Lanthanum tribenzyl complexes as convenient starting materials for organolanthanum chemistry

Bambirra, Sergio; Meetsma, Auke; Hessen, Bart

Published in:
Organometallics

DOI:
10.1021/om060262v

Publication date:
2006

```
# CIF-file generated for C33H45LaO3                  P21/c      Q1009
#==============================================================================
data_Q1009
#==============================================================================

# 0. AUDIT DETAILS

_audit_creation_date                 '2005-06-03  08:26:39'
_audit_creation_method
;
 PLATON <TABLE ACC> option
 SHELXL97-2 & Manual Editing
;
_audit_update_record
;
 ?
;

#==============================================================================

# 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,
     Materials Science Center,
     Groningen University,
     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              'Organometallics'
# Publication choise 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 :  2005-11-11  13:356:39

 Consider this CIF submission for deposition of the first
 X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : Q1009)
;

#==============================================================================

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?

_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              ?

_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
;
 ?
;
_publ_section_title_footnote
;
 ?
;

# The loop structure below should contain the names and adresses 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
;
   'Bambirra, Sergio'
;
 ? # author related footnote
;
;
 Center for Catalytic Olefin Polymerization,
 Stratingh Institute for Chemistry and Chemical Engineering,
 University of Groningen, Nijenborgh 4,
 NL-9747 AG Groningen, The Netherlands
;
```

```
   'Meetsma, Auke'
;
 ? # author related footnote
;
;
 Center for Catalytic Olefin Polymerization,
 Stratingh Institute for Chemistry and Chemical Engineering,
 University of Groningen, Nijenborgh 4,
 NL-9747 AG Groningen, The Netherlands
;
   'Hessen, Bart'
;
 ? # author related footnote
;
;
 Center for Catalytic Olefin Polymerization,
 Stratingh Institute for Chemistry and Chemical Engineering,
 University of Groningen, Nijenborgh 4,
 NL-9747 AG Groningen, The Netherlands

;

#===============================================================================

# 4. TEXT

_publ_section_synopsis
;
 ?
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
; ?
;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
The final difference Fourier map was essentially featureless with a few peaks
 of max. 2.21(10) e/\%A3 within 1.0 \%A from La, but were neglected/rejected,
being artefacts. No other significant peaks (max. = 0.80(10) e/\%A3) having
chemical meaning above the general background were observed in the final
difference Fourier syntheses.
;

# Insert blank lines between references

_publ_section_references
;
 Allen, F.H. (2000). Acta Cryst. B58, 380-388.

 Beurskens, P.T., Beurskens, G., Gelder, R. de   Garc\'ia-Granda, S.
  Gould, R.O.  Isra\"el, & Smits, J.M.M. (1999).
  The DIRDIF99 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.
```

Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

Bruker, (2000). SMART, SAINT, SADABS, XPREP and SHELXTL/NT.
Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

International Tables for Crystallography (1983). Vol. A.
Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
(Present distributor Kluwer Academic Publishers, Dordrecht).

International Tables for Crystallography (1992). Vol. C.
Edited by A.J.C Wilson, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2005). Extended version of the program PLUTO.
Groningen University, The Netherlands. (unpublished).

Sheldrick, G.M. SHELXL97. Program for Crystal Structure
Refinement. University of G\"ottingen, Germany, 1997.

Sheldrick, G.M. SADABS. Version 2.03
Multi-Scan Absorption Correction Program.
University of G\"ottingen, Germany, 2001

Spek, A.L. (1987). Acta Cryst. C43, 1233-1235.

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

Spek, A.L. (1990). Acta Cryst. A46, C-34.

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

_publ_section_figure_captions
;
Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. Perspective ORTEP drawing of the title compound.
Displacement ellipsoids for non-H are represented at the 50%
probability level.
The H-atoms have been omitted to improve clarity.
;

