Electronic Supplementary Material (ESI) for Chemical Science

data_SX232

#==
CHEMICAL DATA

_chemical_formula_sum   'C126 H84 La3 N3 O21'
_chemical_formula_moiety   'C126 H84 La3 N3 O21'
_chemical_formula_weight   2392.7
_chemical_melting_point   ?
_chemical_absolute_configuration 'CHOOSE rm ad rmad syn or unk'

#==
CRYSTAL DATA
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_symmetry_space_group_name_H-M   'P 65'
_symmetry_space_group_name_Hall 'P 65'
_symmetry_Int_Tables_number   170
loop_
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_symmetry_equiv_pos_as_xyz
1 +X,+Y,+Z
2 +X-Y,+X,5/6+Z

3 -Y,+X-Y,2/3+Z
4 -X,-Y,1/2+Z
5 -X+Y,-X,1/3+Z
6 +Y,-X+Y,1/6+Z
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_cell_length_b 34.2658(14)
_cell_length_c 21.8681(14)
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 120.0000
_cell_volume 22236.3(19)
_cell_formula_units_Z 6
_cell_measurement_reflns_used 46092
_cell_measurement_theta_min 2.60
_cell_measurement_theta_max 25.00
_cell_measurement_temperature 173
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_exptl_crystal_description unknown
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_exptl_crystal_size_min 0.200
_exptl_crystal_density_diffrn 1.072
_exptl_crystal_density_meas ?
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 7200.00
_exptl_absorpt_coefficient_mu 0.899
_exptl_absorpt_correction_type multi-scan
_exptl_absorpt_process_details 'REQAB (Rigaku, 1998)'
_exptl_absorpt_correction_T_min 0.461
_exptl_absorpt_correction_T_max 0.835

#==
EXPERIMENTAL DATA

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_diffrn_detector_area_resol_mean 7.111
_diffrn_reflns_number 63729
_diffrn_reflns_av_R_equivalents 0.0771
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#=============================================================================
# REFINEMENT DATA

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   Refinement was performed using all reflections. The weighted
   R-factor (wR) and goodness of fit (S) are based on F^2^.
   R-factor (gt) are based on F. The threshold expression of
   F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt).
;
_reflns_number_total             25026
_reflns_number_gt                16509
_reflns_threshold_expression     F^2^>2.0\s(F^2^)
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_refine_ls_R_factor_gt           0.0905
_refine_ls_wR_factor_ref         0.2573
_refine_ls_number_restraints     1539
_refine_ls_hydrogen_treatment    constr
_refine_ls_number_reflns         25026
_refine_ls_number_parameters     1339
_refine_ls_goodness_of_fit_ref   1.048
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'w = 1/[\s^2^(Fo^2^)+(0.1357P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_hydrogens   geom
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_refine_ls_shift/su_max          0.066
_refine_diff_density_max         3.33
_refine_diff_density_min         -0.93
_refine_ls_extinction_method     none
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_refine_ls_abs_structure_details
'Flack, H. D. (1983), Acta Cryst. A39, 876-881.  11708 Friedel Pairs'
_refine_ls_abs_structure_Flack   -0.03(2)

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_atom_type_symbol
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_atom_type_scat_source
C C 0.0033 0.0016
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
H H 0.0000 0.0000
;
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International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.4)
;
La La -0.2871 2.4523
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International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
O O 0.0106 0.0060
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
N N 0.0061 0.0033
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
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#===
ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_occupancy
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_atom_site_calc_flag
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_atom_site_disorder_assembly
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La2A La 0.40953(4) 0.69778(4) 0.37481(12) 0.0408(3) Uani 1 6 d . . .
La3A La 0.36418(4) 0.62098(4) 0.54099(12) 0.0418(3) Uani 1 6 d . . .
O1 O 0.1301(4) 0.0385(4) 0.6928(6) 0.0473(10) Uani 1 6 d . . .
O2 O -0.0148(5) -0.1156(5) 0.6403(6) 0.070(2) Uani 1 6 d . . .
O3 O -0.0183(4) -0.0250(5) 0.6195(6) 0.0573(19) Uani 1 6 d . . .
O4 O 0.0574(4) -0.0365(3) 0.5518(5) 0.0418(9) Uani 1 6 d . . .
O5 O 0.0495(4) -0.0542(5) 0.7727(6) 0.0544(17) Uani 1 6 d . . .
O6 O 0.0357(4) 0.0244(4) 0.7263(6) 0.0517(10) Uani 1 6 d . . .
O10 O 0.4301(4) 0.7149(4) 0.2615(6) 0.0465(17) Uani 1 6 d . . .
O11 O 0.3449(4) 0.6474(4) 0.3177(6) 0.0505(16) Uani 1 6 d . . .
O12 O 0.4906(3) 0.7287(4) 0.3914(4) 0.0403(8) Uani 1 6 d . . .
O13 O 0.3431(5) 0.6913(5) 0.4258(6) 0.0550(18) Uani 1 6 d . . .
O14 O 0.4343(5) 0.7799(4) 0.3999(6) 0.0593(17) Uani 1 6 d . . .
O15 O 0.4143(4) 0.7123(4) 0.4938(6) 0.0451(11) Uani 1 6 d . . .
O20 O 0.3119(4) 0.6347(4) 0.4843(7) 0.0570(16) Uani 1 6 d . . .
O21 O 0.3582(5) 0.6817(4) 0.5916(6) 0.063(2) Uani 1 6 d . . .
O22 O 0.3920(4) 0.5696(4) 0.5591(5) 0.0446(9) Uani 1 6 d . . .

O23 O 0.3816(4) 0.6172(4) 0.4267(6) 0.0443(6) Uani 1 6 d . . .
O24 O 0.3017(4) 0.5408(4) 0.5154(6) 0.0515(9) Uani 1 6 d . . .
O25 O 0.4450(4) 0.6763(5) 0.5635(6) 0.0606(19) Uani 1 6 d . . .
O26 O 0.4280(4) 0.6355(4) 0.3527(5) 0.0437(7) Uani 1 6 d . . .
O30 O 0.0858(5) -0.0752(4) 0.6541(6) 0.0706(16) Uani 1 6 d . . .
O37 O -0.2524(4) -0.6229(4) 0.4927(6) 0.0470(13) Uani 1 6 d . . .
N16 N 0.1250(4) -0.1081(5) 0.6337(6) 0.0726(17) Uani 1 6 d . . .
N17A N 0.4669(5) 0.5751(7) 0.5296(8) 0.0474(14) Uiso 0.439(11) 6 d . . .
N17B N 0.4144(6) 0.5171(5) 0.5938(7) 0.0479(15) Uiso 0.561(11) 6 d . . .
N18A N 0.5581(6) 0.7934(5) 0.3647(6) 0.0420(11) Uiso 0.585(12) 6 d . . .
N18B N 0.5560(8) 0.7430(7) 0.4219(8) 0.0413(11) Uiso 0.415(12) 6 d . . .
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C5 C -0.1749(3) -0.5783(3) 0.5397(6) 0.0501(11) Uani 1 6 d . . .
C7 C -0.1324(6) 0.3198(6) 0.6418(9) 0.0527(10) Uani 1 6 d . . .
C8 C -0.2454(6) 0.2619(6) 0.7068(10) 0.0530(11) Uani 1 6 d . . .
C9 C 0.1707(7) 0.1042(7) 0.6432(9) 0.0472(9) Uani 1 6 d . . .
C11 C -0.0930(6) 0.3191(6) 0.6465(9) 0.0526(9) Uani 1 6 d . . .
C12 C 0.1331(6) 0.0624(7) 0.6509(10) 0.0482(10) Uani 1 6 d . . .
C14 C 0.1638(5) -0.3732(5) 0.5490(8) 0.0545(9) Uani 1 6 d . . .
C15 C -0.0041(6) 0.0178(6) 0.7519(10) 0.0515(9) Uani 1 6 d . . .
C16A C 0.4296(4) 0.5839(6) 0.5369(7) 0.0472(12) Uiso 0.439(11) 6 d . . .
C16B C 0.5012(10) 0.6122(9) 0.4937(14) 0.049(2) Uiso 0.439(11) 6 d . . .
C16C C 0.4938(9) 0.5530(10) 0.5343(14) 0.048(2) Uiso 0.439(11) 6 d . . .
C16D C 0.4186(6) 0.5556(6) 0.5608(8) 0.0471(12) Uiso 0.561(11) 6 d . . .
C16E C 0.3720(7) 0.4946(9) 0.6276(12) 0.048(2) Uiso 0.561(11) 6 d . . .
C16F C 0.4280(8) 0.4853(8) 0.6147(11) 0.051(2) Uiso 0.561(11) 6 d . . .
C17A C 0.5321(4) 0.7486(5) 0.3943(7) 0.0410(9) Uiso 0.585(12) 6 d . . .
C17B C 0.6057(5) 0.8266(7) 0.3577(10) 0.044(2) Uiso 0.585(12) 6 d . . .
C17C C 0.5435(7) 0.8202(8) 0.3308(11) 0.045(2) Uiso 0.585(12) 6 d . . .
C17D C 0.5303(5) 0.7590(6) 0.3862(10) 0.0410(9) Uiso 0.415(12) 6 d . . .
C17E C 0.6026(7) 0.7575(10) 0.4389(13) 0.043(2) Uiso 0.415(12) 6 d . . .
C17F C 0.5389(10) 0.7009(8) 0.4561(14) 0.041(2) Uiso 0.415(12) 6 d . . .
C18 C 0.4596(6) 0.3314(7) 0.5178(10) 0.0462(8) Uani 1 6 d . . .
C19 C 0.1727(7) 0.1383(6) 0.6127(9) 0.0469(10) Uani 1 6 d . . .
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C21 C 0.0354(6) 0.2870(6) 0.6635(7) 0.0514(9) Uani 1 6 d . . .
C22 C 0.0688(7) -0.2126(6) 0.4820(9) 0.0480(8) Uani 1 6 d . . .
C23 C 0.0435(5) -0.1254(6) 0.5251(7) 0.0460(8) Uani 1 6 d . . .
C25 C 0.0689(6) -0.1724(6) 0.4802(8) 0.0471(8) Uani 1 6 d . . .
C26 C 0.2547(6) 0.1848(6) 0.6211(9) 0.0464(9) Uani 1 6 d . . .
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C30 C 0.0135(4) 0.0900(4) 0.7001(6) 0.0526(9) Uani 1 6 d . . .
C31 C 0.4172(6) 0.3328(8) 0.5194(8) 0.0453(7) Uani 1 6 d . . .
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C33 C 0.2112(6) 0.2100(6) 0.5562(8) 0.0467(9) Uani 1 6 d . . .
C34 C 0.0403(6) -0.3743(6) 0.5208(6) 0.0517(8) Uani 1 6 d . . .
C35 C 0.0839(7) -0.2940(7) 0.5105(6) 0.0514(8) Uani 1 6 d . . .
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C38 C 0.1993(3) -0.3475(4) 0.5060(5) 0.0550(9) Uani 1 6 d . . .
C39 C 0.0968(6) -0.0947(6) 0.4502(8) 0.0449(9) Uani 1 6 d . . .
C40 C 0.1982(3) -0.3151(4) 0.4689(6) 0.0550(9) Uani 1 6 d . . .
C41 C 0.3769(6) 0.2940(6) 0.5414(6) 0.0455(8) Uani 1 6 d . . .

