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Pentaarylfullerenes as noncoordinating cyclopentadienyl anions

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2008-09-24 # 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            ' Inorg. Chem.'
# 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 : 2008-08-11  11:06:42

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"A remarkable Lewis acid-base adduct: preparation..."
Compound :
Your Reference number :

Please consider this CIF submission for deposition at the Cambridge Data
Base.

Consider this CIF submission for deposition of the fifth X-ray structure
of a manuscript to be submitted to : Inorg. Chem.
(Our Compound_Identification_Code : ql482)

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2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_to_coeditor ?

_journal_date_from_coeditor ?

_journal_date_accepted ?

_journal_date_printers_first ?

_journal_date_printers_final ?

_journal_date_proofs_out ?

_journal_date_proofs_in ?

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_journal_codен_ASTM ?

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_journal_year ?

_journal_volume ?

_journal_issue ?

_journal_page_first ?

_journal_page_last ?

_journal_suppl_publ_number ?

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3. TITLE AND AUTHOR LIST

_publ_section_title

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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_
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_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
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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)
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_publ_section_exptl_prep
;

;
_publ_section_exptl_refinement
;
Refinement was frustrated by a disorder problem: from the solution, it was
clear that the position of the C7 was disordered. The smeared electron density
for C7 has been described by two site occupancy factors with a s.o.f. value of
0.5.

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 $U(\text{H}) = 1.2 U(\text{C})$ or $U(\text{methyl C})$. The methyl-groups were refined as rigid groups, which were allowed to rotate freely. Assigned values of bond distances: secondary C-H = 0.99 Å, and methyl C-H = 0.98 Å.

_publ_section_related_literature

;
;

Insert blank lines between references

_publ_section_references

;
Allen, F. H. (2002). *Acta Cryst.* B**58**, 380--388.

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.

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Wilson, A. J. C. (1992). *International Tables for Crystallography, Volume C*, Kluwer Academic Publishers, Dordrecht, The Netherlands.

;

_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

'C14 H34 N3 O2 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

'C38 H54 B N3 O2 Zr'

_chemical_formula_iupac ?

_chemical_formula_weight 686.90

_chemical_compound_source 'see text'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

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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'

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

_symmetry_cell_setting tetragonal

_symmetry_space_group_name_Hall 'P 4cw 2c'

_symmetry_space_group_name_H-M 'P 43 2 2'

_symmetry_Int_Tables_number 95

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

```
1 x,y,z
2 -y,x,3/4+z
3 -x,-y,1/2+z
4 y,-x,1/4+z
5 x,-y,1/2-z
6 y,x,1/4-z
7 -x,y,-z
8 -y,-x,3/4-z
```

```
_cell_length_a          9.2409(11)
_cell_length_b          9.2409(11)
_cell_length_c         42.481(9)
_cell_angle_alpha       90
_cell_angle_beta        90
_cell_angle_gamma       90
_cell_volume            3627.6(10)
_cell_formula_units_Z    4
```

```
_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used  3254
_cell_measurement_theta_min    2.63
_cell_measurement_theta_max    21.60
_cell_special_details
```

;

The final unit cell was obtained from the xyz centroids of 3254 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 'block'
_exptl_crystal_colour      'colorless'
_exptl_crystal_size_max    0.39
_exptl_crystal_size_mid    0.22
_exptl_crystal_size_min    0.17
_exptl_crystal_size_rad    ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.258
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       1456
_exptl_absorpt_coefficient_mu 0.339
_exptl_absorpt_correction_type 'multi-scan'
_exptl_absorpt_process_details '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min 0.8663
_exptl_absorpt_correction_T_max 0.9441
```

#=====

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 '
```

```

_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, 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_n_index_h
_diffrn_standard_refl_n_index_k
_diffrn_standard_refl_n_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                24726
_diffrn_reflns_av_R_equivalents      0.0990
_diffrn_reflns_av_sigmaI/netI        0.0564
_diffrn_reflns_limit_h_min           -10
_diffrn_reflns_limit_h_max           11
_diffrn_reflns_limit_k_min           -10
_diffrn_reflns_limit_k_max           11
_diffrn_reflns_limit_l_min           -53
_diffrn_reflns_limit_l_max           53
_diffrn_reflns_theta_min             2.40
_diffrn_reflns_theta_max             26.36
_diffrn_measured_fraction_theta_max  0.999
_diffrn_reflns_theta_full            25.00
_diffrn_measured_fraction_theta_full 0.998

_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                 3725
_reflns_number_gt                    3257
_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 (Bruker, 2007)'