#==

5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety
'C33 H45 La O3'
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

```
'C33 H45 La O3'
_chemical_formula_iupac              ?
_chemical_formula_weight               628.62
_chemical_compound_source           'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 O   O    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
La  La   -0.2871    2.4523
 '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

_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                         14.092(1)
_cell_length_b                         10.443(1)
_cell_length_c                         20.773(2)
_cell_angle_alpha                      90
_cell_angle_beta                      100.879(2)
_cell_angle_gamma                      90
_cell_volume                          3002.1(5)
_cell_formula_units_Z                  4

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      6060
_cell_measurement_theta_min        2.69
_cell_measurement_theta_max       27.47
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   6060 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'block'
_exptl_crystal_colour            'yellow'
_exptl_crystal_size_max           0.51
_exptl_crystal_size_mid           0.42
_exptl_crystal_size_min           0.37
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.391
_exptl_crystal_density_method     'not measured'
```

```
_exptl_crystal_F_000              1296
_exptl_absorpt_coefficient_mu     1.453
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min    0.5136
_exptl_absorpt_correction_T_max    0.6154

#===============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_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            'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean      '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number              0
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?
_diffrn_standards_decay_%             0

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              26265
_diffrn_reflns_av_R_equivalents    0.0317
_diffrn_reflns_av_sigmaI/netI      0.0302
_diffrn_reflns_limit_h_min         -18
_diffrn_reflns_limit_h_max         18
_diffrn_reflns_limit_k_min         -13
_diffrn_reflns_limit_k_max         13
_diffrn_reflns_limit_l_min         -27
_diffrn_reflns_limit_l_max         27
_diffrn_reflns_theta_min           3.33
_diffrn_reflns_theta_max           28.28
_diffrn_measured_fraction_theta_max    0.996
_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 (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total              7422
_reflns_number_gt                 6624
_reflns_threshold_expression      I>2\s(I)

_computing_data_collection          'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement          'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction           'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2004)
 PLATON (Spek, 2003)
;
_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^)+(0.0420P)^2^+1.2911P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    difmap
_refine_ls_hydrogen_treatment     refall
_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          7422
_refine_ls_number_parameters      514
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0337
_refine_ls_R_factor_gt            0.0290
_refine_ls_wR_factor_ref          0.0716
_refine_ls_wR_factor_gt           0.0696
_refine_ls_goodness_of_fit_ref    1.043
_refine_ls_restrained_S_all       1.043
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000
```

```
_refine_diff_density_max         2.209
_refine_diff_density_min        -0.588
_refine_diff_density_rms         0.098

_vrn_publ_code_frame_time_sec     10.0
_vrn_publ_code_meas_time_hour      8.0

#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_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
La La Uani 0.23078(1) 0.09591(1) 0.15236(1) 1.000 0.0132(1) . .
O1 O Uani 0.07899(11) 0.25214(14) 0.11796(7) 1.000 0.0177(4) . .
O2 O Uani 0.27496(11) 0.25862(15) 0.06380(7) 1.000 0.0191(4) . .
O3 O Uani 0.28032(11) 0.31284(14) 0.21604(7) 1.000 0.0180(4) . .
C1 C Uani 0.42004(16) 0.0640(2) 0.16691(11) 1.000 0.0195(6) . .
C2 C Uani 0.41954(15) 0.0179(2) 0.23187(10) 1.000 0.0173(6) . .
C3 C Uani 0.38742(17) -0.1073(2) 0.24486(11) 1.000 0.0189(6) . .
C4 C Uani 0.38050(16) -0.1461(2) 0.30786(11) 1.000 0.0201(6) . .
C5 C Uani 0.40309(17) -0.0636(2) 0.36110(11) 1.000 0.0205(6) . .
C6 C Uani 0.43402(17) 0.0604(2) 0.34934(11) 1.000 0.0219(6) . .
C7 C Uani 0.44126(17) 0.0998(2) 0.28723(12) 1.000 0.0200(6) . .
C8 C Uani 0.16006(17) 0.0619(2) 0.26058(11) 1.000 0.0196(6) . .
C9 C Uani 0.09581(16) -0.0324(2) 0.22574(10) 1.000 0.0181(6) . .
C10 C Uani 0.00245(17) 0.0017(2) 0.19009(11) 1.000 0.0217(6) . .
C11 C Uani -0.05535(18) -0.0852(3) 0.15038(12) 1.000 0.0259(7) . .
C12 C Uani -0.02601(18) -0.2112(3) 0.14423(12) 1.000 0.0261(7) . .
C13 C Uani 0.06424(18) -0.2481(2) 0.17893(12) 1.000 0.0252(7) . .
C14 C Uani 0.12423(17) -0.1612(2) 0.21813(11) 1.000 0.0214(6) . .
C15 C Uani 0.13444(17) -0.0153(2) 0.04573(11) 1.000 0.0197(6) . .
C16 C Uani 0.22116(16) -0.0806(2) 0.03774(11) 1.000 0.0182(6) . .
C17 C Uani 0.25727(18) -0.1875(2) 0.07775(11) 1.000 0.0219(6) . .
C18 C Uani 0.34599(19) -0.2439(2) 0.07456(12) 1.000 0.0259(7) . .
C19 C Uani 0.4030(2) -0.1976(3) 0.03201(12) 1.000 0.0296(8) . .
C20 C Uani 0.36995(19) -0.0917(3) -0.00762(12) 1.000 0.0265(7) . .
C21 C Uani 0.28226(17) -0.0351(2) -0.00455(11) 1.000 0.0209(6) . .
C22 C Uani 0.06040(18) 0.3676(2) 0.15306(12) 1.000 0.0240(7) . .