C42 C 0.0395(6) -0.2487(6) 0.5247(9) 0.0495(8) Uani 1 6 d . . .
C43 C 0.3354(6) 0.2941(6) 0.5399(6) 0.0452(7) Uani 1 6 d . . .
C44 C -0.1617(6) 0.2638(6) 0.7182(9) 0.0529(10) Uani 1 6 d . . .
C45 C 0.0745(6) -0.0447(6) 0.5028(9) 0.0426(8) Uani 1 6 d . . .
C46 C -0.0055(6) 0.3277(6) 0.6678(7) 0.0517(9) Uani 1 6 d . . .
C47 C 0.1250(6) -0.3338(8) 0.5162(11) 0.0535(8) Uani 1 6 d . . .
C48 C 0.2952(6) 0.2584(6) 0.5598(8) 0.0460(8) Uani 1 6 d . . .
C49 C 0.2349(3) -0.3559(4) 0.5013(5) 0.0553(10) Uani 1 6 d . . .
C50 C 0.4861(6) 0.3492(6) 0.4739(9) 0.0467(9) Uani 1 6 d . . .
C51 C 0.0097(4) 0.1283(3) 0.6938(5) 0.0527(9) Uani 1 6 d . . .
C52 C 0.1452(6) 0.4132(6) 0.5797(9) 0.0524(9) Uani 1 6 d . . .
C53 C 0.0404(7) -0.2929(7) 0.5191(6) 0.0504(7) Uani 1 6 d . . .
C54 C 0.2112(6) 0.1148(6) 0.6679(9) 0.0473(10) Uani 1 6 d . . .
C55 C 0.0269(6) 0.1584(6) 0.6374(9) 0.0528(9) Uani 1 6 d . . .
C56 C 0.0818(6) -0.3346(8) 0.5115(7) 0.0520(8) Uani 1 6 d . . .
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C66 C -0.0962(3) -0.4957(3) 0.5532(6) 0.0515(10) Uani 1 6 d . . .
C67 C -0.0523(6) -0.4541(6) 0.5543(9) 0.0516(10) Uani 1 6 d . . .
C69 C 0.2693(3) -0.3320(4) 0.4595(6) 0.0557(10) Uani 1 6 d . . .
C70 C 0.5742(5) 0.3170(6) 0.5044(8) 0.0475(9) Uani 1 6 d . . .
C71 C 0.1962(6) 0.4949(6) 0.5945(9) 0.0529(10) Uani 1 6 d . . .
C72 C 0.0341(6) 0.3270(6) 0.6573(7) 0.0514(8) Uani 1 6 d . . .
C73 C 0.2681(3) -0.2997(4) 0.4223(5) 0.0558(11) Uani 1 6 d . . .
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C77 C 0.0015(6) -0.3313(7) 0.5276(6) 0.0509(8) Uani 1 6 d . . .
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C79 C 0.3406(6) 0.4186(6) 0.4983(8) 0.0453(7) Uani 1 6 d . . .
C80 C 0.5362(5) 0.3216(5) 0.5091(8) 0.0471(9) Uani 1 6 d . . .
C81 C -0.0076(4) 0.0605(3) 0.7484(6) 0.0522(9) Uani 1 6 d . . .
C82 C 0.3733(6) 0.3696(6) 0.4959(7) 0.0449(7) Uani 1 6 d . . .
C83 C 0.3374(6) 0.4551(6) 0.4813(8) 0.0453(7) Uani 1 6 d . . .
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C85 C 0.1070(6) 0.3724(6) 0.5983(9) 0.0517(10) Uani 1 6 d . . .
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C87 C 0.3668(6) 0.5287(6) 0.4301(7) 0.0444(7) Uani 1 6 d . . .
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C90 C 0.2268(6) 0.4956(6) 0.5586(10) 0.0530(10) Uani 1 6 d . . .
C91 C 0.0216(6) 0.1955(6) 0.6421(10) 0.0527(9) Uani 1 6 d . . .
C92 C 0.3990(6) 0.5615(6) 0.3918(8) 0.0442(6) Uani 1 6 d . . .
C93 C -0.2097(6) 0.2941(6) 0.6718(9) 0.0529(10) Uani 1 6 d . . .
C94 C -0.0222(5) 0.1739(6) 0.7353(9) 0.0523(9) Uani 1 6 d . . .
C95 C 0.5068(6) 0.3028(5) 0.5565(8) 0.0468(9) Uani 1 6 d . . .
C96 C 0.2736(6) 0.5379(6) 0.5545(10) 0.0535(10) Uani 1 6 d . . .
C97 C 0.6033(5) 0.3352(6) 0.4588(8) 0.0479(10) Uani 1 6 d . . .
C98 C -0.1289(4) -0.5002(3) 0.5115(6) 0.0511(10) Uani 1 6 d . . .

C99 C 0.3730(6) 0.4117(6) 0.4737(8) 0.0451(7) Uani 1 6 d . . .
C100 C -0.1682(3) -0.5415(3) 0.5048(5) 0.0506(11) Uani 1 6 d . . .
C101 C 0.3683(6) 0.4865(5) 0.4454(7) 0.0447(7) Uani 1 6 d . . .
C102 C 0.1800(6) 0.4131(6) 0.5445(10) 0.0526(10) Uani 1 6 d . . .
C103 C -0.1677(6) 0.2949(6) 0.6751(9) 0.0528(10) Uani 1 6 d . . .
C104 C 0.5305(6) 0.3490(6) 0.4645(8) 0.0473(9) Uani 1 6 d . . .
C105 C -0.0458(6) -0.4186(6) 0.5232(9) 0.0515(9) Uani 1 6 d . . .
C106 C 0.1557(6) -0.3119(6) 0.4757(9) 0.0544(9) Uani 1 6 d . . .
C107 C 0.1199(6) 0.4505(6) 0.6474(8) 0.0525(10) Uani 1 6 d . . .
C108 C 0.3364(6) 0.3312(7) 0.5178(7) 0.0453(8) Uani 1 6 d . . .
C109 C -0.0866(6) 0.2888(5) 0.6874(8) 0.0525(9) Uani 1 6 d . . .
C111 C 0.0396(5) -0.1694(5) 0.5254(7) 0.0471(8) Uani 1 6 d . . .
C112 C 0.4338(6) 0.5118(6) 0.3822(8) 0.0445(7) Uani 1 6 d . . .
C113 C -0.1154(6) -0.4629(6) 0.4805(8) 0.0514(10) Uani 1 6 d . . .
C114 C -0.2381(6) 0.2369(6) 0.7479(9) 0.0532(11) Uani 1 6 d . . .
C116 C -0.1029(3) -0.5324(4) 0.5881(5) 0.0515(11) Uani 1 6 d . . .
C119 C 0.4676(6) 0.3055(5) 0.5648(9) 0.0465(9) Uani 1 6 d . . .
C120 C -0.0366(4) 0.1076(4) 0.7842(5) 0.0525(9) Uani 1 6 d . . .
C121 C 0.5623(6) 0.3664(6) 0.4169(8) 0.0480(10) Uani 1 6 d . . .
C122 C -0.2181(4) -0.6224(4) 0.5326(8) 0.0487(12) Uani 1 6 d . . .
C124 C -0.0785(6) -0.4243(6) 0.4840(8) 0.0516(10) Uani 1 6 d . . .
C125 C 0.1286(6) -0.3688(5) 0.5567(8) 0.0541(9) Uani 1 6 d . . .
C128 C 0.4339(6) 0.5559(6) 0.3669(8) 0.0445(7) Uani 1 6 d . . .
C131 C 0.2326(4) -0.2912(4) 0.4270(6) 0.0556(10) Uani 1 6 d . . .
C132 C 0.1514(6) 0.4525(6) 0.6090(10) 0.0526(9) Uani 1 6 d . . .
C134 C -0.1987(6) 0.2375(6) 0.7545(9) 0.0532(10) Uani 1 6 d . . .
C135 C 0.5987(5) 0.3597(6) 0.4105(8) 0.0482(10) Uani 1 6 d . . .
C136 C 0.2210(6) 0.4533(6) 0.5341(9) 0.0530(10) Uani 1 6 d . . .
C142 C -0.2893(6) 0.2591(6) 0.6974(10) 0.0531(12) Uani 1 6 d . . .
C149 C 0.4023(6) 0.6056(6) 0.3877(9) 0.0442(6) Uani 1 6 d . . .
C150 C 0.6440(5) 0.3275(6) 0.4542(8) 0.0480(11) Uani 1 6 d . . .
C151 C 0.3097(5) -0.3385(6) 0.4575(9) 0.0557(11) Uani 1 6 d . . .
C152 C 0.0847(5) -0.1119(5) 0.6632(8) 0.0719(17) Uani 1 6 d . . .
C153 C 0.1547(7) -0.0642(5) 0.6038(9) 0.074(2) Uani 1 6 d . . .
C154 C 0.1554(6) -0.1248(6) 0.6170(9) 0.0741(19) Uani 1 6 d . . .
H7 H -0.13407 0.33937 0.61256 0.0633 Uiso 1 6 calc R . .
H11 H -0.0683 0.33955 0.62201 0.0631 Uiso 1 6 calc R . .
H14 H 0.16621 -0.39479 0.5734 0.0653 Uiso 1 6 calc R . .
H15A H 0.14043 -0.04561 0.60521 0.1113 Uiso 1 6 calc R . .
H15B H 0.15974 -0.06926 0.56111 0.1113 Uiso 1 6 calc R . .
H15C H 0.18369 -0.04874 0.6253 0.1113 Uiso 1 6 calc R . .
H15D H 0.14498 -0.15425 0.63618 0.1112 Uiso 1 6 calc R . .
H15E H 0.1859 -0.10353 0.63131 0.1112 Uiso 1 6 calc R . .
H15F H 0.15558 -0.12783 0.57251 0.1112 Uiso 1 6 calc R . .
H16A H 0.43757 0.61131 0.51649 0.0566 Uiso 0.439(11) 6 calc R . .
H16B H 0.52668 0.60723 0.48688 0.0734 Uiso 0.439(11) 6 calc R . .
H16C H 0.51159 0.64055 0.51579 0.0734 Uiso 0.439(11) 6 calc R . .
H16D H 0.48844 0.61361 0.45423 0.0734 Uiso 0.439(11) 6 calc R . .
H16E H 0.52232 0.57086 0.51236 0.0726 Uiso 0.439(11) 6 calc R . .
H16F H 0.4772 0.52285 0.51636 0.0726 Uiso 0.439(11) 6 calc R . .
H16G H 0.50009 0.55061 0.57749 0.0726 Uiso 0.439(11) 6 calc R . .
H16H H 0.44543 0.57217 0.53757 0.0565 Uiso 0.561(11) 6 calc R . .
H16I H 0.36933 0.46797 0.64838 0.0726 Uiso 0.561(11) 6 calc R . .
H16J H 0.34676 0.48525 0.59924 0.0726 Uiso 0.561(11) 6 calc R . .