```



```

_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 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.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
'calc w=1/[\s2(Fo2)+(0.0437P)2+0.5134P] 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
;
The absolute structure of the molecule actually chosen was
determined by Flack's x-refinement.

(Flack & Bernardinelli, 1999, 2000)
;
_chemical_absolute_configuration  'ad'
_refine_ls_abs_structure_Flack    0.01(6)
_refine_ls_number_reflns          3725
_refine_ls_number_parameters      217
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0581
_refine_ls_R_factor_gt            0.0472
_refine_ls_wR_factor_ref          0.0991
_refine_ls_wR_factor_gt           0.0945
_refine_ls_goodness_of_fit_ref    1.060
_refine_ls_restrained_S_all       1.060
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

```

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_refine_diff_density_max      0.623
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_refine_diff_density_rms      0.062

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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Zr1 Zr Uani 0.00000 0.02750(4) 0.00000 1.000 0.0279(1) . .
O11 O Uani 0.1363(2) 0.0309(2) 0.04420(5) 1.000 0.0344(7) . .
N11 N Uani 0.00000 -0.1890(4) 0.00000 1.000 0.0297(11) . .
N12 N Uani -0.1647(3) 0.1402(3) 0.02061(6) 1.000 0.0370(10) . .
C11 C Uani 0.1261(4) -0.2791(4) -0.00707(9) 1.000 0.0490(16) . .
C12 C Uani -0.1413(5) 0.2876(4) 0.03132(10) 1.000 0.0583(16) . .
C13 C Uani -0.3152(4) 0.0987(5) 0.02394(11) 1.000 0.0657(19) . .
C14 C Uani 0.1249(6) -0.0674(6) 0.07000(9) 1.000 0.085(2) . .
C15 C Uani 0.2241(4) -0.0146(4) 0.09574(8) 1.000 0.0471(13) . .
C16 C Uani 0.2814(6) 0.1279(5) 0.08349(9) 1.000 0.076(2) . .
C17A C Uani 0.2675(9) 0.1265(9) 0.05009(16) 0.500 0.036(3) . .
C17B C Uani 0.1829(10) 0.1628(9) 0.06021(19) 0.500 0.045(3) . .
C21 C Uani 0.8647(3) 0.6645(3) 0.11698(7) 1.000 0.0232(10) . .
C22 C Uani 0.9154(3) 0.5774(4) 0.09206(7) 1.000 0.0274(10) . .
C23 C Uani 1.0604(4) 0.5476(4) 0.08726(7) 1.000 0.0313(10) . .
C24 C Uani 1.1644(4) 0.6023(4) 0.10715(7) 1.000 0.0313(11) . .
C25 C Uani 1.1202(3) 0.6896(4) 0.13205(7) 1.000 0.0323(11) . .
C26 C Uani 0.9744(4) 0.7197(3) 0.13646(7) 1.000 0.0305(10) . .
C27 C Uani 0.6445(3) 0.5949(3) 0.15601(6) 1.000 0.0241(10) . .
C28 C Uani 0.7414(3) 0.5386(4) 0.17833(7) 1.000 0.0301(10) . .
C29 C Uani 0.6956(4) 0.4638(4) 0.20495(7) 1.000 0.0382(11) . .
C210 C Uani 0.5508(4) 0.4414(3) 0.21052(7) 1.000 0.0355(10) . .
C211 C Uani 0.4511(3) 0.4936(3) 0.18892(7) 1.000 0.0317(9) . .
C212 C Uani 0.4981(3) 0.5674(3) 0.16230(6) 1.000 0.0272(9) . .
B2 B Uani 0.6925(4) 0.6925(4) 0.12500 1.000 0.0242(10) . .
H161' H Uiso 0.38418 0.13993 0.08952 1.000 0.0908 . .
H171' H Uiso 0.25139 0.22541 0.04184 0.500 0.0429 . .
H172' H Uiso 0.09814 0.21199 0.06963 0.500 0.0543 . .
H11 H Uiso 0.15104 -0.33707 0.01146 1.000 0.0735 . .
H11' H Uiso 0.20818 -0.21701 -0.01268 1.000 0.0735 . .
H11" H Uiso 0.10359 -0.34341 -0.02474 1.000 0.0735 . .
H12 H Uiso -0.20199 0.35375 0.01904 1.000 0.0877 . .
H12' H Uiso -0.03926 0.31343 0.02848 1.000 0.0877 . .
H12" H Uiso -0.16681 0.29503 0.05365 1.000 0.0877 . .
H13 H Uiso -0.34264 0.10240 0.04621 1.000 0.0987 . .
H13' H Uiso -0.32858 0.00011 0.01596 1.000 0.0987 . .
H13" H Uiso -0.37609 0.16559 0.01189 1.000 0.0987 . .
H14 H Uiso 0.15340 -0.16597 0.06329 1.000 0.1024 . .
```