C23 C Uani -0.03071(18) 0.4265(2) 0.11306(13) 1.000 0.0242(7) . .
C24 C Uani -0.08695(17) 0.3066(2) 0.08596(12) 1.000 0.0239(7) . .
C25 C Uani -0.00788(16) 0.2227(2) 0.06877(11) 1.000 0.0200(6) . .
C26 C Uani 0.37205(16) 0.2846(2) 0.05250(11) 1.000 0.0215(6) . .
C27 C Uani 0.3627(2) 0.4018(3) 0.00880(14) 1.000 0.0306(8) . .
C28 C Uani 0.2638(2) 0.3791(3) -0.03445(14) 1.000 0.0372(9) . .
C29 C Uani 0.20563(18) 0.3241(3) 0.01401(12) 1.000 0.0257(7) . .
C30 C Uani 0.26771(18) 0.3366(2) 0.28344(11) 1.000 0.0210(6) . .
C31 C Uani 0.3260(2) 0.4559(3) 0.30569(13) 1.000 0.0275(7) . .
C32 C Uani 0.32005(19) 0.5299(2) 0.24181(12) 1.000 0.0251(7) . .
C33 C Uani 0.32865(18) 0.4231(2) 0.19390(12) 1.000 0.0217(7) . .
H1 H Uiso 0.429(2) 0.005(3) 0.1343(15) 1.000 0.034(8) . .
H1' H Uiso 0.455(2) 0.140(3) 0.1661(14) 1.000 0.032(8) . .
H3 H Uiso 0.373(2) -0.165(3) 0.2101(13) 1.000 0.026(7) . .
H4 H Uiso 0.359(2) -0.229(3) 0.3148(13) 1.000 0.023(7) . .
H5 H Uiso 0.399(2) -0.092(2) 0.4043(14) 1.000 0.024(7) . .
H6 H Uiso 0.448(2) 0.121(3) 0.3867(15) 1.000 0.033(8) . .
```

```
H7 H Uiso 0.4638(18) 0.179(3) 0.2813(12) 1.000 0.016(6) . .
H8 H Uiso 0.214(2) 0.033(3) 0.2956(14) 1.000 0.030(7) . .
H8' H Uiso 0.126(2) 0.132(3) 0.2724(14) 1.000 0.031(8) . .
H10 H Uiso -0.018(2) 0.089(3) 0.1948(16) 1.000 0.037(9) . .
H11 H Uiso -0.119(2) -0.053(3) 0.1289(15) 1.000 0.032(8) . .
H12 H Uiso -0.0647(19) -0.271(3) 0.1185(13) 1.000 0.022(7) . .
H13 H Uiso 0.085(2) -0.332(3) 0.1780(14) 1.000 0.035(8) . .
H14 H Uiso 0.187(2) -0.186(3) 0.2416(13) 1.000 0.023(7) . .
H15 H Uiso 0.088(2) -0.066(3) 0.0643(16) 1.000 0.038(9) . .
H15' H Uiso 0.107(2) 0.034(3) 0.0118(13) 1.000 0.021(7) . .
H17 H Uiso 0.217(2) -0.215(3) 0.1080(13) 1.000 0.023(7) . .
H18 H Uiso 0.366(2) -0.315(3) 0.1018(14) 1.000 0.028(7) . .
H19 H Uiso 0.461(2) -0.233(3) 0.0305(15) 1.000 0.040(9) . .
H20 H Uiso 0.409(2) -0.056(3) -0.0376(14) 1.000 0.028(7) . .
H21 H Uiso 0.262(2) 0.035(3) -0.0322(13) 1.000 0.023(7) . .
H22 H Uiso 0.121(2) 0.424(3) 0.1565(16) 1.000 0.038(9) . .
H22' H Uiso 0.051(2) 0.341(3) 0.1982(14) 1.000 0.032(8) . .
H23 H Uiso -0.0108(19) 0.476(3) 0.0758(13) 1.000 0.022(7) . .
H23' H Uiso -0.065(2) 0.475(3) 0.1392(14) 1.000 0.028(7) . .
H24 H Uiso -0.115(2) 0.267(3) 0.1204(14) 1.000 0.024(7) . .
H24' H Uiso -0.133(2) 0.324(3) 0.0499(15) 1.000 0.037(8) . .
H25 H Uiso -0.019(2) 0.132(3) 0.0717(13) 1.000 0.024(7) . .
H25' H Uiso 0.0040(19) 0.243(2) 0.0244(13) 1.000 0.021(7) . .
H26 H Uiso 0.394(2) 0.212(3) 0.0325(13) 1.000 0.024(7) . .
H26' H Uiso 0.414(2) 0.301(3) 0.0950(14) 1.000 0.028(7) . .
H27 H Uiso 0.354(3) 0.487(4) 0.0386(17) 1.000 0.052(10) . .
H27' H Uiso 0.423(2) 0.406(3) -0.0163(15) 1.000 0.028(8) . .
H28 H Uiso 0.272(3) 0.314(4) -0.0717(18) 1.000 0.060(11) . .
H28' H Uiso 0.236(3) 0.453(4) -0.0536(17) 1.000 0.050(10) . .
H29 H Uiso 0.170(3) 0.389(3) 0.0368(17) 1.000 0.043(9) . .
H29' H Uiso 0.158(2) 0.266(3) -0.0063(14) 1.000 0.029(7) . .
H30 H Uiso 0.287(2) 0.262(3) 0.3090(14) 1.000 0.027(7) . .
H30' H Uiso 0.203(2) 0.349(3) 0.2822(13) 1.000 0.023(7) . .
H31 H Uiso 0.390(3) 0.436(3) 0.3224(16) 1.000 0.040(9) . .
H31' H Uiso 0.297(2) 0.503(3) 0.3380(15) 1.000 0.041(9) . .
H32 H Uiso 0.264(2) 0.569(3) 0.2310(14) 1.000 0.026(7) . .
H32' H Uiso 0.372(2) 0.594(3) 0.2425(14) 1.000 0.028(8) . .
H33 H Uiso 0.2986(17) 0.440(2) 0.1476(12) 1.000 0.010(6) . .
H33' H Uiso 0.394(2) 0.406(2) 0.1939(13) 1.000 0.018(7) . .

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
La 0.0131(1) 0.0111(1) 0.0146(1) -0.0016(1) 0.0007(1) -0.0003(1)
O1 0.0152(7) 0.0151(7) 0.0210(7) -0.0061(6) -0.0012(6) 0.0018(6)
O2 0.0174(7) 0.0204(8) 0.0189(7) 0.0028(6) 0.0018(6) 0.0003(6)
O3 0.0201(7) 0.0151(7) 0.0188(7) -0.0040(6) 0.0035(6) -0.0034(6)
C1 0.0162(10) 0.0217(11) 0.0200(10) 0.0022(9) 0.0020(8) 0.0015(9)
C2 0.0129(9) 0.0177(10) 0.0199(10) -0.0001(8) -0.0004(8) 0.0029(8)
C3 0.0193(10) 0.0168(10) 0.0191(10) -0.0043(8) 0.0000(8) 0.0018(8)
C4 0.0204(10) 0.0146(10) 0.0241(11) 0.0008(9) 0.0010(9) 0.0007(9)
C5 0.0219(11) 0.0205(11) 0.0178(10) 0.0004(8) 0.0003(9) 0.0021(9)
C6 0.0213(11) 0.0220(11) 0.0206(11) -0.0054(9) -0.0009(9) -0.0007(9)
C7 0.0182(10) 0.0160(10) 0.0247(11) -0.0015(8) 0.0013(9) -0.0012(9)
C8 0.0215(11) 0.0165(10) 0.0214(10) -0.0017(9) 0.0053(9) -0.0008(9)
C9 0.0187(10) 0.0180(10) 0.0188(10) 0.0015(8) 0.0068(8) -0.0014(9)
C10 0.0202(11) 0.0204(11) 0.0249(11) 0.0048(9) 0.0054(9) 0.0000(9)
C11 0.0191(11) 0.0330(13) 0.0245(12) 0.0078(10) 0.0010(9) -0.0049(10)
C12 0.0237(11) 0.0283(12) 0.0252(11) -0.0003(10) 0.0018(9) -0.0110(10)
C13 0.0267(12) 0.0182(11) 0.0306(12) -0.0015(9) 0.0053(10) -0.0047(10)
C14 0.0185(10) 0.0204(11) 0.0244(11) 0.0008(9) 0.0018(9) -0.0002(9)
```

```
C15 0.0189(10) 0.0186(10) 0.0200(10) -0.0051(9) -0.0001(8) 0.0001(9)
C16 0.0196(10) 0.0158(10) 0.0176(10) -0.0068(8) -0.0002(8) -0.0017(8)
C17 0.0258(12) 0.0192(11) 0.0206(10) -0.0039(9) 0.0042(9) -0.0010(9)
C18 0.0332(13) 0.0214(11) 0.0222(11) -0.0004(9) 0.0029(10) 0.0075(10)
C19 0.0301(13) 0.0316(14) 0.0279(12) -0.0001(10) 0.0076(10) 0.0127(11)
C20 0.0270(12) 0.0315(13) 0.0216(11) 0.0008(9) 0.0065(10) 0.0033(10)
C21 0.0235(11) 0.0191(11) 0.0188(10) -0.0009(9) 0.0007(8) 0.0023(9)
C22 0.0214(11) 0.0199(11) 0.0280(12) -0.0107(9) -0.0020(9) 0.0046(9)
C23 0.0227(11) 0.0199(11) 0.0283(12) -0.0062(9) 0.0003(10) 0.0072(9)
C24 0.0170(10) 0.0254(12) 0.0273(12) -0.0040(10) -0.0009(9) 0.0041(9)
C25 0.0171(10) 0.0193(11) 0.0214(10) -0.0047(9) -0.0018(8) -0.0011(9)
C26 0.0190(10) 0.0236(11) 0.0222(11) 0.0035(9) 0.0049(9) 0.0005(9)