H16K H 0.37153 0.51533 0.65803 0.0726 Uiso 0.561(11) 6 calc R . .
H16L H 0.40313 0.46062 0.63703 0.0767 Uiso 0.561(11) 6 calc R . .
H16M H 0.45426 0.50075 0.64168 0.0767 Uiso 0.561(11) 6 calc R . .
H16N H 0.43595 0.47302 0.5793 0.0767 Uiso 0.561(11) 6 calc R . .
H17A H 0.54714 0.73551 0.41505 0.0492 Uiso 0.585(12) 6 calc R . .
H17B H 0.6239 0.81629 0.37931 0.0666 Uiso 0.585(12) 6 calc R . .
H17C H 0.61155 0.85548 0.37483 0.0666 Uiso 0.585(12) 6 calc R . .
H17D H 0.6136 0.83045 0.31416 0.0666 Uiso 0.585(12) 6 calc R . .
H17E H 0.5105 0.80385 0.32824 0.0677 Uiso 0.585(12) 6 calc R . .
H17F H 0.55626 0.82577 0.28954 0.0677 Uiso 0.585(12) 6 calc R . .
H17G H 0.55378 0.84893 0.35185 0.0677 Uiso 0.585(12) 6 calc R . .
H17H H 0.54159 0.78646 0.3641 0.0492 Uiso 0.415(12) 6 calc R . .
H17I H 0.62266 0.78766 0.42223 0.0640 Uiso 0.415(12) 6 calc R . .
H17J H 0.61114 0.73627 0.42236 0.0640 Uiso 0.415(12) 6 calc R . .
H17K H 0.60533 0.75844 0.48359 0.0640 Uiso 0.415(12) 6 calc R . .
H17L H 0.506 0.68343 0.45242 0.0612 Uiso 0.415(12) 6 calc R . .
H17M H 0.54724 0.70765 0.49925 0.0612 Uiso 0.415(12) 6 calc R . .
H17N H 0.55196 0.68342 0.43943 0.0612 Uiso 0.415(12) 6 calc R . .
H19 H 0.14499 0.13522 0.59927 0.0563 Uiso 1 6 calc R . .
H20 H 0.32033 0.22811 0.61991 0.0553 Uiso 1 6 calc R . .
H21 H 0.06242 0.28631 0.65647 0.0617 Uiso 1 6 calc R . .
H22 H 0.0879 -0.21715 0.45516 0.0576 Uiso 1 6 calc R . .
H23 H 0.02397 -0.12149 0.55202 0.0552 Uiso 1 6 calc R . .
H27 H 0.25041 0.27062 0.51182 0.0555 Uiso 1 6 calc R . .
H29 H 0.44362 0.39318 0.4854 0.0543 Uiso 1 6 calc R . .
H30 H 0.03067 0.08405 0.67138 0.0631 Uiso 1 6 calc R . .
H32 H -0.06642 0.22266 0.70054 0.0623 Uiso 1 6 calc R . .
H33 H 0.1833 0.20475 0.53972 0.0561 Uiso 1 6 calc R . .
H34 H 0.03992 -0.40224 0.52176 0.0620 Uiso 1 6 calc R . .
H35 H 0.11179 -0.26703 0.50463 0.0617 Uiso 1 6 calc R . .
H39 H 0.11702 -0.06945 0.42623 0.0539 Uiso 1 6 calc R . .
H41 H 0.37803 0.2686 0.55667 0.0546 Uiso 1 6 calc R . .
H46 H -0.00585 0.3551 0.66379 0.0620 Uiso 1 6 calc R . .
H49 H 0.23569 -0.37799 0.52666 0.0664 Uiso 1 6 calc R . .
H50 H 0.47815 0.36397 0.44389 0.0560 Uiso 1 6 calc R . .
H54 H 0.21052 0.09226 0.69396 0.0567 Uiso 1 6 calc R . .
H55 H 0.03982 0.1522 0.60295 0.0633 Uiso 1 6 calc R . .
H57 H 0.11029 -0.13912 0.40939 0.0550 Uiso 1 6 calc R . .
H58 H -0.12036 0.2396 0.74872 0.0632 Uiso 1 6 calc R . .
H62 H -0.01148 -0.27131 0.58542 0.0592 Uiso 1 6 calc R . .
H64 H 0.42738 0.43571 0.42005 0.0536 Uiso 1 6 calc R . .
H65 H -0.14671 -0.59878 0.60525 0.0611 Uiso 1 6 calc R . .
H67 H -0.02835 -0.45281 0.57783 0.0619 Uiso 1 6 calc R . .
H70 H 0.57938 0.30037 0.5348 0.0570 Uiso 1 6 calc R . .
H71 H 0.20208 0.52246 0.61286 0.0635 Uiso 1 6 calc R . .
H73 H 0.29165 -0.28334 0.39372 0.0670 Uiso 1 6 calc R . .
H75 H 0.27675 0.15405 0.68377 0.0560 Uiso 1 6 calc R . .
H77 H -0.02558 -0.33059 0.533 0.0611 Uiso 1 6 calc R . .
H78 H -0.00724 -0.20412 0.59044 0.0583 Uiso 1 6 calc R . .
H79 H 0.32012 0.3979 0.52741 0.0544 Uiso 1 6 calc R . .
H83 H 0.3128 0.45803 0.49531 0.0544 Uiso 1 6 calc R . .
H84 H 0.06001 0.41106 0.68751 0.0620 Uiso 1 6 calc R . .
H85 H 0.10313 0.34463 0.58322 0.0620 Uiso 1 6 calc R . .
H87 H 0.34358 0.53301 0.44679 0.0533 Uiso 1 6 calc R . .