```

H14' H Uiso 0.02381 -0.07092 0.07771 1.000 0.1024 . .
H15 H Uiso 0.30402 -0.08401 0.09938 1.000 0.0564 . .
H15' H Uiso 0.17040 -0.00071 0.11568 1.000 0.0564 . .
H161 H Uiso 0.22530 0.20920 0.09251 1.000 0.0908 . .
H171 H Uiso 0.35509 0.08541 0.04008 0.500 0.0429 . .
H172 H Uiso 0.22804 0.22962 0.04488 0.500 0.0543 . .
H22 H Uiso 0.84676 0.53721 0.07790 1.000 0.0328 . .
H23 H Uiso 1.08857 0.48859 0.07000 1.000 0.0374 . .
H24 H Uiso 1.26395 0.58107 0.10396 1.000 0.0375 . .
H25 H Uiso 1.19007 0.72873 0.14609 1.000 0.0386 . .
H26 H Uiso 0.94754 0.78065 0.15349 1.000 0.0364 . .
H28 H Uiso 0.84226 0.55220 0.17514 1.000 0.0362 . .
H29 H Uiso 0.76515 0.42787 0.21944 1.000 0.0460 . .
H210 H Uiso 0.51968 0.39104 0.22880 1.000 0.0427 . .
H211 H Uiso 0.35053 0.47894 0.19233 1.000 0.0381 . .
H212 H Uiso 0.42777 0.60086 0.14770 1.000 0.0326 . .

