	H18"	2.56	.	.	no
H124'	C18	3.00	.	.	no
H16	C213	3.00	.	1_554	no
H16	C214	3.02	.	1_554	no
H16	C215	3.05	.	1_554	no
H16	C218	2.95	.	1_554	no
H16	C216	3.00	.	1_554	no
H16	C217	2.96	.	1_554	no
H16'	C110	2.98	.	.	no

H16'	H220	2.41	.	1_554	no
H16'	H110'	2.36	.	.	no
H16'	H119'	2.33	.	.	no
H16"	H120	2.53	.	.	no
H16"	C17	2.86	.	.	no
H16"	H17	2.48	.	.	no
H17	H16"	2.48	.	.	no
H17	C16	3.04	.	.	no
H17'	C18	2.81	.	.	no
H17'	H18'	2.42	.	.	no
H17'	H121	2.42	.	.	no
H18'	O1	2.70	.	.	no
H18'	C17	3.05	.	.	no
H18'	C121	2.97	.	.	no
H18'	C124	3.09	.	.	no
H18'	H17'	2.42	.	.	no
H18'	H121	2.41	.	.	no
H18'	C211	3.06	.	2_656	no
H18'	H211	2.51	.	2_656	no
H18"	H19	2.43	.	.	no
H18"	H124'	2.56	.	.	no
H18"	C25	3.08	.	2_666	no
H18"	C19	2.76	.	.	no
H19	C18	3.05	.	.	no
H19	H18"	2.43	.	.	no
H19'	H118"	2.60	.	.	no
H19'	H110	2.35	.	.	no
H19'	C221	2.97	.	2_566	no
H19'	C110	2.79	.	.	no
H19'	C222	2.96	.	2_566	no
H19"	C216	2.79	.	2_666	no
H19"	C218	3.06	.	2_666	no
H19"	C215	2.86	.	2_666	no
H19"	C217	2.88	.	2_666	no
H19"	C214	3.05	.	2_666	no
H22	H117'	2.60	.	2_566	no
H22	C219	2.69	.	.	no
H22	C224	2.58	.	.	no
H22	H224	2.42	.	.	no
H23	H117'	2.48	.	2_566	no
H24	H25	2.31	.	2_666	no
H25	C24	3.00	.	2_666	no
H25	H24	2.31	.	2_666	no
H26	C213	2.99	.	.	no
H26	C27	3.04	.	.	no
H28	C21	2.71	.	.	no
H28	C26	2.91	.	.	no
H29	C223	3.10	.	2_556	no
H29	C224	2.93	.	2_556	no
H29	H224	2.58	.	2_556	no
H29	C116	2.94	.	.	no
H29	H116	2.56	.	.	no
H110	H19'	2.35	.	.	no
H110	H119"	2.43	.	.	no
H110	C19	2.98	.	.	no
H110	H118'	2.32	.	.	no
H110	C119	3.08	.	.	no
H110	C118	2.97	.	.	no
H116	C124	2.87	.	.	no
H116	C117	2.92	.	.	no
H116	O1	2.80	.	.	no
H116	H122'	2.57	.	.	no
H116	H29	2.56	.	.	no
H116	H117	2.30	.	.	no
H116	H124	2.32	.	.	no
H117	H116	2.30	.	.	no

H117	H124	2.26	.	.	no
H117	C116	2.84	.	.	no
H118	C117	3.09	.	.	no
H118	H218	2.42	.	2_566	no
H120	H119'	2.59	.	2_555	no
H120	H119''	2.43	.	.	no
H120	H16''	2.53	.	.	no
H120	Zr1	2.95	.	.	no
H120	C16	2.91	.	.	no
H120	C119	2.96	.	.	no
H120	H120	2.54	.	2_555	no
H121	C212	2.94	.	2_656	no
H121	H17'	2.42	.	.	no
H121	C211	2.76	.	2_656	no
H121	C17	3.03	.	.	no
H121	H18'	2.41	.	.	no
H122	C28	2.86	.	2_656	no
H122	C29	2.78	.	2_656	no
H122	C210	3.09	.	2_656	no
H124	H117	2.26	.	.	no
H124	H117''	2.57	.	.	no
H124	H116	2.32	.	.	no
H124	C25	3.10	.	.	no
H124	C112	3.04	.	.	no
H124	C116	3.09	.	.	no
H124	C117	2.70	.	.	no
H210	H123'	2.56	.	2_656	no
H210	H224	2.57	.	2_556	no
H211	C112	3.07	.	2_556	no
H211	H18'	2.51	.	2_656	no
H212	C213	2.84	.	.	no
H212	C214	2.79	.	.	no
H212	H214	2.52	.	.	no
H214	C27	2.70	.	.	no
H214	C212	2.69	.	.	no
H214	H212	2.52	.	.	no
H214	C121	3.04	.	2_656	no
H216	H217	2.52	.	2_667	no
H217	H110''	2.56	.	1_556	no
H217	C216	2.97	.	2_667	no
H217	C217	2.82	.	2_667	no
H217	H216	2.52	.	2_667	no
H217	H217	2.19	.	2_667	no
H218	C219	2.95	.	.	no
H218	C220	2.87	.	.	no
H218	H220	2.45	.	.	no
H218	C118	2.99	.	2_566	no
H218	H118	2.42	.	2_566	no
H220	C16	2.94	.	1_556	no
H220	C213	2.79	.	.	no
H220	C218	2.65	.	.	no
H220	H110'	2.57	.	1_556	no
H220	H16'	2.41	.	1_556	no
H220	H218	2.45	.	.	no
H221	H120'	2.59	.	2_556	no
H222	C19	3.03	.	2_566	no
H223	H123'	2.59	.	1_455	no
H224	C21	2.93	.	.	no
H224	C22	2.82	.	.	no
H224	C27	3.06	.	.	no
H224	C28	3.09	.	.	no
H224	H22	2.42	.	.	no
H224	H29	2.58	.	2_556	no
H224	H210	2.57	.	2_556	no

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