H88 H -0.04719 0.04915 0.82352 0.0626 Uiso 1 6 calc R . .
H91 H 0.03534 0.21715 0.61044 0.0632 Uiso 1 6 calc R . .
H93 H -0.21319 0.31468 0.64668 0.0635 Uiso 1 6 calc R . .
H94 H -0.03959 0.17843 0.76531 0.0628 Uiso 1 6 calc R . .
H95 H 0.51326 0.28664 0.58614 0.0562 Uiso 1 6 calc R . .
H100 H -0.19056 -0.54467 0.47634 0.0607 Uiso 1 6 calc R . .
H102 H 0.17564 0.38562 0.52774 0.0631 Uiso 1 6 calc R . .
H106 H 0.1515 -0.29256 0.44867 0.0653 Uiso 1 6 calc R . .
H107 H 0.12425 0.4776 0.66552 0.0629 Uiso 1 6 calc R . .
H108 H 0.30853 0.33087 0.5172 0.0544 Uiso 1 6 calc R . .
H112 H 0.45575 0.50601 0.36483 0.0534 Uiso 1 6 calc R . .
H113 H -0.13608 -0.46434 0.45038 0.0617 Uiso 1 6 calc R . .
H114 H -0.2623 0.21754 0.77388 0.0639 Uiso 1 6 calc R . .
H116 H -0.08054 -0.52926 0.61657 0.0619 Uiso 1 6 calc R . .
H119 H 0.4477 0.2917 0.59833 0.0558 Uiso 1 6 calc R . .
H120 H -0.05372 0.1136 0.81296 0.0629 Uiso 1 6 calc R . .
H121 H 0.55854 0.38415 0.38664 0.0576 Uiso 1 6 calc R . .
H124 H -0.07461 -0.39995 0.45896 0.0620 Uiso 1 6 calc R . .
H125 H 0.10602 -0.3864 0.586 0.0649 Uiso 1 6 calc R . .
H128 H 0.45664 0.57832 0.34168 0.0534 Uiso 1 6 calc R . .
H131 H 0.23177 -0.26914 0.40165 0.0667 Uiso 1 6 calc R . .
H134 H -0.19632 0.21916 0.78524 0.0639 Uiso 1 6 calc R . .
H135 H 0.6187 0.37053 0.37657 0.0578 Uiso 1 6 calc R . .
H136 H 0.2445 0.45301 0.51153 0.0636 Uiso 1 6 calc R . .
H152 H 0.06225 -0.13725 0.68487 0.0863 Uiso 1 6 calc R . .

loop_
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La2A 0.0327(5) 0.0282(5) 0.0650(6) 0.0179(5) 0.0033(5) 0.0085(5)
La3A 0.0280(5) 0.0280(5) 0.0662(6) 0.0116(4) 0.0106(5) 0.0062(5)
O1 0.0289(11) 0.0346(14) 0.068(2) 0.0078(10) 0.0025(13) 0.0160(13)
O2 0.068(3) 0.0336(17) 0.067(5) -0.0057(17) 0.046(4) -0.013(2)
O3 0.0242(16) 0.103(6) 0.051(4) 0.036(2) 0.016(2) 0.023(3)
O4 0.037(2) 0.0323(16) 0.0563(10) 0.0175(15) 0.0194(14) 0.0089(12)
O5 0.036(4) 0.056(4) 0.0623(15) 0.016(3) 0.007(3) 0.030(3)
O6 0.0481(19) 0.0290(16) 0.078(2) 0.0194(14) 0.0188(17) -0.0027(14)
O10 0.034(4) 0.061(4) 0.0618(11) 0.036(4) -0.0029(15) 0.020(2)
O11 0.0393(18) 0.037(3) 0.075(3) 0.0187(19) -0.007(2) 0.006(2)
O12 0.0383(8) 0.0413(10) 0.0418(11) 0.0203(8) -0.0001(6) 0.0007(7)
O13 0.052(2) 0.066(5) 0.071(4) 0.048(3) 0.007(2) 0.016(3)
O14 0.070(4) 0.0345(14) 0.086(4) 0.036(3) -0.032(5) 0.0001(17)
O15 0.029(3) 0.0300(8) 0.0652(11) 0.0068(12) 0.0104(15) 0.0054(10)
O20 0.021(2) 0.037(3) 0.113(5) 0.0142(18) 0.011(2) 0.015(3)
O21 0.064(5) 0.0245(18) 0.090(5) 0.015(2) 0.039(3) 0.011(2)
O22 0.0458(12) 0.0450(11) 0.0483(13) 0.0268(10) 0.0001(7) 0.0008(7)
O23 0.0451(16) 0.0321(8) 0.0631(10) 0.0250(10) 0.0087(11) 0.0111(8)

O24 0.0314(10) 0.0279(11) 0.089(2) 0.0098(9) 0.0110(12) 0.0033(13)
O25 0.0345(17) 0.0441(15) 0.086(4) 0.0068(16) -0.007(3) 0.009(3)
O26 0.0432(16) 0.0316(9) 0.0638(14) 0.0242(10) 0.0087(12) 0.0125(10)
O30 0.098(4) 0.058(2) 0.091(4) 0.066(3) -0.017(3) -0.012(3)
O37 0.040(2) 0.0254(19) 0.071(3) 0.0123(18) 0.012(2) 0.022(2)
N16 0.099(4) 0.060(2) 0.093(4) 0.066(3) -0.016(4) -0.014(3)
C4 0.0395(18) 0.0312(14) 0.0632(13) 0.0180(14) 0.0199(14) 0.0085(13)
C5 0.0396(18) 0.0298(16) 0.076(2) 0.0136(16) 0.0120(19) 0.0182(17)
C7 0.0352(15) 0.0314(17) 0.091(2) 0.0160(13) 0.0147(17) 0.0047(17)
C8 0.0350(16) 0.0323(19) 0.090(2) 0.0157(15) 0.0144(18) 0.0051(19)
C9 0.0312(12) 0.0341(12) 0.0664(18) 0.0090(10) 0.0034(14) 0.0159(13)
C11 0.0354(15) 0.0309(16) 0.091(2) 0.0160(13) 0.0148(17) 0.0045(17)
C12 0.0309(12) 0.0352(12) 0.0659(19) 0.0072(9) 0.0041(13) 0.0163(13)
C14 0.0403(17) 0.0382(18) 0.084(2) 0.0192(15) 0.0162(19) 0.0157(17)
C15 0.0476(18) 0.0285(15) 0.080(2) 0.0198(14) 0.0188(16) -0.0015(14)
C18 0.0362(13) 0.0387(14) 0.0680(17) 0.0220(12) 0.0074(15) 0.0166(14)
C19 0.0321(13) 0.0342(13) 0.0667(19) 0.0107(11) 0.0037(15) 0.0154(13)
C20 0.0328(13) 0.0337(13) 0.0678(17) 0.0138(11) 0.0043(15) 0.0160(13)
C21 0.0371(13) 0.0284(13) 0.0888(19) 0.0163(11) 0.0158(14) 0.0028(14)
C22 0.0408(17) 0.0306(13) 0.0723(16) 0.0177(14) 0.0189(16) 0.0100(13)
C23 0.0401(18) 0.0314(14) 0.0660(15) 0.0175(14) 0.0196(15) 0.0093(14)
C25 0.0406(17) 0.0307(14) 0.0698(15) 0.0178(14) 0.0193(15) 0.0095(13)
C26 0.0323(12) 0.0338(13) 0.0674(18) 0.0123(11) 0.0037(14) 0.0156(13)
C27 0.0340(13) 0.0336(13) 0.0682(18) 0.0147(12) 0.0046(15) 0.0160(13)
C28 0.0415(15) 0.0287(13) 0.0865(19) 0.0179(11) 0.0175(15) 0.0024(14)
C29 0.0365(13) 0.0351(12) 0.0680(16) 0.0207(11) 0.0080(15) 0.0162(13)
C30 0.0463(17) 0.0292(15) 0.083(2) 0.0193(13) 0.0185(16) 0.0007(14)
C31 0.0357(12) 0.0361(13) 0.0680(16) 0.0208(11) 0.0075(14) 0.0167(13)
C32 0.0374(14) 0.0288(13) 0.089(2) 0.0162(11) 0.0160(15) 0.0034(15)
C33 0.0338(13) 0.0339(13) 0.0679(18) 0.0134(12) 0.0042(15) 0.0157(14)
C34 0.0399(15) 0.0323(14) 0.0814(18) 0.0170(14) 0.0162(17) 0.0140(15)
C35 0.0401(16) 0.0324(14) 0.0801(17) 0.0169(13) 0.0174(16) 0.0131(14)
C36 0.0385(14) 0.0285(12) 0.0882(19) 0.0168(11) 0.0165(14) 0.0028(14)
C38 0.0404(17) 0.0391(18) 0.084(2) 0.0189(15) 0.0164(18) 0.0156(17)
C39 0.0400(19) 0.0305(14) 0.0656(15) 0.0186(15) 0.0201(15) 0.0081(13)
C40 0.0405(17) 0.0387(18) 0.084(2) 0.0187(15) 0.0170(18) 0.0157(17)
C41 0.0354(12) 0.0353(12) 0.0683(16) 0.0195(11) 0.0068(15) 0.0165(13)
C42 0.0409(16) 0.0312(13) 0.0746(16) 0.0166(13) 0.0185(15) 0.0112(13)
C43 0.0347(12) 0.0341(11) 0.0682(16) 0.0183(11) 0.0064(14) 0.0167(12)
C44 0.0353(14) 0.0317(17) 0.091(2) 0.0160(13) 0.0146(17) 0.0049(17)
C45 0.038(2) 0.0315(14) 0.0583(11) 0.0177(15) 0.0204(14) 0.0083(13)
C46 0.0357(13) 0.0288(13) 0.090(2) 0.0159(11) 0.0152(14) 0.0037(15)
C47 0.0401(15) 0.0360(16) 0.0833(19) 0.0184(14) 0.0166(17) 0.0151(16)
C48 0.0340(12) 0.0339(12) 0.0682(16) 0.0156(11) 0.0050(14) 0.0159(12)
C49 0.0405(18) 0.0397(19) 0.084(2) 0.0191(16) 0.0166(19) 0.0155(19)
C50 0.0365(14) 0.0402(16) 0.0679(19) 0.0226(13) 0.0073(16) 0.0168(15)
C51 0.0453(17) 0.0292(14) 0.084(2) 0.0189(13) 0.0183(16) 0.0013(14)
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C55 0.0443(17) 0.0293(15) 0.085(2) 0.0185(13) 0.0184(16) 0.0017(14)
C56 0.0399(15) 0.0333(14) 0.0817(17) 0.0176(13) 0.0167(16) 0.0140(14)
C57 0.0405(19) 0.0303(14) 0.0679(16) 0.0185(15) 0.0197(15) 0.0086(13)
C58 0.0354(14) 0.0312(16) 0.091(2) 0.0160(13) 0.0146(16) 0.0047(17)