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12

```

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O11 0.0398(13) 0.0309(13) 0.0326(12) 0.0009(10) -0.0096(10) -0.0054(11)
N11 0.028(2) 0.0323(19) 0.0288(18) 0.0000 -0.0030(18) 0.0000
N12 0.0426(19) 0.0338(17) 0.0346(15) -0.0063(13) -0.0054(14) 0.0056(13)
C11 0.051(3) 0.047(2) 0.049(3) -0.0079(19) -0.010(2) 0.0125(19)
C12 0.083(3) 0.039(2) 0.053(3) -0.014(2) 0.023(2) -0.009(2)
C13 0.042(3) 0.060(3) 0.095(4) -0.032(3) -0.019(3) 0.009(2)
C14 0.115(4) 0.108(4) 0.033(2) 0.029(2) -0.022(2) -0.078(3)
C15 0.059(2) 0.055(3) 0.0274(18) 0.0070(19) -0.0033(16) -0.015(2)
C16 0.102(4) 0.082(4) 0.043(2) 0.022(2) -0.032(3) -0.058(3)
C17A 0.040(5) 0.044(5) 0.024(4) 0.002(3) -0.001(3) -0.025(4)
C17B 0.059(6) 0.037(5) 0.039(5) 0.006(4) -0.014(4) -0.004(4)
C21 0.0285(18) 0.0203(17) 0.0208(16) 0.0006(13) 0.0030(13) -0.0015(14)
C22 0.0301(19) 0.0306(19) 0.0214(15) -0.0007(14) -0.0015(14) -0.0007(15)
C23 0.0320(18) 0.032(2) 0.0298(16) -0.0023(15) 0.0056(14) 0.0017(15)
C24 0.0269(19) 0.037(2) 0.0299(18) 0.0075(16) 0.0061(15) 0.0059(16)
C25 0.0250(19) 0.044(2) 0.0279(18) 0.0029(16) -0.0030(14) -0.0035(16)
C26 0.033(2) 0.0350(17) 0.0235(15) -0.0042(13) 0.0034(15) 0.0015(16)
C27 0.0320(19) 0.0220(17) 0.0183(14) -0.0045(12) -0.0033(13) 0.0027(12)
C28 0.0304(17) 0.034(2) 0.0259(16) -0.0004(14) -0.0026(14) -0.0063(15)
C29 0.049(2) 0.040(2) 0.0257(17) 0.0101(16) -0.0085(15) -0.0051(18)
C210 0.053(2) 0.0317(18) 0.0218(15) -0.0006(13) 0.0065(15) -0.0056(15)
C211 0.0320(16) 0.0314(18) 0.0318(15) -0.0051(15) 0.0094(12) -0.0024(13)
C212 0.0300(18) 0.0277(15) 0.0238(14) -0.0029(11) 0.0012(13) 0.0051(14)
B2 0.0263(17) 0.0263(17) 0.020(2) 0.0009(15) -0.0009(15) 0.001(2)

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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_
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_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Zr1      O11      2.261(2)      .      .      yes
Zr1      N11      2.001(4)      .      .      yes
Zr1      N12      2.042(3)      .      .      yes
Zr1      O11      2.261(2)      .      7_555      yes
Zr1      N12      2.042(3)      .      7_555      yes
O11      C14      1.427(5)      .      .      yes
O11      C17A     1.521(9)      .      .      yes
O11      C17B     1.461(9)      .      .      yes
N11      C11      1.463(4)      .      .      yes
N11      C11      1.463(4)      .      7_555      yes
N12      C12      1.452(5)      .      .      yes
N12      C13      1.450(5)      .      .      yes
C14      C15      1.508(6)      .      .      no
C15      C16      1.512(6)      .      .      no
C16      C17A     1.425(8)      .      .      no
C16      C17B     1.382(10)     .      .      no
C17A     C17B     0.953(12)     .      .      no
C11      H11      0.9800        .      .      no
C11      H11'     0.9800        .      .      no
C11      H11"     0.9800        .      .      no
C12      H12      0.9800        .      .      no
C12      H12'     0.9800        .      .      no
C12      H12"     0.9800        .      .      no
C13      H13      0.9800        .      .      no
C13      H13'     0.9800        .      .      no