C27 0.0309(14) 0.0300(14) 0.0318(13) 0.0090(10) 0.0085(11) 0.0027(11)
C28 0.0275(13) 0.0509(18) 0.0318(14) 0.0208(13) 0.0024(11) 0.0004(13)
C29 0.0195(11) 0.0313(13) 0.0249(11) 0.0090(10) 0.0004(9) 0.0033(10)
C30 0.0220(11) 0.0226(11) 0.0191(10) -0.0057(9) 0.0060(9) -0.0023(9)
C31 0.0254(12) 0.0295(13) 0.0273(12) -0.0116(10) 0.0045(10) -0.0079(11)
C32 0.0241(12) 0.0170(11) 0.0344(13) -0.0070(9) 0.0062(10) -0.0045(10)
C33 0.0236(12) 0.0167(10) 0.0255(12) -0.0049(9) 0.0063(9) -0.0048(9)

#=============================================================================

# 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
;

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
 La      O1       2.6779(16)                    .       .                 yes
 La      O2       2.6630(15)                    .       .                 yes
 La      O3       2.6497(15)                    .       .                 yes
 La      C1         2.648(2)                    .       .                 yes
 La      C8         2.649(2)                    .       .                 yes
 La      C15        2.639(2)                    .       .                 yes
 O1      C22        1.458(3)                    .       .                 yes
 O1      C25        1.471(3)                    .       .                 yes
 O2      C26        1.457(3)                    .       .                 yes
 O2      C29        1.453(3)                    .       .                 yes
 O3      C30        1.465(3)                    .       .                 yes
 O3      C33        1.456(3)                    .       .                 yes
 C1      C2         1.434(3)                    .       .                 no
 C2      C3         1.426(3)                    .       .                 no
 C2      C7         1.419(3)                    .       .                 no
 C3      C4         1.391(3)                    .       .                 no
 C4      C5         1.391(3)                    .       .                 no
 C5      C6         1.402(3)                    .       .                 no
 C6      C7         1.376(3)                    .       .                 no
 C8      C9         1.437(3)                    .       .                 no
 C9      C10        1.428(3)                    .       .                 no
 C9      C14        1.421(3)                    .       .                 no
 C10     C11        1.383(4)                    .       .                 no
 C11     C12        1.392(4)                    .       .                 no
 C12     C13        1.393(4)                    .       .                 no
 C13     C14        1.393(3)                    .       .                 no
```

```
 C15     C16        1.436(3)                    .      .                 no
 C16     C17        1.427(3)                    .      .                 no
 C16     C21        1.423(3)                    .      .                 no
 C17     C18        1.395(4)                    .      .                 no
 C18     C19        1.389(4)                    .      .                 no
 C19     C20        1.405(4)                    .      .                 no
 C20     C21        1.382(4)                    .      .                 no
 C22     C23        1.521(4)                    .      .                 no
 C23     C24        1.531(3)                    .      .                 no
 C24     C25        1.512(3)                    .      .                 no
 C26     C27        1.515(4)                    .      .                 no
 C27     C28        1.528(4)                    .      .                 no
 C28     C29        1.525(4)                    .      .                 no
 C30     C31        1.516(4)                    .      .                 no
 C31     C32        1.524(4)                    .      .                 no
 C32     C33        1.515(3)                    .      .                 no
 C1      H1          0.94(3)                    .      .                 no
 C1      H1'         0.94(3)                    .      .                 no
 C3      H3          0.93(3)                    .      .                 no
 C4      H4          0.94(3)                    .      .                 no
 C5      H5          0.96(3)                    .      .                 no
 C6      H6          0.99(3)                    .      .                 no
 C7      H7          0.90(3)                    .      .                 no
 C8      H8          1.00(3)                    .      .                 no
 C8      H8'         0.93(3)                    .      .                 no
 C10     H10         0.97(3)                    .      .                 no
 C11     H11         0.98(3)                    .      .                 no
 C12     H12         0.93(3)                    .      .                 no
 C13     H13         0.93(3)                    .      .                 no
 C14     H14         0.96(3)                    .      .                 no
 C15     H15         0.98(3)                    .      .                 no
 C15     H15'        0.90(3)                    .      .                 no
 C17     H17         0.97(3)                    .      .                 no
 C18     H18         0.94(3)                    .      .                 no
 C19     H19         0.90(3)                    .      .                 no
 C20     H20         0.98(3)                    .      .                 no
 C21     H21         0.94(3)                    .      .                 no
 C22     H22         1.03(3)                    .      .                 no