C60 0.0413(14) 0.0322(11) 0.0669(15) 0.0233(11) 0.0106(14) 0.0137(12)
C61 0.0360(13) 0.0293(13) 0.090(2) 0.0161(11) 0.0154(14) 0.0039(14)
C62 0.0411(17) 0.0315(14) 0.0728(16) 0.0162(14) 0.0186(16) 0.0113(14)
C63 0.0348(12) 0.0284(12) 0.090(2) 0.0142(11) 0.0141(14) 0.0031(14)
C64 0.0404(14) 0.0325(11) 0.0673(15) 0.0229(11) 0.0101(14) 0.0143(12)
C65 0.0396(19) 0.0308(16) 0.077(2) 0.0137(16) 0.0115(19) 0.0177(17)
C66 0.0399(17) 0.0308(14) 0.079(2) 0.0140(15) 0.0127(18) 0.0170(16)
C67 0.0398(17) 0.0311(14) 0.079(2) 0.0144(15) 0.0135(17) 0.0161(16)
C69 0.0406(18) 0.040(2) 0.085(2) 0.0190(16) 0.017(2) 0.0155(19)
C70 0.0371(16) 0.0426(19) 0.068(2) 0.0239(14) 0.0078(17) 0.0163(18)
C71 0.0341(12) 0.0285(13) 0.089(2) 0.0104(10) 0.0132(14) 0.0024(15)
C72 0.0357(12) 0.0283(12) 0.0894(19) 0.0155(11) 0.0152(14) 0.0032(14)
C73 0.0406(18) 0.040(2) 0.085(2) 0.0188(17) 0.0171(19) 0.0157(19)
C74 0.0448(16) 0.0289(14) 0.085(2) 0.0191(12) 0.0182(16) 0.0016(14)
C75 0.0315(13) 0.0339(13) 0.0673(19) 0.0109(11) 0.0031(15) 0.0158(13)
C77 0.0399(16) 0.0313(13) 0.0798(17) 0.0164(14) 0.0166(16) 0.0134(14)
C78 0.0410(18) 0.0315(14) 0.0709(16) 0.0164(14) 0.0191(16) 0.0106(14)
C79 0.0401(15) 0.0331(12) 0.0677(16) 0.0219(11) 0.0100(14) 0.0146(12)
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C82 0.0372(13) 0.0339(11) 0.0679(15) 0.0209(10) 0.0083(14) 0.0160(12)
C83 0.0408(15) 0.0330(12) 0.0674(16) 0.0224(11) 0.0103(14) 0.0141(13)
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C87 0.0420(15) 0.0323(10) 0.0659(14) 0.0238(11) 0.0106(14) 0.0129(12)
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La1 O30 2.532(18) yes . .
La1 C45 3.06(2) yes . 6_555
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La2A O23 2.680(13) yes . .
La2A O26 2.559(15) yes . .
La2A O37 2.850(12) yes . 2_564
La2A C122 2.982(9) yes . 2_564
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La3A O10 2.661(16) yes . 5_565
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La3A O20 2.411(16) yes . .
La3A O21 2.454(16) yes . .
La3A O22 2.416(15) yes . .
La3A O23 2.588(13) yes . .
La3A O24 2.561(10) yes . .
La3A O25 2.500(11) yes . .
La3A O37 2.617(14) yes . 6_665
La3A C96 2.998(15) yes . .
La3A C142 3.05(2) yes . 2_664
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O2 C45 1.16(2) yes . 6_555
O3 C15 1.09(2) yes . 2_554
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O5 C12 1.32(3) yes . 6_555
O6 C15 1.39(3) yes . .
O10 C96 1.31(2) yes . 3_664
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O24 C96 1.26(3) yes . .
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N16 C152 1.47(2) yes . .
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O1 La1 C45 161.8(5) yes . . 6_555
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O3 La1 O6 72.5(5) yes . . .

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O3 La1 C45 66.8(5) yes . . 6_555
O4 La1 O4 119.8(3) yes . . 6_555
O4 La1 O5 148.5(5) yes . . .
O4 La1 O5 64.3(3) yes . . 2_554
O4 La1 O6 133.5(4) yes . . .
O4 La1 O30 73.1(4) yes . . .
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O4 La1 O5 63.3(4) yes 6_555 . .
O4 La1 O5 155.1(4) yes 6_555 . 2_554
O4 La1 O6 83.8(4) yes 6_555 . .
O4 La1 O30 102.1(4) yes 6_555 . .
O4 La1 C45 25.5(5) yes 6_555 . 6_555
O5 La1 O5 127.8(4) yes . . 2_554
O5 La1 O6 76.9(5) yes . . .
O5 La1 O30 75.7(5) yes . . .
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O5 La1 O6 78.4(4) yes 2_554 . .
O5 La1 O30 102.5(4) yes 2_554 . .
O5 La1 C45 150.9(5) yes 2_554 . 6_555
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O30 La1 C45 89.6(4) yes . . 6_555
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O10 La2A O12 85.5(4) yes . . .
O10 La2A O13 126.8(5) yes . . .
O10 La2A O14 93.0(4) yes . . .
O10 La2A O15 157.8(3) yes . . .
O10 La2A O23 124.1(4) yes . . .
O10 La2A O26 81.6(5) yes . . .
O10 La2A O37 70.0(5) yes . . 2_564
O10 La2A C122 81.8(5) yes . . 2_564
O10 La2A C149 101.4(5) yes . . .
O11 La2A O12 146.7(5) yes . . .
O11 La2A O13 71.6(5) yes . . .
O11 La2A O14 126.0(6) yes . . .
O11 La2A O15 127.1(4) yes . . .
O11 La2A O23 75.6(4) yes . . .
O11 La2A O26 79.9(5) yes . . .
O11 La2A O37 72.0(5) yes . . 2_564
O11 La2A C122 100.6(5) yes . . 2_564
O11 La2A C149 74.5(5) yes . . .
O12 La2A O13 140.7(4) yes . . .
O12 La2A O14 79.2(5) yes . . .
O12 La2A O15 79.8(4) yes . . .
O12 La2A O23 97.3(4) yes . . .
O12 La2A O26 71.9(4) yes . . .
O12 La2A O37 124.4(4) yes . . 2_564
O12 La2A C122 101.2(4) yes . . 2_564
O12 La2A C149 85.6(5) yes . . .
O13 La2A O14 77.5(5) yes . . .
O13 La2A O15 62.2(4) yes . . .
O13 La2A O23 82.9(5) yes . . .
O13 La2A O26 128.2(4) yes . . .

O13 La2A O37 62.0(5) yes . . 2_564
O13 La2A C122 67.3(5) yes . . 2_564
O13 La2A C149 105.9(5) yes . . .
O14 La2A O15 68.0(4) yes . . .
O14 La2A O23 142.5(4) yes . . .
O14 La2A O26 150.9(4) yes . . .
O14 La2A O37 54.5(5) yes . . 2_564
O14 La2A C122 25.6(5) yes . . 2_564
O14 La2A C149 158.1(5) yes . . .
O15 La2A O23 74.5(4) yes . . .
O15 La2A O26 109.0(4) yes . . .
O15 La2A O37 105.0(4) yes . . 2_564
O15 La2A C122 84.8(5) yes . . 2_564
O15 La2A C149 94.0(5) yes . . .
O23 La2A O26 48.0(4) yes . . .
O23 La2A O37 138.0(4) yes . . 2_564
O23 La2A C122 149.3(5) yes . . 2_564
O23 La2A C149 24.9(5) yes . . .
O26 La2A O37 144.6(4) yes . . 2_564
O26 La2A C122 162.5(4) yes . . 2_564
O26 La2A C149 23.2(4) yes . . .
O37 La2A C122 28.8(4) yes 2_564 . 2_564
O37 La2A C149 146.5(5) yes 2_564 . .
C122 La2A C149 172.8(5) yes 2_564 . .
O10 La3A O15 136.5(4) yes 5_565 . .
O10 La3A O20 75.0(4) yes 5_565 . .
O10 La3A O21 82.4(4) yes 5_565 . .
O10 La3A O22 95.4(3) yes 5_565 . .
O10 La3A O23 125.4(4) yes 5_565 . .
O10 La3A O24 50.2(4) yes 5_565 . .
O10 La3A O25 142.3(4) yes 5_565 . .
O10 La3A O37 72.3(4) yes 5_565 . 6_665
O10 La3A C96 25.8(5) yes 5_565 . .
O10 La3A C142 149.6(4) yes 5_565 . 2_664
O15 La3A O20 72.7(4) yes . . .
O15 La3A O21 60.1(4) yes . . .
O15 La3A O22 127.4(4) yes . . .
O15 La3A O23 71.5(4) yes . . .
O15 La3A O24 143.6(4) yes . . .
O15 La3A O25 54.5(5) yes . . .
O15 La3A O37 104.8(4) yes . . 6_665
O15 La3A C96 146.3(6) yes . . .
O15 La3A C142 29.8(5) yes . . 2_664
O20 La3A O21 71.4(5) yes . . .
O20 La3A O22 146.0(4) yes . . .
O20 La3A O23 74.1(5) yes . . .
O20 La3A O24 78.1(4) yes . . .
O20 La3A O25 127.0(5) yes . . .
O20 La3A O37 126.0(4) yes . . 6_665
O20 La3A C96 73.7(5) yes . . .
O20 La3A C142 102.5(5) yes . . 2_664
O21 La3A O22 140.7(4) yes . . .
O21 La3A O23 126.7(5) yes . . .
O21 La3A O24 129.0(5) yes . . .