C13      H13"     0.9800        .      .      no
C14      H14      0.9900        .      .      no
C14      H14'     0.9900        .      .      no
C15      H15      0.9900        .      .      no
C15      H15'     0.9900        .      .      no
C16      H161'    0.9900        .      .      no
C16      H161     0.9900        .      .      no
C17A     H171'    0.9900        .      .      no
C17A     H171     0.9900        .      .      no
C17A     H172     1.0400        .      .      no
C17B     H171'    1.1600        .      .      no
C17B     H172'    0.9900        .      .      no
C17B     H172     0.9900        .      .      no
C21      C22      1.410(4)      .      .      no
C21      C26      1.405(4)      .      .      no
C21      B2       1.648(5)      .      .      yes
C22      C23      1.383(5)      .      .      no
C23      C24      1.376(5)      .      .      no
C24      C25      1.392(5)      .      .      no
C25      C26      1.388(5)      .      .      no
C27      C28      1.404(4)      .      .      no
C27      B2       1.657(3)      .      .      yes
C27      C212     1.402(4)      .      .      no
C28      C29      1.391(5)      .      .      no
C29      C210     1.375(5)      .      .      no
C22      H22      0.9500        .      .      no

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C23	H23	0.9500	.	.	no
C24	H24	0.9500	.	.	no
C25	H25	0.9500	.	.	no
C26	H26	0.9500	.	.	no
C28	H28	0.9500	.	.	no
C29	H29	0.9500	.	.	no
C210	C211	1.387(4)	.	.	no
C211	C212	1.390(4)	.	.	no
C210	H210	0.9500	.	.	no
C211	H211	0.9500	.	.	no
C212	H212	0.9500	.	.	no

loop_

_geom_angle_atom_site_label_1

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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

O11	Zr1	N11	90.80(5)	.	.	.	yes
O11	Zr1	N12	92.98(9)	.	.	.	yes
O11	Zr1	O11	178.41(7)	.	.	7_555	yes
O11	Zr1	N12	86.20(9)	.	.	7_555	yes
N11	Zr1	N12	120.67(8)	.	.	.	yes
O11	Zr1	N11	90.80(5)	7_555	.	.	yes
N11	Zr1	N12	120.67(8)	.	.	7_555	yes
O11	Zr1	N12	86.20(9)	7_555	.	.	yes
N12	Zr1	N12	118.65(11)	.	.	7_555	yes
O11	Zr1	N12	92.98(9)	7_555	.	7_555	yes
Zr1	O11	C14	126.0(2)	.	.	.	yes
Zr1	O11	C17A	126.1(3)	.	.	.	yes
Zr1	O11	C17B	124.2(3)	.	.	.	yes
C14	O11	C17A	107.6(4)	.	.	.	yes
C14	O11	C17B	101.3(4)	.	.	.	yes
C17A	O11	C17B	37.2(5)	.	.	.	yes
Zr1	N11	C11	124.68(19)	.	.	.	yes
Zr1	N11	C11	124.68(19)	.	.	7_555	yes
C11	N11	C11	110.6(3)	.	.	7_555	yes
Zr1	N12	C12	120.1(2)	.	.	.	yes
Zr1	N12	C13	128.5(2)	.	.	.	yes
C12	N12	C13	111.1(3)	.	.	.	yes
O11	C14	C15	107.8(4)	.	.	.	yes
C14	C15	C16	104.2(3)	.	.	.	no
C15	C16	C17A	107.7(5)	.	.	.	no
C15	C16	C17B	102.6(5)	.	.	.	no
C17A	C16	C17B	39.7(5)	.	.	.	no
O11	C17A	C16	104.0(5)	.	.	.	yes
O11	C17A	C17B	68.0(7)	.	.	.	yes
C16	C17A	C17B	67.8(7)	.	.	.	no
O11	C17B	C16	109.4(6)	.	.	.	yes
O11	C17B	C17A	74.8(7)	.	.	.	yes
C16	C17B	C17A	72.6(7)	.	.	.	no
N11	C11	H11	109.00	.	.	.	no
N11	C11	H11'	109.00	.	.	.	no
N11	C11	H11''	109.00	.	.	.	no
H11	C11	H11'	109.00	.	.	.	no
H11	C11	H11''	110.00	.	.	.	no
H11'	C11	H11''	109.00	.	.	.	no
N12	C12	H12	109.00	.	.	.	no

N12	C12	H12'	109.00	.	.	.	no
N12	C12	H12"	109.00	.	.	.	no
H12	C12	H12'	109.00	.	.	.	no
H12	C12	H12"	110.00	.	.	.	no