 C22     H22'        1.01(3)                    .      .                 no
 C23     H23         1.01(3)                    .      .                 no
 C23     H23'        0.94(3)                    .      .                 no
 C24     H24         0.97(3)                    .      .                 no
 C24     H24'        0.91(3)                    .      .                 no
 C25     H25         0.96(3)                    .      .                 no
 C25     H25'        0.99(3)                    .      .                 no
 C26     H26         0.94(3)                    .      .                 no
 C26     H26'        0.98(3)                    .      .                 no
 C27     H27         1.10(4)                    .      .                 no
 C27     H27'        1.08(3)                    .      .                 no
 C28     H28         1.05(4)                    .      .                 no
 C28     H28'        0.92(4)                    .      .                 no
 C29     H29         1.01(4)                    .      .                 no
 C29     H29'        0.94(3)                    .      .                 no
 C30     H30         0.95(3)                    .      .                 no
 C30     H30'        0.92(3)                    .      .                 no
 C31     H31         0.93(4)                    .      .                 no
 C31     H31'        0.98(3)                    .      .                 no
 C32     H32         0.88(3)                    .      .                 no
 C32     H32'        0.99(3)                    .      .                 no
 C33     H33         0.99(2)                    .      .                 no
 C33     H33'        0.94(3)                    .      .                 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	La	O2	72.90(5)	.	.	.	yes
O1	La	O3	74.59(5)	.	.	.	yes
O1	La	C1	147.54(6)	.	.	.	yes
O1	La	C8	84.18(6)	.	.	.	yes
O1	La	C15	77.62(6)	.	.	.	yes
O2	La	O3	74.06(5)	.	.	.	yes
O2	La	C1	78.31(6)	.	.	.	yes
O2	La	C8	147.80(6)	.	.	.	yes
O2	La	C15	81.45(6)	.	.	.	yes
O3	La	C1	83.44(6)	.	.	.	yes
O3	La	C8	78.28(6)	.	.	.	yes
O3	La	C15	147.21(6)	.	.	.	yes
C1	La	C8	114.73(7)	.	.	.	yes
C1	La	C15	112.83(7)	.	.	.	yes
C8	La	C15	115.91(7)	.	.	.	yes
La	O1	C22	125.47(13)	.	.	.	yes
La	O1	C25	125.17(11)	.	.	.	yes
C22	O1	C25	108.40(16)	.	.	.	yes
La	O2	C26	125.40(12)	.	.	.	yes
La	O2	C29	125.36(14)	.	.	.	yes
C26	O2	C29	108.88(17)	.	.	.	yes
La	O3	C30	123.62(12)	.	.	.	yes
La	O3	C33	127.84(12)	.	.	.	yes
C30	O3	C33	108.44(16)	.	.	.	yes
La	C1	C2	88.05(13)	.	.	.	yes
C1	C2	C3	122.96(19)	.	.	.	no
C1	C2	C7	121.43(19)	.	.	.	no
C3	C2	C7	115.26(19)	.	.	.	no
C2	C3	C4	121.8(2)	.	.	.	no
C3	C4	C5	121.4(2)	.	.	.	no
C4	C5	C6	117.8(2)	.	.	.	no
C5	C6	C7	121.3(2)	.	.	.	no
C2	C7	C6	122.5(2)	.	.	.	no
La	C8	C9	88.09(13)	.	.	.	yes
C8	C9	C10	121.43(19)	.	.	.	no
C8	C9	C14	122.7(2)	.	.	.	no
C10	C9	C14	115.46(19)	.	.	.	no
C9	C10	C11	121.8(2)	.	.	.	no
C10	C11	C12	121.5(2)	.	.	.	no
C11	C12	C13	118.2(2)	.	.	.	no
C12	C13	C14	121.1(2)	.	.	.	no
C9	C14	C13	121.9(2)	.	.	.	no
La	C15	C16	89.53(14)	.	.	.	yes
C15	C16	C17	121.5(2)	.	.	.	no
C15	C16	C21	122.7(2)	.	.	.	no
C17	C16	C21	115.5(2)	.	.	.	no
C16	C17	C18	121.8(2)	.	.	.	no
C17	C18	C19	121.0(2)	.	.	.	no
C18	C19	C20	118.7(3)	.	.	.	no
C19	C20	C21	120.7(2)	.	.	.	no
C16	C21	C20	122.4(2)	.	.	.	no
O1	C22	C23	105.90(18)	.	.	.	yes
C22	C23	C24	101.25(17)	.	.	.	no
C23	C24	C25	101.96(19)	.	.	.	no
O1	C25	C24	105.57(17)	.	.	.	yes
O2	C26	C27	105.60(19)	.	.	.	yes
C26	C27	C28	101.2(2)	.	.	.	no
C27	C28	C29	102.4(2)	.	.	.	no
O2	C29	C28	105.9(2)	.	.	.	yes
O3	C30	C31	105.91(19)	.	.	.	yes
C30	C31	C32	102.3(2)	.	.	.	no

C31	C32	C33	101.57(19)	.	.	.	no
O3	C33	C32	105.94(19)	.	.	.	yes
La	C1	H1	105.6(18)	.	.	.	no
La	C1	H1'	114.4(18)	.	.	.	no
C2	C1	H1	118.8(19)	.	.	.	no
C2	C1	H1'	113.4(18)	.	.	.	no
H1	C1	H1'	114(3)	.	.	.	no
C2	C3	H3	118.4(18)	.	.	.	no
C4	C3	H3	119.8(18)	.	.	.	no
C3	C4	H4	119.7(16)	.	.	.	no
C5	C4	H4	118.8(16)	.	.	.	no
C4	C5	H5	120.6(14)	.	.	.	no
C6	C5	H5	121.7(14)	.	.	.	no
C5	C6	H6	118.4(17)	.	.	.	no
C7	C6	H6	120.3(18)	.	.	.	no
C2	C7	H7	118.0(16)	.	.	.	no
C6	C7	H7	119.5(16)	.	.	.	no
La	C8	H8	107.7(16)	.	.	.	no
La	C8	H8'	114.4(18)	.	.	.	no
C9	C8	H8	118.8(18)	.	.	.	no
C9	C8	H8'	111.3(18)	.	.	.	no
H8	C8	H8'	114(2)	.	.	.	no
C9	C10	H10	116.5(18)	.	.	.	no
C11	C10	H10	121.7(18)	.	.	.	no
C10	C11	H11	115.5(18)	.	.	.	no
C12	C11	H11	122.9(18)	.	.	.	no
C11	C12	H12	122.4(19)	.	.	.	no
C13	C12	H12	119.4(19)	.	.	.	no
C12	C13	H13	120.9(18)	.	.	.	no
C14	C13	H13	118.0(18)	.	.	.	no
C9	C14	H14	116.8(19)	.	.	.	no
C13	C14	H14	121.3(18)	.	.	.	no
La	C15	H15	100.6(19)	.	.	.	no
La	C15	H15'	118.9(19)	.	.	.	no
C16	C15	H15	115.9(18)	.	.	.	no
C16	C15	H15'	115.5(18)	.	.	.	no
H15	C15	H15'	114(3)	.	.	.	no
C16	C17	H17	115.0(18)	.	.	.	no
C18	C17	H17	123.2(18)	.	.	.	no
C17	C18	H18	118.2(17)	.	.	.	no
C19	C18	H18	120.8(17)	.	.	.	no
C18	C19	H19	121(2)	.	.	.	no
C20	C19	H19	120(2)	.	.	.	no
C19	C20	H20	120.6(18)	.	.	.	no
C21	C20	H20	118.8(18)	.	.	.	no
C16	C21	H21	119.2(18)	.	.	.	no
C20	C21	H21	118.4(18)	.	.	.	no
O1	C22	H22	106.4(17)	.	.	.	no
O1	C22	H22'	107.7(18)	.	.	.	no
C23	C22	H22	114.2(17)	.	.	.	no
C23	C22	H22'	111.9(17)	.	.	.	no
H22	C22	H22'	110(2)	.	.	.	no
C22	C23	H23	107.3(16)	.	.	.	no
C22	C23	H23'	112.0(18)	.	.	.	no
C24	C23	H23	109.6(16)	.	.	.	no
C24	C23	H23'	111.5(18)	.	.	.	no
H23	C23	H23'	114(2)	.	.	.	no
C23	C24	H24	109.4(18)	.	.	.	no
C23	C24	H24'	112(2)	.	.	.	no
C25	C24	H24	110.3(18)	.	.	.	no
C25	C24	H24'	111.3(19)	.	.	.	no
H24	C24	H24'	111(3)	.	.	.	no
O1	C25	H25	106.6(17)	.	.	.	no
O1	C25	H25'	109.7(15)	.	.	.	no
C24	C25	H25	114.8(17)	.	.	.	no
C24	C25	H25'	110.9(14)	.	.	.	no