O21 La3A O25 78.3(5) yes . . .
O21 La3A O37 62.6(5) yes . . 6_665
O21 La3A C96 106.0(6) yes . . .
O21 La3A C142 68.5(5) yes . . 2_664
O22 La3A O23 86.4(4) yes . . .
O22 La3A O24 71.2(4) yes . . .
O22 La3A O25 80.2(5) yes . . .
O22 La3A O37 79.2(4) yes . . 6_665
O22 La3A C96 83.7(5) yes . . .
O22 La3A C142 101.5(4) yes . . 2_664
O23 La3A O24 79.9(4) yes . . .
O23 La3A O25 91.9(4) yes . . .
O23 La3A O37 158.5(4) yes . . 6_665
O23 La3A C96 101.7(5) yes . . .
O23 La3A C142 81.0(5) yes . . 2_664
O24 La3A O25 150.6(6) yes . . .
O24 La3A O37 109.9(5) yes . . 6_665
O24 La3A C96 24.5(6) yes . . .
O24 La3A C142 160.0(5) yes . . 2_664
O25 La3A O37 70.1(4) yes . . 6_665
O25 La3A C96 158.2(6) yes . . .
O25 La3A C142 24.7(5) yes . . 2_664
O37 La3A C96 92.6(5) yes 6_665 . .
O37 La3A C142 86.2(5) yes 6_665 . 2_664
C96 La3A C142 174.3(6) yes . . 2_664
La1 O1 C12 96.0(10) yes . . .
La1 O2 C45 99.7(15) yes . . 6_555
La1 O3 C15 135.7(16) yes . . 2_554
La1 O4 La1 107.6(4) yes . . 2_554
La1 O4 C45 156.9(14) yes . . .
La1 O4 C45 87.8(10) yes 2_554 . .
La1 O5 La1 107.8(6) yes . . 6_555
La1 O5 C12 157.0(14) yes . . 6_555
La1 O5 C12 92.6(10) yes 6_555 . 6_555
La1 O6 C15 126.3(9) yes . . .
La2A O10 La3A 110.9(5) yes . . 3_664
La2A O10 C96 146.9(12) yes . . 3_664
La3A O10 C96 91.7(11) yes 3_664 . 3_664
La2A O11 C150 145.6(12) yes . . 2_554
La2A O13 C151 137.3(15) yes . . 1_565
La2A O14 C122 95.7(8) yes . . 2_564
La2A O15 La3A 101.5(4) yes . . .
La2A O15 C142 119.0(11) yes . . 2_664
La3A O15 C142 80.2(9) yes . . 2_664
La3A O20 C151 142.1(10) yes . . 1_565
La3A O21 C150 134.2(12) yes . . 6_565
La2A O23 La3A 109.3(5) yes . . .
La2A O23 C149 94.0(10) yes . . .
La3A O23 C149 145.9(14) yes . . .
La3A O24 C96 97.6(10) yes . . .
La3A O25 C142 101.9(13) yes . . 2_664
La2A O26 C149 101.8(14) yes . . .
La1 O30 C152 147.0(11) yes . . .
La2A O37 La3A 103.7(4) yes 6_445 . 2_544

La2A O37 C122 80.6(7) yes 6_445 . .
La3A O37 C122 124.9(11) yes 2_544 . .
C152 N16 C153 115.0(16) yes . . .
C152 N16 C154 153.5(14) yes . . .
C153 N16 C154 91.4(14) yes . . .
C16A N17A C16B 107(2) yes . . .
C16A N17A C16C 160.6(18) yes . . .
C16B N17A C16C 93(2) yes . . .
C16D N17B C16E 111(2) yes . . .
C16D N17B C16F 156.2(19) yes . . .
C16E N17B C16F 92.9(18) yes . . .
C17A N18A C17B 135.4(19) yes . . .
C17A N18A C17C 131.3(16) yes . . .
C17B N18A C17C 93.3(15) yes . . .
C17D N18B C17E 139.7(19) yes . . .
C17D N18B C17F 128(2) yes . . .
C17E N18B C17F 92(2) yes . . .
C23 C4 C39 119(2) yes . . .
C23 C4 C45 121.2(18) yes . . .
C39 C4 C45 119.3(15) yes . . .
C65 C5 C100 120.0(7) yes . . .
C65 C5 C122 120.9(10) yes . . .
C100 C5 C122 119.1(11) yes . . .
C11 C7 C103 123(2) yes . . .
C93 C8 C114 120(2) yes . . .
C93 C8 C142 116(2) yes . . .
C114 C8 C142 124.1(16) yes . . .
C12 C9 C19 127(2) yes . . .
C12 C9 C54 122(2) yes . . .
C19 C9 C54 111.7(16) yes . . .
C7 C11 C109 123.9(15) yes . . .
O1 C12 O5 123.6(15) yes . . 2_554
O1 C12 C9 121.4(18) yes . . .
O5 C12 C9 114.7(19) yes 2_554 . .
C38 C14 C125 124.5(17) yes . . .
O3 C15 O6 128(2) yes 6_555 . .
O3 C15 C81 116(2) yes 6_555 . .
O6 C15 C81 111.5(13) yes . . .
O22 C16A N17A 144.6(19) yes . . .
O22 C16D N17B 128.1(16) yes . . .
O12 C17A N18A 118.5(17) yes . . .
O12 C17D N18B 104.5(17) yes . . .
C31 C18 C50 119(2) yes . . .
C31 C18 C119 119.1(17) yes . . .
C50 C18 C119 121(2) yes . . .
C9 C19 C89 126(2) yes . . .
C26 C20 C48 127(2) yes . . .
C36 C21 C72 117(2) yes . . .
C25 C22 C42 121(2) yes . . .
C4 C23 C111 127.6(19) yes . . .
C22 C25 C57 128(2) yes . . .
C22 C25 C111 113.3(16) yes . . .
C57 C25 C111 119(2) yes . . .
C20 C26 C75 128(2) yes . . .

C20 C26 C89 117(2) yes . . .
C75 C26 C89 115.0(15) yes . . .
C33 C27 C48 122.0(18) yes . . .
C36 C28 C91 120.8(17) yes . . .
C36 C28 C94 119.7(18) yes . . .
C91 C28 C94 120(2) yes . . .
C31 C29 C82 121.9(15) yes . . .
C51 C30 C81 120.0(13) yes . . .
C18 C31 C29 120.0(16) yes . . .
C18 C31 C41 119(2) yes . . .
C29 C31 C41 121(2) yes . . .
C36 C32 C61 121.7(16) yes . . .
C27 C33 C89 121.3(19) yes . . .
C56 C34 C86 123(2) yes . . .
C53 C35 C56 118.2(16) yes . . .
C21 C36 C28 116(2) yes . . .
C21 C36 C32 123(2) yes . . .
C28 C36 C32 120.3(15) yes . . .
C14 C38 C40 121.1(14) yes . . .
C14 C38 C49 118.9(13) yes . . .
C40 C38 C49 120.0(10) yes . . .
C4 C39 C57 119.1(16) yes . . .
C38 C40 C106 114.2(11) yes . . .
C38 C40 C131 120.0(13) yes . . .
C106 C40 C131 125.6(14) yes . . .
C31 C41 C43 119(2) yes . . .
C22 C42 C53 116.0(19) yes . . .
C22 C42 C62 124(2) yes . . .
C53 C42 C62 119.9(16) yes . . .
C41 C43 C48 123(2) yes . . .
C41 C43 C108 117.2(14) yes . . .
C48 C43 C108 120(2) yes . . .
C58 C44 C103 124.3(16) yes . . .
C58 C44 C134 121(2) yes . . .
C103 C44 C134 115(2) yes . . .
La1 C45 O2 58.3(12) yes 2_554 . 2_554
La1 C45 O4 66.7(10) yes 2_554 . .
La1 C45 C4 168.3(13) yes 2_554 . .
O2 C45 O4 119.5(17) yes 2_554 . .
O2 C45 C4 117.1(19) yes 2_554 . .
O4 C45 C4 121.4(15) yes . . .
C61 C46 C72 120(2) yes . . .
C56 C47 C106 119(2) yes . . .
C56 C47 C125 119.8(16) yes . . .
C106 C47 C125 119(2) yes . . .
C20 C48 C27 113.3(14) yes . . .
C20 C48 C43 123(2) yes . . .
C27 C48 C43 123.6(19) yes . . .
C38 C49 C69 120.0(12) yes . . .
C18 C50 C104 126(2) yes . . .
C30 C51 C55 122.0(14) yes . . .
C30 C51 C74 120.0(10) yes . . .
C55 C51 C74 117.5(14) yes . . .
C85 C52 C102 121(2) yes . . .