H12'	C12	H12"	109.00	.	.	.	no
N12	C13	H13	109.00	.	.	.	no
N12	C13	H13'	109.00	.	.	.	no
N12	C13	H13"	109.00	.	.	.	no
H13	C13	H13'	109.00	.	.	.	no
H13	C13	H13"	109.00	.	.	.	no
H13'	C13	H13"	109.00	.	.	.	no
O11	C14	H14	110.00	.	.	.	no
O11	C14	H14'	110.00	.	.	.	no
C15	C14	H14	110.00	.	.	.	no
C15	C14	H14'	110.00	.	.	.	no
H14	C14	H14'	108.00	.	.	.	no
C14	C15	H15	111.00	.	.	.	no
C14	C15	H15'	111.00	.	.	.	no
C16	C15	H15	111.00	.	.	.	no
C16	C15	H15'	111.00	.	.	.	no
H15	C15	H15'	109.00	.	.	.	no
C15	C16	H161'	110.00	.	.	.	no
C15	C16	H161	110.00	.	.	.	no
C17A	C16	H161'	110.00	.	.	.	no
C17A	C16	H161	110.00	.	.	.	no
C17B	C16	H161'	142.00	.	.	.	no
C17B	C16	H161	76.00	.	.	.	no
H161'	C16	H161	108.00	.	.	.	no
O11	C17A	H171'	111.00	.	.	.	no
O11	C17A	H171	111.00	.	.	.	no
O11	C17A	H172	103.00	.	.	.	no
C16	C17A	H171'	111.00	.	.	.	no
C16	C17A	H171	111.00	.	.	.	no
C16	C17A	H172	104.00	.	.	.	no
C17B	C17A	H171'	73.00	.	.	.	no
C17B	C17A	H171	178.00	.	.	.	no
C17B	C17A	H172	59.00	.	.	.	no
H171'	C17A	H171	109.00	.	.	.	no
H171'	C17A	H172	14.00	.	.	.	no
H171	C17A	H172	123.00	.	.	.	no
O11	C17B	H171'	105.00	.	.	.	no
O11	C17B	H172'	110.00	.	.	.	no
O11	C17B	H172	110.00	.	.	.	no
C16	C17B	H171'	104.00	.	.	.	no
C16	C17B	H172'	110.00	.	.	.	no
C16	C17B	H172	110.00	.	.	.	no
C17A	C17B	H171'	55.00	.	.	.	no
C17A	C17B	H172'	173.00	.	.	.	no
C17A	C17B	H172	65.00	.	.	.	no
H171'	C17B	H172'	118.00	.	.	.	no
H171'	C17B	H172	10.00	.	.	.	no
H172'	C17B	H172	108.00	.	.	.	no
C22	C21	C26	114.2(3)	.	.	.	no
C22	C21	B2	124.5(2)	.	.	.	yes
C26	C21	B2	121.2(2)	.	.	.	yes
C21	C22	C23	123.1(3)	.	.	.	no
C22	C23	C24	120.9(3)	.	.	.	no
C23	C24	C25	118.3(3)	.	.	.	no
C24	C25	C26	120.2(3)	.	.	.	no
C21	C26	C25	123.2(3)	.	.	.	no
C28	C27	C212	114.8(2)	.	.	.	no

C28	C27	B2	124.6(3)	.	.	.	yes
C212	C27	B2	120.6(2)	.	.	.	yes
C27	C28	C29	122.6(3)	.	.	.	no
C28	C29	C210	120.7(3)	.	.	.	no
C23	C22	H22	118.00	.	.	.	no
C21	C22	H22	118.00	.	.	.	no
C22	C23	H23	120.00	.	.	.	no
C24	C23	H23	120.00	.	.	.	no
C25	C24	H24	121.00	.	.	.	no
C23	C24	H24	121.00	.	.	.	no
C26	C25	H25	120.00	.	.	.	no
C24	C25	H25	120.00	.	.	.	no
C21	C26	H26	118.00	.	.	.	no
C25	C26	H26	118.00	.	.	.	no
C27	C28	H28	119.00	.	.	.	no
C29	C28	H28	119.00	.	.	.	no
C210	C29	H29	120.00	.	.	.	no
C28	C29	H29	120.00	.	.	.	no
C29	C210	C211	118.7(3)	.	.	.	no
C210	C211	C212	120.1(3)	.	.	.	no
C27	C212	C211	123.1(2)	.	.	.	no
C29	C210	H210	121.00	.	.	.	no
C211	C210	H210	121.00	.	.	.	no
C212	C211	H211	120.00	.	.	.	no
C210	C211	H211	120.00	.	.	.	no
C27	C212	H212	118.00	.	.	.	no
C211	C212	H212	118.00	.	.	.	no
C27	B2	C27	109.9(2)	.	.	6_555	yes
C21	B2	C27	109.7(2)	6_555	.	6_555	yes
C21	B2	C27	109.7(2)	.	.	.	yes
C21	B2	C21	110.2(3)	.	.	6_555	yes
C21	B2	C27	108.62(18)	.	.	6_555	yes
C21	B2	C27	108.62(18)	6_555	.	.	yes

loop_

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_geom_torsion_atom_site_label_3
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_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
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N11	Zr1	O11	C14	-37.2(3)	.	.	.	.	no
N11	Zr1	O11	C17A	135.1(4)	.	.	.	.	no
N11	Zr1	O11	C17B	-179.0(4)	.	.	.	.	no
N12	Zr1	O11	C14	83.6(3)	.	.	.	.	no
N12	Zr1	O11	C17A	-104.1(4)	.	.	.	.	no
N12	Zr1	O11	C17B	-58.2(4)	.	.	.	.	no