```
 H25     C25     H25'        109(2)              .       .       .          no
 O2      C26     H26      108.5(18)              .       .       .          no
 O2      C26     H26'     108.2(17)              .       .       .          no
 C27     C26     H26      112.6(17)              .       .       .          no
 C27     C26     H26'     111.6(18)              .       .       .          no
 H26     C26     H26'        110(2)              .       .       .          no
 C26     C27     H27      108.8(19)              .       .       .          no
 C26     C27     H27'     109.6(17)              .       .       .          no
 C28     C27     H27         106(2)              .       .       .          no
 C28     C27     H27'     115.9(16)              .       .       .          no
 H27     C27     H27'        115(3)              .       .       .          no
 C27     C28     H28         109(2)              .       .       .          no
 C27     C28     H28'        113(3)              .       .       .          no
 C29     C28     H28         113(2)              .       .       .          no
 C29     C28     H28'        111(3)              .       .       .          no
 H28     C28     H28'        109(3)              .       .       .          no
 O2      C29     H29         108(2)              .       .       .          no
 O2      C29     H29'     110.0(19)              .       .       .          no
 C28     C29     H29         116(2)              .       .       .          no
 C28     C29     H29'     111.9(18)              .       .       .          no
 H29     C29     H29'        105(3)              .       .       .          no
 O3      C30     H30      108.7(18)              .       .       .          no
 O3      C30     H30'     107.3(17)              .       .       .          no
 C31     C30     H30      114.9(18)              .       .       .          no
 C31     C30     H30'     111.8(19)              .       .       .          no
 H30     C30     H30'        108(3)              .       .       .          no
 C30     C31     H31         111(2)              .       .       .          no
 C30     C31     H31'     110.4(18)              .       .       .          no
 C32     C31     H31         109(2)              .       .       .          no
 C32     C31     H31'     112.3(18)              .       .       .          no
 H31     C31     H31'        111(3)              .       .       .          no
 C31     C32     H32      110.9(19)              .       .       .          no
 C31     C32     H32'     114.3(17)              .       .       .          no
 C33     C32     H32      110.7(19)              .       .       .          no
 C33     C32     H32'     110.9(17)              .       .       .          no
 H32     C32     H32'        108(3)              .       .       .          no
 O3      C33     H33      107.9(13)              .       .       .          no
 O3      C33     H33'     111.6(14)              .       .       .          no
 C32     C33     H33      115.7(13)              .       .       .          no
 C32     C33     H33'     109.9(15)              .       .       .          no
 H33     C33     H33'        106(2)              .       .       .          no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 O2      La      O1      C22      -95.59(15)     .       .       .       .   no
 O2      La      O1      C25       97.00(15)     .       .       .       .   no
 O3      La      O1      C22      -17.90(15)     .       .       .       .   no
 O3      La      O1      C25      174.69(15)     .       .       .       .   no
 C1      La      O1      C22      -67.05(19)     .       .       .       .   no
 C1      La      O1      C25      125.54(16)     .       .       .       .   no
 C8      La      O1      C22       61.51(16)     .       .       .       .   no
 C8      La      O1      C25     -105.90(15)     .       .       .       .   no
 C15     La      O1      C22      179.67(16)     .       .       .       .   no
 C15     La      O1      C25       12.27(15)     .       .       .       .   no
 O1      La      O2      C26      162.03(15)     .       .       .       .   no
 O1      La      O2      C29      -25.66(17)     .       .       .       .   no
 O3      La      O2      C26       83.65(15)     .       .       .       .   no
```

O3	La	O2	C29	-104.05(17)	.	.	.	.	no
C1	La	O2	C26	-2.79(15)	.	.	.	.	no
C1	La	O2	C29	169.52(18)	.	.	.	.	no
C8	La	O2	C26	115.45(17)	.	.	.	.	no
C8	La	O2	C29	-72.2(2)	.	.	.	.	no
C15	La	O2	C26	-118.37(15)	.	.	.	.	no
C15	La	O2	C29	53.94(17)	.	.	.	.	no
O1	La	O3	C30	94.58(15)	.	.	.	.	no
O1	La	O3	C33	-89.59(16)	.	.	.	.	no
O2	La	O3	C30	170.79(16)	.	.	.	.	no
O2	La	O3	C33	-13.39(16)	.	.	.	.	no
C1	La	O3	C30	-109.54(16)	.	.	.	.	no
C1	La	O3	C33	66.29(17)	.	.	.	.	no
C8	La	O3	C30	7.46(15)	.	.	.	.	no
C8	La	O3	C33	-176.72(17)	.	.	.	.	no
C15	La	O3	C30	127.59(17)	.	.	.	.	no
C15	La	O3	C33	-56.6(2)	.	.	.	.	no
O1	La	C1	C2	129.18(12)	.	.	.	.	no
O2	La	C1	C2	156.97(13)	.	.	.	.	no
O3	La	C1	C2	81.95(12)	.	.	.	.	no
C8	La	C1	C2	8.10(14)	.	.	.	.	no
C15	La	C1	C2	-127.62(12)	.	.	.	.	no
O1	La	C8	C9	83.31(13)	.	.	.	.	no
O2	La	C8	C9	127.56(13)	.	.	.	.	no
O3	La	C8	C9	158.73(14)	.	.	.	.	no
C1	La	C8	C9	-124.21(13)	.	.	.	.	no
C15	La	C8	C9	10.11(15)	.	.	.	.	no
O1	La	C15	C16	158.86(13)	.	.	.	.	no
O2	La	C15	C16	84.60(13)	.	.	.	.	no
O3	La	C15	C16	126.33(13)	.	.	.	.	no
C1	La	C15	C16	11.20(15)	.	.	.	.	no
C8	La	C15	C16	-123.97(13)	.	.	.	.	no
O2	La	C8	H8	-112.7(19)	.	.	.	.	no
O2	La	C8	H8'	15(2)	.	.	.	.	no
O3	La	C8	H8	-81.6(19)	.	.	.	.	no
O3	La	C8	H8'	46(2)	.	.	.	.	no
C1	La	C8	H8	-4.5(19)	.	.	.	.	no
C1	La	C8	H8'	123(2)	.	.	.	.	no
C15	La	C8	H8	129.8(19)	.	.	.	.	no
C15	La	C8	H8'	-103(2)	.	.	.	.	no
O1	La	C15	H15	-84.9(19)	.	.	.	.	no
O1	La	C15	H15'	40(2)	.	.	.	.	no
O2	La	C15	H15	-159.1(19)	.	.	.	.	no
O2	La	C15	H15'	-35(2)	.	.	.	.	no
O3	La	C15	H15	-117.4(19)	.	.	.	.	no
O3	La	C15	H15'	7(2)	.	.	.	.	no
C1	La	C15	H15	127.5(19)	.	.	.	.	no
C1	La	C15	H15'	-108(2)	.	.	.	.	no
C8	La	C15	H15	-7.7(19)	.	.	.	.	no
C8	La	C15	H15'	117(2)	.	.	.	.	no
O3	La	C1	H1'	-33.0(19)	.	.	.	.	no
C8	La	C1	H1	128(2)	.	.	.	.	no
O1	La	C1	H1	-111(2)	.	.	.	.	no
O1	La	C1	H1'	14.2(19)	.	.	.	.	no
O2	La	C1	H1	-84(2)	.	.	.	.	no
O2	La	C1	H1'	42.0(19)	.	.	.	.	no
O3	La	C1	H1	-159(2)	.	.	.	.	no
C15	La	C1	H1	-8(2)	.	.	.	.	no
C15	La	C1	H1'	117.5(19)	.	.	.	.	no
C8	La	C1	H1'	-106.8(19)	.	.	.	.	no
O1	La	C8	H8'	-29(2)	.	.	.	.	no
O1	La	C8	H8	-157.0(19)	.	.	.	.	no
La	O1	C25	C24	156.55(12)	.	.	.	.	no
C25	O1	C22	C23	-13.6(2)	.	.	.	.	no
La	O1	C22	C23	177.23(13)	.	.	.	.	no
C22	O1	C25	C24	-12.7(2)	.	.	.	.	no

La	O2	C26	C27	-168.23(14)	.	.	.	.	no