C85 C52 C132 115.9(19) yes . . .
C102 C52 C132 121.5(14) yes . . .
C35 C53 C42 122.5(15) yes . . .
C35 C53 C77 120(2) yes . . .
C42 C53 C77 117(2) yes . . .
C9 C54 C75 131(2) yes . . .
C51 C55 C91 112.2(17) yes . . .
C34 C56 C35 120(2) yes . . .
C34 C56 C47 122(2) yes . . .
C35 C56 C47 116.4(17) yes . . .
C25 C57 C39 123.0(19) yes . . .
C44 C58 C109 117.8(19) yes . . .
C64 C60 C101 119.9(15) yes . . .
C64 C60 C112 117(2) yes . . .
C101 C60 C112 123(2) yes . . .
C32 C61 C46 117(2) yes . . .
C32 C61 C109 123.2(14) yes . . .
C46 C61 C109 120(2) yes . . .
C42 C62 C78 114.2(17) yes . . .
C72 C63 C84 114.6(17) yes . . .
C72 C63 C85 123.7(19) yes . . .
C84 C63 C85 121.6(15) yes . . .
C60 C64 C99 116(2) yes . . .
C5 C65 C116 120.0(10) yes . . .
C67 C66 C98 119.9(12) yes . . .
C67 C66 C116 119.6(13) yes . . .
C98 C66 C116 120.0(7) yes . . .
C66 C67 C105 120.5(19) yes . . .
C49 C69 C73 120.0(12) yes . . .
C49 C69 C151 120.1(13) yes . . .
C73 C69 C151 119.7(11) yes . . .
C80 C70 C97 122.0(19) yes . . .
C90 C71 C132 124.1(19) yes . . .
C21 C72 C46 120.8(15) yes . . .
C21 C72 C63 120.2(19) yes . . .
C46 C72 C63 119.0(19) yes . . .
C69 C73 C131 120.0(10) yes . . .
C51 C74 C94 126.3(12) yes . . .
C51 C74 C120 120.0(12) yes . . .
C94 C74 C120 113.7(13) yes . . .
C26 C75 C54 117(2) yes . . .
C53 C77 C86 121(2) yes . . .
C62 C78 C111 128(2) yes . . .
C83 C79 C99 120.0(16) yes . . .
C70 C80 C95 121.1(18) yes . . .
C70 C80 C104 117.8(15) yes . . .
C95 C80 C104 121.0(19) yes . . .
C15 C81 C30 118.1(14) yes . . .
C15 C81 C88 121.8(12) yes . . .
C30 C81 C88 120.0(13) yes . . .
C29 C82 C99 121.3(13) yes . . .
C29 C82 C108 113.3(19) yes . . .
C99 C82 C108 125(2) yes . . .
C79 C83 C101 121(2) yes . . .

C63 C84 C107 117.6(18) yes . . .
C52 C85 C63 122(2) yes . . .
C34 C86 C77 118.0(15) yes . . .
C34 C86 C105 122(2) yes . . .
C77 C86 C105 119(2) yes . . .
C92 C87 C101 120.7(19) yes . . .
C81 C88 C120 120.0(10) yes . . .
C19 C89 C26 118(2) yes . . .
C19 C89 C33 122.0(19) yes . . .
C26 C89 C33 119.5(15) yes . . .
C71 C90 C96 120.4(19) yes . . .
C71 C90 C136 119.6(15) yes . . .
C96 C90 C136 118.2(19) yes . . .
C28 C91 C55 129.7(19) yes . . .
C87 C92 C128 120(2) yes . . .
C87 C92 C149 119.2(19) yes . . .
C128 C92 C149 119.1(14) yes . . .
C8 C93 C103 118(2) yes . . .
C28 C94 C74 113.8(18) yes . . .
C80 C95 C119 125.1(19) yes . . .
La3A C96 O10 62.5(9) yes . . 5_565
La3A C96 O24 57.8(8) yes . . .
La3A C96 C90 177.5(15) yes . . .
O10 C96 O24 120.1(15) yes 5_565 . .
O10 C96 C90 118.9(19) yes 5_565 . .
O24 C96 C90 120.9(18) yes . . .
C70 C97 C135 124.3(19) yes . . .
C70 C97 C150 120.0(18) yes . . .
C135 C97 C150 115.6(15) yes . . .
C66 C98 C100 120.0(10) yes . . .
C66 C98 C113 110.9(10) yes . . .
C100 C98 C113 128.9(13) yes . . .
C64 C99 C79 123(2) yes . . .
C64 C99 C82 121(2) yes . . .
C79 C99 C82 115.4(15) yes . . .
C5 C100 C98 120.0(10) yes . . .
C60 C101 C83 120(2) yes . . .
C60 C101 C87 118.8(14) yes . . .
C83 C101 C87 121(2) yes . . .
C52 C102 C136 120.8(19) yes . . .
C7 C103 C44 114(2) yes . . .
C7 C103 C93 126(2) yes . . .
C44 C103 C93 120.5(15) yes . . .
C50 C104 C80 111.7(14) yes . . .
C50 C104 C121 131.1(19) yes . . .
C80 C104 C121 117(2) yes . . .
C67 C105 C86 118.5(19) yes . . .
C67 C105 C124 117.0(15) yes . . .
C86 C105 C124 124.2(17) yes . . .
C40 C106 C47 124(2) yes . . .
C84 C107 C132 123(2) yes . . .
C43 C108 C82 127(2) yes . . .
C11 C109 C58 117(2) yes . . .
C11 C109 C61 117.8(14) yes . . .

C58 C109 C61 125.3(19) yes . . .
C23 C111 C25 111.5(13) yes . . .
C23 C111 C78 129.1(18) yes . . .
C25 C111 C78 119.4(19) yes . . .
C60 C112 C128 120(2) yes . . .
C98 C113 C124 130.8(19) yes . . .
C8 C114 C134 124.5(17) yes . . .
C65 C116 C66 120.0(10) yes . . .
C18 C119 C95 115.0(16) yes . . .
C74 C120 C88 120.0(12) yes . . .
C104 C121 C135 125.3(19) yes . . .
La2A C122 O14 58.6(7) yes 6_445 . 6_445
La2A C122 O37 70.6(5) yes 6_445 . .
La2A C122 C5 170.1(11) yes 6_445 . .
O14 C122 O37 129.2(10) yes 6_445 . .
O14 C122 C5 113.5(13) yes 6_445 . .
O37 C122 C5 117.2(11) yes . . .
C105 C124 C113 120.2(19) yes . . .
C14 C125 C47 116.9(15) yes . . .
C92 C128 C112 117.4(14) yes . . .
C40 C131 C73 120.0(12) yes . . .
C52 C132 C71 114.4(19) yes . . .
C52 C132 C107 120.2(15) yes . . .
C71 C132 C107 125.4(19) yes . . .
C44 C134 C114 122(2) yes . . .
C97 C135 C121 113.7(16) yes . . .
C90 C136 C102 119(2) yes . . .
La3A C142 O15 70.0(9) yes 6_455 . 6_455
La3A C142 O25 53.5(10) yes 6_455 . 6_455
La3A C142 C8 167.5(15) yes 6_455 . .
O15 C142 O25 123.3(18) yes 6_455 . 6_455
O15 C142 C8 115.2(13) yes 6_455 . .
O25 C142 C8 119.6(19) yes 6_455 . .
La2A C149 O23 61.0(10) yes . . .
La2A C149 O26 55.0(12) yes . . .
La2A C149 C92 178.2(13) yes . . .
O23 C149 O26 115.4(19) yes . . .
O23 C149 C92 120.6(15) yes . . .
O26 C149 C92 123(2) yes . . .
O11 C150 O21 123.0(18) yes 6_555 . 2_654
O11 C150 C97 122.4(15) yes 6_555 . .
O21 C150 C97 112.7(17) yes 2_654 . .
O13 C151 O20 122.1(19) yes 1_545 . 1_545
O13 C151 C69 114.5(18) yes 1_545 . .
O20 C151 C69 123.3(14) yes 1_545 . .
O30 C152 N16 106.6(12) yes . . .
C11 C7 H7 118.267 no . . .
C103 C7 H7 118.289 no . . .
C7 C11 H11 118.056 no . . .
C109 C11 H11 118.081 no . . .
C38 C14 H14 117.764 no . . .
C125 C14 H14 117.757 no . . .
O22 C16A H16A 107.704 no . . .
N17A C16A H16A 107.690 no . . .