N12	Zr1	O11	C14	-157.9(3)	7_555	.	.	.	no
N12	Zr1	O11	C17A	14.4(4)	7_555	.	.	.	no
N12	Zr1	O11	C17B	60.3(4)	7_555	.	.	.	no
O11	Zr1	N11	C11	-70.60(19)	.	.	.	.	no
O11	Zr1	N11	C11	109.40(19)	.	.	.	7_555	no
N12	Zr1	N11	C11	-164.5(2)	.	.	.	.	no
N12	Zr1	N11	C11	15.5(2)	.	.	.	7_555	no
O11	Zr1	N11	C11	109.40(19)	7_555	.	.	.	no
N12	Zr1	N11	C11	15.5(2)	7_555	.	.	.	no
O11	Zr1	N12	C12	63.7(3)	.	.	.	.	no

O11	Zr1	N12	C13	-122.9(3)	.	.	.	.	no
N11	Zr1	N12	C12	156.4(2)	.	.	.	.	no
N11	Zr1	N12	C13	-30.2(3)	.	.	.	.	no
O11	Zr1	N12	C12	-114.9(3)	7_555	.	.	.	no
O11	Zr1	N12	C13	58.5(3)	7_555	.	.	.	no
N12	Zr1	N12	C12	-23.6(3)	7_555	.	.	.	no
N12	Zr1	N12	C13	149.8(3)	7_555	.	.	.	no
Zr1	O11	C14	C15	-173.5(2)	.	.	.	.	no
C17A	O11	C14	C15	13.0(5)	.	.	.	.	no
C17B	O11	C14	C15	-25.0(5)	.	.	.	.	no
Zr1	O11	C17A	C16	159.6(3)	.	.	.	.	no
Zr1	O11	C17A	C17B	101.0(6)	.	.	.	.	no
C14	O11	C17A	C16	-26.9(6)	.	.	.	.	no
C14	O11	C17A	C17B	-85.5(7)	.	.	.	.	no
C17B	O11	C17A	C16	58.6(7)	.	.	.	.	no
Zr1	O11	C17B	C16	-171.2(4)	.	.	.	.	no
Zr1	O11	C17B	C17A	-106.4(6)	.	.	.	.	no
C14	O11	C17B	C16	39.5(7)	.	.	.	.	no
C14	O11	C17B	C17A	104.3(7)	.	.	.	.	no
C17A	O11	C17B	C16	-64.9(7)	.	.	.	.	no
O11	C14	C15	C16	5.0(5)	.	.	.	.	no
C14	C15	C16	C17A	-22.4(6)	.	.	.	.	no
C14	C15	C16	C17B	18.5(5)	.	.	.	.	no
C15	C16	C17A	O11	29.9(6)	.	.	.	.	no
C15	C16	C17A	C17B	88.6(8)	.	.	.	.	no
C17B	C16	C17A	O11	-58.7(7)	.	.	.	.	no
C15	C16	C17B	O11	-36.2(6)	.	.	.	.	no
C15	C16	C17B	C17A	-102.5(7)	.	.	.	.	no
C17A	C16	C17B	O11	66.3(7)	.	.	.	.	no
O11	C17A	C17B	C16	116.5(5)	.	.	.	.	no
C16	C17A	C17B	O11	-116.5(5)	.	.	.	.	no
C26	C21	C22	C23	0.5(5)	.	.	.	.	no
B2	C21	C22	C23	-175.3(3)	.	.	.	.	no
C22	C21	C26	C25	-1.1(4)	.	.	.	.	no
B2	C21	C26	C25	174.8(3)	.	.	.	.	no
C22	C21	B2	C27	103.7(3)	.	.	.	.	no
C22	C21	B2	C21	-136.7(3)	.	.	.	6_555	no
C22	C21	B2	C27	-16.4(4)	.	.	.	6_555	no
C26	C21	B2	C27	-71.7(3)	.	.	.	.	no
C26	C21	B2	C21	47.9(3)	.	.	.	6_555	no
C26	C21	B2	C27	168.1(3)	.	.	.	6_555	no
C21	C22	C23	C24	0.3(5)	.	.	.	.	no
C22	C23	C24	C25	-0.6(5)	.	.	.	.	no
C23	C24	C25	C26	0.1(5)	.	.	.	.	no
C24	C25	C26	C21	0.8(5)	.	.	.	.	no
C212	C27	C28	C29	-1.2(5)	.	.	.	.	no
B2	C27	C28	C29	176.4(3)	.	.	.	.	no
C28	C27	B2	C21	20.5(4)	.	.	.	.	no
C28	C27	B2	C21	-100.1(3)	.	.	.	6_555	no
C28	C27	B2	C27	139.8(3)	.	.	.	6_555	no
C212	C27	B2	C21	-162.0(2)	.	.	.	.	no
C212	C27	B2	C21	77.4(3)	.	.	.	6_555	no
C212	C27	B2	C27	-42.7(4)	.	.	.	6_555	no
C28	C27	C212	C211	1.6(4)	.	.	.	.	no
B2	C27	C212	C211	-176.1(3)	.	.	.	.	no
C27	C28	C29	C210	0.1(5)	.	.	.	.	no
C28	C29	C210	C211	0.6(5)	.	.	.	.	no
C29	C210	C211	C212	-0.2(4)	.	.	.	.	no
C210	C211	C212	C27	-1.0(4)	.	.	.	.	no

loop_

_geom_contact_atom_site_label_1					
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_geom_contact_site_symmetry_1					
_geom_contact_site_symmetry_2					
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O11	N11	3.040(3)	.	.	no
O11	N12	3.124(3)	.	.	no
O11	N12	2.944(3)	.	7_555	no
O11	C13	3.392(5)	.	7_555	no
N11	O11	3.040(3)	.	.	no
N11	C14	3.382(5)	.	.	no
N11	O11	3.040(3)	.	7_555	no
N11	C14	3.382(5)	.	7_555	no
N12	O11	3.124(3)	.	.	no
N12	O11	2.944(3)	.	7_555	no
N12	C17A	3.153(7)	.	7_555	no
N12	C17B	3.444(8)	.	7_555	no
N12	H171'	2.8800	.	7_555	no