C29	O2	C26	C27	18.4(2)	.	.	.	.	no
C26	O2	C29	C28	7.0(3)	.	.	.	.	no
La	O2	C29	C28	-166.42(15)	.	.	.	.	no
C33	O3	C30	C31	-9.7(2)	.	.	.	.	no
La	O3	C30	C31	166.86(14)	.	.	.	.	no
C30	O3	C33	C32	-15.7(2)	.	.	.	.	no
La	O3	C33	C32	168.02(14)	.	.	.	.	no
La	C1	C2	C3	76.7(2)	.	.	.	.	no
La	C1	C2	C7	-96.3(2)	.	.	.	.	no
C1	C2	C3	C4	-174.8(2)	.	.	.	.	no
C7	C2	C3	C4	-1.5(3)	.	.	.	.	no
C1	C2	C7	C6	174.9(2)	.	.	.	.	no
C3	C2	C7	C6	1.4(3)	.	.	.	.	no
C2	C3	C4	C5	1.1(4)	.	.	.	.	no
C3	C4	C5	C6	-0.5(3)	.	.	.	.	no
C4	C5	C6	C7	0.4(4)	.	.	.	.	no
C5	C6	C7	C2	-1.0(4)	.	.	.	.	no
La	C8	C9	C14	82.6(2)	.	.	.	.	no
La	C8	C9	C10	-90.1(2)	.	.	.	.	no
C8	C9	C14	C13	-173.7(2)	.	.	.	.	no
C14	C9	C10	C11	-0.7(3)	.	.	.	.	no
C8	C9	C10	C11	172.5(2)	.	.	.	.	no
C10	C9	C14	C13	-0.6(3)	.	.	.	.	no
C9	C10	C11	C12	1.3(4)	.	.	.	.	no
C10	C11	C12	C13	-0.5(4)	.	.	.	.	no
C11	C12	C13	C14	-0.8(4)	.	.	.	.	no
C12	C13	C14	C9	1.4(4)	.	.	.	.	no
La	C15	C16	C21	-96.9(2)	.	.	.	.	no
La	C15	C16	C17	75.7(2)	.	.	.	.	no
C21	C16	C17	C18	-0.8(3)	.	.	.	.	no
C15	C16	C21	C20	174.0(2)	.	.	.	.	no
C15	C16	C17	C18	-173.9(2)	.	.	.	.	no
C17	C16	C21	C20	1.1(3)	.	.	.	.	no
C16	C17	C18	C19	0.1(4)	.	.	.	.	no
C17	C18	C19	C20	0.5(4)	.	.	.	.	no
C18	C19	C20	C21	-0.3(4)	.	.	.	.	no
C19	C20	C21	C16	-0.5(4)	.	.	.	.	no
O1	C22	C23	C24	33.8(2)	.	.	.	.	no
C22	C23	C24	C25	-40.5(2)	.	.	.	.	no
C23	C24	C25	O1	33.4(2)	.	.	.	.	no
O2	C26	C27	C28	-35.8(2)	.	.	.	.	no
C26	C27	C28	C29	39.0(3)	.	.	.	.	no
C27	C28	C29	O2	-29.1(3)	.	.	.	.	no
O3	C30	C31	C32	30.7(2)	.	.	.	.	no
C30	C31	C32	C33	-39.1(3)	.	.	.	.	no
C31	C32	C33	O3	34.2(2)	.	.	.	.	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

La	C4	4.324(2)	.	.	no
La	C6	4.545(2)	.	.	no
La	C11	4.447(3)	.	.	no
La	C13	4.383(2)	.	.	no
La	C18	4.340(2)	.	.	no
La	H3	3.46(3)	.	.	no
La	H7	3.92(3)	.	.	no
La	H10	3.77(3)	.	.	no
La	H14	3.59(3)	.	.	no
La	H17	3.37(3)	.	.	no
La	H21	3.99(3)	.	.	no

O1	O2	3.173(2)	.	.	no
O1	O3	3.228(2)	.	.	no
O1	C10	3.295(3)	.	.	no
O1	C15	3.332(3)	.	.	no
O1	C29	3.141(3)	.	.	no
O2	O3	3.200(2)	.	.	no
O2	C1	3.353(3)	.	.	no
O2	O1	3.173(2)	.	.	no
O2	C33	3.171(3)	.	.	no
O2	C21	3.390(3)	.	.	no
O3	O1	3.228(2)	.	.	no
O3	O2	3.200(2)	.	.	no
O3	C7	3.319(3)	.	.	no
O3	C8	3.345(3)	.	.	no
O3	C22	3.180(3)	.	.	no
O1	H29	2.71(4)	.	.	no
O1	H10	2.85(3)	.	.	no
O2	H33	2.55(2)	.	.	no
O3	H22	2.62(3)	.	.	no
C1	O2	3.353(3)	.	.	no
C1	C26	3.287(3)	.	.	no
C4	La	4.324(2)	.	.	no
C6	La	4.545(2)	.	.	no
C7	O3	3.319(3)	.	.	no
C7	C30	3.468(3)	.	.	no
C8	C30	3.238(3)	.	.	no
C8	O3	3.345(3)	.	.	no
C10	C25	3.400(3)	.	.	no
C10	O1	3.295(3)	.	.	no
C11	La	4.447(3)	.	.	no
C13	La	4.383(2)	.	.	no
C15	C25	3.285(3)	.	.	no
C15	O1	3.332(3)	.	.	no
C15	C25	3.454(3)	.	3_555	no
C18	La	4.340(2)	.	.	no
C21	O2	3.390(3)	.	.	no
C25	C29	3.572(3)	.	.	no
C25	C15	3.454(3)	.	3_555	no
C25	C10	3.400(3)	.	.	no
C26	C33	3.431(3)	.	.	no
C29	C25	3.572(3)	.	.	no
C30	C7	3.468(3)	.	.	no
C33	C26	3.431(3)	.	.	no
C1	H26'	2.88(3)	.	.	no
C1	H31	2.96(4)	.	2_645	no
C2	H33'	3.02(3)	.	2_645	no
C2	H32'	2.99(3)	.	2_645	no
C3	H14	2.93(3)	.	.	no
C4	H32'	3.03(3)	.	1_545	no
C4	H14	2.84(3)	.	.	no
C4	H8	2.97(3)	.	.	no
C5	H8	2.93(3)	.	.	no
C5	H27'	3.00(3)	.	4_555	no
C5	H26'	2.93(3)	.	2_645	no
C6	H27'	2.85(3)	.	4_555	no
C6	H30	2.96(3)	.	.	no
C6	H18	3.10(3)	.	2_655	no
C7	H32'	2.82(3)	.	2_645	no
C7	H33'	3.05(3)	.	2_645	no
C7	H30	2.86(3)	.	.	no
C8	H30	2.81(3)	.	.	no
C8	H30'	3.08(3)	.	.	no
C8	H23'	2.83(3)	.	2_545	no
C9	H23'	2.92(3)	.	2_545	no
C10	H25	2.78(3)	.	.	no
C10	H22'	3.07(3)	.	2_545	no

C11	H30'	2.80(3)	.	2_545	no
C11	H15	2.95(3)	.	.	no
C11	H25	2.90(3)	.	.	no
C12	H8'	2.93(3)	.	2_545	no
C12	H15	2.94(3)	.	.	no
C13	H17	2.85(3)	.	.	no
C14	H17	2.90(3)	.	.	no
C15	H25	2.93(3)	.	3_555	no
C15	H25	2.79(3)	.	.	no
C17	H3	2.93(3)	.	.	no
C18	H3	2.89(3)	.	.	no
C18	H27	2.92(4)	.	1_545	no
C18	H1	3.02(3)	.	.	no
C19	H1	2.97(3)	.	.	no
C19	H6	3.08(3)	.	2_645	no
C20	H1	3.08(3)	.	.	no
C21	H26	3.05(3)	.	.	no
C22	H30'	3.04(3)	.	.	no
C25	H15'	2.94(3)	.	.	no
C25	H29'	3.08(3)	.	.	no
C25	H10	2.99(3)	.	.	no
C26	H33	2.90(2)	.	.	no
C26	H1'	2.86(3)	.	.	no
C27	H5	3.06(3)	.	4_554	no
C27	H6	3.01(3)	.	4_554	no
C29	H25'	3.01(3)	.	.	no
C29	H33	3.08(2)	.	.	no
C30	H8'	2.90(3)	.	.	no
C32	H4	2.94(3)	.	1_565	no
C33	H22	2.88(3)	.	.	no
C33	H26'	2.87(3)	.	.	no
H1	C18	3.02(3)	.	.	no
H1	C19	2.97(3)	.	.	no
H1	C20	3.08(3)	.	.	no
H1	H3	2.59(4)	.	.	no
H1'	C26	2.86(3)	.	.	no
H1'	H7	2.41(4)	.	.	no
H1'	H26'	2.24(4)	.	.	no
H3	La	3.46(3)	.	.	no
H3	C17	2.93(3)	.	.	no
H3	C18	2.89(3)	.	.	no
H3	H1	2.59(4)	.	.	no
H4	C32	2.94(3)	.	1_545	no
H4	H32'	2.41(4)	.	1_545	no
H5	C27	3.06(3)	.	4_555	no
H5	H27'	2.53(4)	.	4_555	no
H6	C19	3.08(3)	.	2_655	no
H6	H19	2.47(4)	.	2_655	no
H6	C27	3.01(3)	.	4_555	no
H6	H27'	2.13(4)	.	4_555	no
H7	La	3.92(3)	.	.	no
H7	H1'	2.41(4)	.	.	no
H8	C4	2.97(3)	.	.	no
H8	C5	2.93(3)	.	.	no
H8	H14	2.54(4)	.	.	no
H8	H30	2.60(4)	.	.	no
H8'	C30	2.90(3)	.	.	no
H8'	H10	2.38(4)	.	.	no
H8'	H30'	2.50(4)	.	.	no
H8'	C12	2.93(3)	.	2_555	no
H10	La	3.77(3)	.	.	no
H10	O1	2.85(3)	.	.	no
H10	C25	2.99(3)	.	.	no
H10	H8'	2.38(4)	.	.	no
H10	H25	2.59(4)	.	.	no
H11	H30'	2.59(4)	.	2_545	no

H11	H21	2.57(4)	.	3_555	no
H12	H29'	2.45(4)	.	3_555	no
H14	La	3.59(3)	.	.	no
H14	C3	2.93(3)	.	.	no
H14	C4	2.84(3)	.	.	no
H14	H8	2.54(4)	.	.	no
H15	C11	2.95(3)	.	.	no
H15	C12	2.94(3)	.	.	no
H15	H17	2.44(4)	.	.	no
H15	H25	2.58(4)	.	.	no
H15'	C25	2.94(3)	.	.	no
H15'	H21	2.52(4)	.	.	no
H15'	H25	2.57(4)	.	.	no
H15'	H29'	2.58(4)	.	.	no
H15'	H25	2.60(4)	.	3_555	no
H17	La	3.37(3)	.	.	no
H17	C13	2.85(3)	.	.	no
H17	C14	2.90(3)	.	.	no
H17	H15	2.44(4)	.	.	no
H18	H27	2.44(5)	.	1_545	no
H18	C6	3.10(3)	.	2_645	no
H19	H6	2.47(4)	.	2_645	no
H19	H27'	2.49(4)	.	3_655	no
H21	La	3.99(3)	.	.	no
H21	H15'	2.52(4)	.	.	no
H21	H11	2.57(4)	.	3_555	no
H22	O3	2.62(3)	.	.	no
H22	C33	2.88(3)	.	.	no
H22	H33	2.55(4)	.	.	no
H22'	H30'	2.50(4)	.	.	no
H22'	C10	3.07(3)	.	2_555	no
H23'	C8	2.83(3)	.	2_555	no
H23'	C9	2.92(3)	.	2_555	no
H25	C10	2.78(3)	.	.	no
H25	C11	2.90(3)	.	.	no
H25	C15	2.79(3)	.	.	no
H25	H10	2.59(4)	.	.	no
H25	H15	2.58(4)	.	.	no
H25	H15'	2.57(4)	.	.	no
H25	C15	2.93(3)	.	3_555	no
H25	H15'	2.60(4)	.	3_555	no
H25'	C29	3.01(3)	.	.	no
H25'	H29'	2.39(4)	.	.	no
H26	C21	3.05(3)	.	.	no
H26'	C1	2.88(3)	.	.	no
H26'	C33	2.87(3)	.	.	no
H26'	H1'	2.24(4)	.	.	no
H26'	H33	2.57(4)	.	.	no
H26'	H33'	2.39(4)	.	.	no
H26'	C5	2.93(3)	.	2_655	no
H27	C18	2.92(4)	.	1_565	no
H27	H18	2.44(5)	.	1_565	no
H27	H33	2.58(4)	.	.	no
H27'	H19	2.49(4)	.	3_655	no
H27'	C5	3.00(3)	.	4_554	no
H27'	C6	2.85(3)	.	4_554	no
H27'	H5	2.53(4)	.	4_554	no
H27'	H6	2.13(4)	.	4_554	no
H29	O1	2.71(4)	.	.	no
H29'	C25	3.08(3)	.	.	no
H29'	H15'	2.58(4)	.	.	no
H29'	H25'	2.39(4)	.	.	no
H29'	H12	2.45(4)	.	3_555	no
H30	C6	2.96(3)	.	.	no
H30	C7	2.86(3)	.	.	no
H30	C8	2.81(3)	.	.	no