N17A C16B H16B 109.463 no . . .
N17A C16B H16C 109.466 no . . .
N17A C16B H16D 109.467 no . . .
H16B C16B H16C 109.473 no . . .
H16B C16B H16D 109.463 no . . .
H16C C16B H16D 109.495 no . . .
N17A C16C H16E 109.465 no . . .
N17A C16C H16F 109.488 no . . .
N17A C16C H16G 109.464 no . . .
H16E C16C H16F 109.468 no . . .
H16E C16C H16G 109.475 no . . .
H16F C16C H16G 109.467 no . . .
O22 C16D H16H 115.951 no . . .
N17B C16D H16H 115.914 no . . .
N17B C16E H16I 109.475 no . . .
N17B C16E H16J 109.465 no . . .
N17B C16E H16K 109.469 no . . .
H16I C16E H16J 109.477 no . . .
H16I C16E H16K 109.484 no . . .
H16J C16E H16K 109.456 no . . .
N17B C16F H16L 109.472 no . . .
N17B C16F H16M 109.485 no . . .
N17B C16F H16N 109.479 no . . .
H16L C16F H16M 109.474 no . . .
H16L C16F H16N 109.467 no . . .
H16M C16F H16N 109.450 no . . .
O12 C17A H17A 120.731 no . . .
N18A C17A H17A 120.738 no . . .
N18A C17B H17B 109.475 no . . .
N18A C17B H17C 109.475 no . . .
N18A C17B H17D 109.465 no . . .
H17B C17B H17C 109.467 no . . .
H17B C17B H17D 109.479 no . . .
H17C C17B H17D 109.466 no . . .
N18A C17C H17E 109.454 no . . .
N18A C17C H17F 109.453 no . . .
N18A C17C H17G 109.476 no . . .
H17E C17C H17F 109.471 no . . .
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H17F C17C H17G 109.487 no . . .
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N18B C17E H17I 109.475 no . . .
N18B C17E H17J 109.471 no . . .
N18B C17E H17K 109.468 no . . .
H17I C17E H17J 109.483 no . . .
H17I C17E H17K 109.458 no . . .
H17J C17E H17K 109.472 no . . .
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N18B C17F H17N 109.477 no . . .
H17L C17F H17M 109.480 no . . .
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C26 C20 H20 116.555 no . . .
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C72 C21 H21 121.267 no . . .
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C42 C22 H22 119.309 no . . .
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C116 C65 H65 119.992 no . . .
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C100 C5 C65 C116 -0.0(17) no . . . .
C65 C5 C122 O14 -2.5(19) no . . . 6_445
C65 C5 C122 O37 173.7(11) no . . . .
C122 C5 C65 C116 -178.8(11) no . . . .
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C100 C5 C122 O37 -5.1(19) no . . . .
C122 C5 C100 C98 178.8(11) no . . . .
C11 C7 C103 C44 -2(3) no . . . .
C11 C7 C103 C93 -179.6(16) no . . . .
C103 C7 C11 C109 3(3) no . . . .
C93 C8 C114 C134 -6(3) no . . . .
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C54 C9 C19 C89 9(3) no . . . .
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O3 C15 C81 C30 -171.3(15) no 6_555 . . .
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C81 C30 C51 C55 -171.8(9) no . . . .
C81 C30 C51 C74 -0.0(16) no . . . .
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C61 C32 C36 C21 -0(2) no . . . .
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C14 C38 C49 C69 179.0(10) no . . . .
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C49 C38 C40 C106 175.8(9) no . . . .
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C106 C47 C56 C35 -56(3) no . . . .
C56 C47 C125 C14 165.2(16) no . . . .
C125 C47 C56 C34 -26(3) no . . . .
C125 C47 C56 C35 140.5(16) no . . . .
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C125 C47 C106 C40 -6(3) no . . . .
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C18 C50 C104 C121 177.9(17) no . . . .
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C132 C52 C85 C63 7(3) no . . . .
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C102 C52 C132 C107 -172.6(19) no . . . .
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C42 C53 C77 C86 -174.3(12) no . . . .
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C51 C55 C91 C28 -8(3) no . . . .
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C44 C58 C109 C61 -177.4(14) no . . . .
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C64 C60 C101 C87 178.8(12) no . . . .
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C64 C60 C112 C128 -177.3(13) no . . . .
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C122 H17E 3.4273 no . 6_445
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C122 H73 3.4117 no . 6_555
C122 H93 3.3559 no . 1_545
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C124 H16G 3.5617 no . 2_544
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C124 H77 2.9870 no . .
C125 H34 2.7649 no . .
C125 H106 3.3138 no . .
C128 H14 3.1238 no . 3_554
C128 H16D 2.7122 no . .
C128 H87 3.2907 no . .
C128 H107 3.1642 no . 3_664
C128 H125 3.1744 no . 3_554
C131 H106 2.7956 no . .
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C132 H102 3.3184 no . .
C134 H58 2.6522 no . .
C135 H70 3.2577 no . .
C136 H17D 3.3326 no . 5_565
C136 H17E 3.5187 no . 5_565

C136 H17F 2.6811 no . 5_565
C136 H71 3.2448 no . .
C136 H83 3.1840 no . .
C136 H95 3.1842 no . 2_554
C136 H119 3.0958 no . 2_554
C142 H16A 3.2079 no . 6_455
C142 H17L 3.0025 no . 6_455
C142 H17M 3.3995 no . 6_455
C142 H93 2.5863 no . .
C142 H100 3.3558 no . 5_555
C142 H114 2.6444 no . .
C149 H14 3.5259 no . 3_554
C149 H71 3.4853 no . 3_664
C149 H87 2.6252 no . .
C149 H128 2.6637 no . .
C150 H49 3.4570 no . 2_554
C150 H70 2.6092 no . .
C150 H135 2.6619 no . .
C151 H49 2.6675 no . .
C151 H70 3.1435 no . 2_544
C151 H73 2.6590 no . .
C151 H135 3.3155 no . 6_555
C152 H15A 2.4654 no . .
C152 H15B 3.1574 no . .
C152 H15C 3.0873 no . .
C152 H15D 3.1155 no . .
C152 H15E 3.4041 no . .
C152 H15F 3.3830 no . .
C152 H23 3.1098 no . .
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C153 H15D 3.0167 no . .
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C154 H15B 2.2036 no . .
C154 H15C 2.2886 no . .
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H7 H16K 2.9526 no . 2_554
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H7 H17E 3.2057 no . 6_455
H7 H17G 2.4458 no . 6_455
H7 H17H 3.5046 no . 6_455
H7 H65 2.3712 no . 1_565
H7 H93 2.5157 no . .
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H11 H17G 3.3415 no . 6_455
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H14 H125 2.2372 no . .

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H15A H15F 3.1907 no . .
H15A H33 3.1574 no . 6_555
H15A H152 3.4146 no . .
H15B H15D 3.1558 no . .
H15B H15E 2.3647 no . .
H15B H15F 1.9556 no . .
H15B H39 3.2914 no . .
H15B H78 3.5287 no . 2_554
H15C H15D 3.1767 no . .
H15C H15E 1.9209 no . .
H15C H15F 2.6447 no . .
H15C H27 2.9614 no . 6_555
H15C H33 2.7775 no . 6_555
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H16A H16D 2.1820 no . .
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H16B H16G 2.5986 no . .
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H16B H113 3.5219 no . 6_665
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H16C H16F 3.5919 no . .
H16C H16G 3.2030 no . .
H16C H100 3.4413 no . 6_665
H16C H113 2.4175 no . 6_665
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H16D H16E 2.6096 no . .
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H16D H128 2.7184 no . .
H16F H64 3.3419 no . .
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H16H H16J 3.4714 no . .
H16H H16K 3.4947 no . .
H16H H16M 3.4647 no . .
H16H H16N 3.3730 no . .
H16H H100 3.3100 no . 6_665
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H16I H16M 2.5463 no . .
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H16I H79 3.3996 no . .
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H16K H16M 3.1353 no . .
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H16M H116 3.4528 no . 6_665
H16N H29 3.5340 no . .
H17A H17B 2.8125 no . .
H17A H107 3.2698 no . 3_664
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H17B H17G 3.1736 no . .
H17C H17E 3.1672 no . .
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H17D H17E 3.1916 no . .
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H17D H17G 2.5651 no . .
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H17D H136 3.5755 no . 3_664
H17F H79 3.5435 no . 3_664
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H17F H102 3.4977 no . 3_664
H17F H136 2.6525 no . 3_664
H17H H17I 3.0365 no . .
H17I H17M 3.1538 no . .
H17I H17N 3.1805 no . .
H17J H17L 3.1885 no . .
H17J H17M 2.5369 no . .
H17J H17N 1.9644 no . .
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H17N H84 2.8236 no . 3_664
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H20 H75 2.6135 no . .
H20 H85 2.9328 no . 6_555
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H27 H33 2.3589 no . .
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H29 H50 2.1000 no . .
H29 H64 2.2993 no . .

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H32 H94 2.5577 no . .
H33 H54 2.3496 no . 2_554
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H34 H125 2.4837 no . .
H35 H106 2.3032 no . .
H39 H57 2.3103 no . .
H39 H78 2.4904 no . 2_554
H39 H88 3.5942 no . 4_554
H39 H120 3.1381 no . 4_554
H41 H119 2.2948 no . .
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H49 H71 3.5478 no . 1_545
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H54 H55 2.9299 no . 6_555
H54 H75 2.2086 no . .
H54 H91 3.4751 no . 6_555
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H57 H120 3.2656 no . 4_554
H58 H134 2.4658 no . .
H62 H77 2.1661 no . .
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H64 H112 2.4216 no . .
H65 H93 2.8370 no . 1_545
H65 H116 2.3400 no . .
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H67 H116 2.4685 no . .
H70 H95 2.3556 no . .
H71 H107 2.5888 no . .
H71 H128 3.4530 no . 5_565
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H73 H131 2.3399 no . .
H75 H85 3.0839 no . 6_555
H75 H91 3.3443 no . 6_555
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H79 H108 2.1380 no . .
H83 H87 2.4758 no . .
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H84 H107 2.2927 no . .
H85 H102 2.4755 no . .
H87 H136 3.4262 no . .
H88 H120 2.3398 no . .
H93 H135 3.3608 no . 5_565
H94 H120 2.2759 no . .
H95 H119 2.3531 no . .
H95 H136 3.1552 no . 6_555
H100 H113 2.4991 no . .
H100 H114 2.9079 no . 3_554
H102 H119 3.2900 no . 2_554
H102 H136 2.3615 no . .

H106 H131 2.6569 no . .
H107 H128 2.3080 no . 5_565
H112 H125 3.2822 no . 3_554
H112 H128 2.5141 no . .
H113 H114 2.5763 no . 3_554
H113 H124 2.1662 no . .
H114 H131 3.1903 no . 4_555
H114 H134 2.2474 no . .
H119 H136 3.4246 no . 6_555
H121 H135 2.3405 no . .
H125 H128 3.3408 no . 5_555

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Additional structures and associated data_? identifiers
should be added at this point if there is more than one
structure analysis in the CIF.
SQUEEZE RESULTS (APPEND TO CIF)
Note: Data are Listed for all Voids in the P1 Unit Cell
i.e. Centre of Gravity, Solvent Accessible Volume,
Recovered number of Electrons in the Void and
Details about the Squeezed Material
loop_
_platon_squeeze_void_nr
_platon_squeeze_void_average_x
_platon_squeeze_void_average_y
_platon_squeeze_void_average_z
_platon_squeeze_void_volume
_platon_squeeze_void_count_electrons
_platon_squeeze_void_content
1 0.042 0.281 0.885 8425 2650 ' '
_platon_squeeze_details ?
_database_code_depnum_ccdc_archive 'CCDC 946972'