C12	C17B	3.437(10)	.	.	no
C13	C17A	3.186(8)	.	7_555	no
C14	C25	3.463(6)	.	1_445	no
C14	C24	3.456(6)	.	1_445	no
C15	C25	3.282(5)	.	1_445	no
C17A	C13	3.186(8)	.	7_555	no
C17B	C12	3.437(10)	.	.	no
C22	C212	3.304(4)	.	6_555	no
C24	C14	3.456(6)	.	1_665	no
C25	C14	3.463(6)	.	1_665	no
C25	C15	3.282(5)	.	1_665	no
C26	C26	3.468(5)	.	6_555	no
C26	C28	3.256(5)	.	.	no
C28	C26	3.256(5)	.	.	no
C12	H172'	2.8300	.	.	no
C12	H12'	3.0500	.	7_555	no
C12	H22	3.0400	.	1_455	no
C13	H171	2.7500	.	7_555	no
C13	H171'	3.0900	.	7_555	no
C16	H211	2.9600	.	6_555	no
C17A	H13'	3.0900	.	7_555	no
C17A	H211	2.8600	.	6_555	no
C17A	H13"	2.8400	.	7_555	no
C17B	H12'	2.8200	.	.	no
C21	H26	2.8600	.	6_555	no
C21	H28	2.6900	.	.	no
C22	H11"	2.9600	.	7_665	no
C23	H14	2.9600	.	1_665	no
C24	H212	2.9800	.	1_655	no
C24	H161'	3.0400	.	6_655	no
C24	H14	2.8400	.	1_665	no
C25	H161'	3.0800	.	6_655	no
C25	H212	3.0300	.	1_655	no
C25	H15	3.0300	.	1_665	no
C25	H13	3.0700	.	6_665	no
C25	H15'	2.9800	.	1_665	no
C26	H28	2.5700	.	.	no
C27	H212	2.7800	.	6_555	no
C27	H22	2.6200	.	6_555	no
C28	H15	2.9500	.	6_655	no
C210	C210	3.525(4)	.	5_565	no
C212	C212	3.296(4)	.	6_555	no

C212	C22	3.304(4)	.	6_555	no
C210	H210	3.0200	.	5_565	no
C211	H24	3.0400	.	6_545	no
C212	H22	2.6400	.	6_555	no
C212	H24	2.9900	.	6_545	no
C212	H212	3.0100	.	6_555	no
H161'	H211	2.5300	.	6_555	no
H161'	C24	3.0400	.	6_545	no
H161'	C25	3.0800	.	6_545	no
H171'	C13	3.0900	.	7_555	no
H171'	H211	2.4900	.	6_555	no
H171'	N12	2.8800	.	7_555	no
H172'	H23	2.5600	.	1_455	no
H172'	C12	2.8300	.	.	no
H172'	H12'	2.3600	.	.	no
H11	H11"	2.4200	.	7_555	no
H11'	H13'	2.3000	.	7_555	no
H11"	C22	2.9600	.	7_645	no
H11"	H11	2.4200	.	7_555	no
H11"	H22	2.5500	.	7_645	no
H12	H13"	2.3900	.	.	no
H12'	C17B	2.8200	.	.	no
H12'	H172'	2.3600	.	.	no
H12'	C12	3.0500	.	7_555	no
H12'	H12'	2.5300	.	7_555	no
H12"	H13	2.4300	.	.	no
H12"	H22	2.4700	.	1_455	no
H12"	H25	2.5400	.	6_445	no
H13	H12"	2.4300	.	.	no
H13	C25	3.0700	.	6_445	no
H13'	C17A	3.0900	.	7_555	no
H13'	H11'	2.3000	.	7_555	no
H13'	H171	2.5200	.	7_555	no
H13"	H12	2.3900	.	.	no
H13"	C17A	2.8400	.	7_555	no
H13"	H13"	2.5000	.	7_455	no
H13"	H171	2.3400	.	7_555	no
H14	C23	2.9600	.	1_445	no
H14	C24	2.8400	.	1_445	no
H14'	H26	2.3900	.	6_445	no
H15	C25	3.0300	.	1_445	no
H15	C28	2.9500	.	6_545	no
H15'	C25	2.9800	.	1_445	no
H15'	H15'	2.3700	.	6_555	no
H22	H11"	2.5500	.	7_665	no
H22	H12"	2.4700	.	1_655	no
H22	C27	2.6200	.	6_555	no
H22	C12	3.0400	.	1_655	no
H22	C212	2.6400	.	6_555	no
H23	H172'	2.5600	.	1_655	no
H24	H212	2.4000	.	1_655	no
H24	C211	3.0400	.	6_655	no
H24	C212	2.9900	.	6_655	no
H25	H212	2.5000	.	1_655	no
H25	H12"	2.5400	.	6_665	no
H26	H14'	2.3900	.	6_665	no
H26	C21	2.8600	.	6_555	no
H26	H28	2.5000	.	.	no
H28	C21	2.6900	.	.	no
H28	C26	2.5700	.	.	no
H28	H26	2.5000	.	.	no

H171	H13"	2.3400	.	7_555	no
H171	C13	2.7500	.	7_555	no
H171	H13'	2.5200	.	7_555	no
H210	C210	3.0200	.	5_565	no
H211	C16	2.9600	.	6_555	no
H211	C17A	2.8600	.	6_555	no
H211	H161'	2.5300	.	6_555	no
H211	H171'	2.4900	.	6_555	no
H212	C24	2.9800	.	1_455	no
H212	C25	3.0300	.	1_455	no
H212	H24	2.4000	.	1_455	no
H212	H25	2.5000	.	1_455	no
H212	C27	2.7800	.	6_555	no
H212	C212	3.0100	.	6_555	no

#===END of Crystallographic Information File