```
 H30     H8          2.60(4)                     .       .                   no
 H30'    C8          3.08(3)                     .       .                   no
 H30'    C22         3.04(3)                     .       .                   no
 H30'    H8'         2.50(4)                     .       .                   no
 H30'    H22'        2.50(4)                     .       .                   no
 H30'    C11         2.80(3)                     .     2_555                 no
 H30'    H11         2.59(4)                     .     2_555                 no
 H31     C1          2.96(4)                     .     2_655                 no
 H32'    C4          3.03(3)                     .     1_565                 no
 H32'    H4          2.41(4)                     .     1_565                 no
 H32'    C2          2.99(3)                     .     2_655                 no
 H32'    C7          2.82(3)                     .     2_655                 no
 H33     O2          2.55(2)                     .       .                   no
 H33     C26         2.90(2)                     .       .                   no
 H33     C29         3.08(2)                     .       .                   no
 H33     H22         2.55(4)                     .       .                   no
 H33     H26'        2.57(4)                     .       .                   no
 H33     H27         2.58(4)                     .       .                   no
 H33'    H26'        2.39(4)                     .       .                   no
 H33'    C2          3.02(3)                     .     2_655                 no
 H33'    C7          3.05(3)                     .     2_655                 no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C33     H33     O2          0.99(2)    2.55(2)   3.171(3)  120.5(15)     .   yes

#===END of Crystallographic Information File
```