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Solid state organisation of C-60 by inclusion crystallisation with triptycenes

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#Belonging to Paper 'Tuning the solid state organisation of C60 ...
#by E.M.Veen, P.M. Postma, H.T.Jonkman, A.L.Spek & B.L.Feringa
Compounds 1 & 2

CIF-file generated for s1269b - compound #1

data_global
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0. AUDIT DETAILS

_audit_creation_date 'May 17 17:51:36 1999'
_audit_creation_method 'PLATON <TABLE ACC> option'
_audit_update_record
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?
;

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1. SUBMISSION DETAILS

_publ_contact_author_name # Name of author for correspondence
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_publ_contact_author_phone '+31 30 2532538'

#####

data_s1269b

#####

5. CHEMICAL DATA

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;
?
;
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_chemical_melting_point ?
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_chemical_formula_structural ?
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_weight 1441.54
_chemical_compound_source 'see text'

loop_
_atom_type_symbol

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

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6. CRYSTAL DATA

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_symmetry_space_group_name_H-M 'P 21/c'

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

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_cell_length_b      9.9958(10)
_cell_length_c      17.661(2)
_cell_angle_alpha    90
_cell_angle_beta     109.882(10)
_cell_angle_gamma    90
_cell_volume         3281.6(6)
_cell_formula_units_Z 2
_cell_measurement_temperature 150

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_exptl_crystal_size_max 0.55
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_exptl_crystal_size_min 0.05
_exptl_crystal_density_diffraction 1.459
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_exptl_absorption_coefficient_mu 0.08

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7. EXPERIMENTAL DATA

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_diffraction_radiation_wavelength 0.71073
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_diffraction_radiation_monochromator graphite

_diffraction_measurement_device_type 'Nonius CAD4T'
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number of measured reflections (redundant set)

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_diffraction_reflections_number 11766
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_diffraction_reflections_limit_k_min -12

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_diffrn_reflms_limit_l_min     -21
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_diffrn_reflms_theta_min       1.10
_diffrn_reflms_theta_max       25.33

# number of unique reflections
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# number of observed reflections (> n sig(I))
_reflms_number_gt              2080
_reflms_threshold_expression    'I>2sigma(I)'

_computing_data_collection      'Locally modified CAD4-Version 5 Software'
_computing_cell_refinement      'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction       'HELENA (Spek, 1997)'
_computing_structure_solution   'SIR97'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_publication_material 'PLATON (Spek, 1990)'

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8. REFINEMENT DATA

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_refine_ls_weighting_scheme       'calc      '
_refine_ls_weighting_details
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_refine_ls_extinction_method       none
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_refine_ls_abs_structure_Flack     none
_refine_ls_number_reflms          5988
_refine_ls_number_parameters       527
_refine_ls_number_restraints       45
_refine_ls_R_factor_all            0.2605
_refine_ls_R_factor_gt             0.0947
_refine_ls_wR_factor_ref           0.2611
_refine_ls_wR_factor_gt            0.1882
_refine_ls_goodness_of_fit_ref     1.003
_refine_ls_restrained_S_all        1.016
_refine_ls_shift/su_max            0.042
_refine_ls_shift/su_mean           0.004
_refine_diff_density_max           0.642
_refine_diff_density_min           -0.428
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9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_thermal_displace_type
_atom_site_fract_x
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_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
C1      C  Uani      0.4219(4)      0.1274(7)      0.1384(5)      1.000      0.034(3)
C2      C  Uani      0.4803(6)      0.2209(7)      0.1462(5)      1.000      0.050(4)
C3      C  Uani      0.5503(5)      0.1487(12)     0.1908(5)      1.000      0.079(5)
C4      C  Uani      0.5280(3)      0.0085(9)      0.2085(3)      1.000      0.034(2)
C5      C  Uani      0.4503(3)      0.0001(8)      0.1745(3)      1.000      0.026(2)
C6      C  Uani      0.4181(4)      -0.1150(7)     0.1365(4)      1.000      0.031(3)
C7      C  Uani      0.4622(5)      -0.2275(7)     0.1333(5)      1.000      0.043(3)

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C8	C	Uani	0.5350(5)	-0.2202(9)	0.1656(5)	1.000	0.047(3)
C9	C	Uani	0.5810(6)	-0.2732(9)	0.1206(6)	1.000	0.070(4)
C10	C	Uani	0.5507(6)	-0.3335(9)	0.0548(7)	1.000	0.065(4)
C11	C	Uani	0.4746(6)	-0.3452(8)	0.0196(6)	1.000	0.053(4)
C12	C	Uani	0.4295(5)	-0.2946(7)	0.0538(6)	1.000	0.045(3)
C13	C	Uani	0.3658(5)	-0.2190(10)	0.0099(6)	1.000	0.063(4)
C14	C	Uani	0.3574(5)	-0.1054(10)	0.0642(5)	1.000	0.046(3)
C15	C	Uani	0.3328(4)	0.0077(13)	0.0283(6)	1.000	0.072(4)
C16	C	Uani	0.3117(4)	0.0313(12)	-0.0619(6)	1.000	0.067(4)
C17	C	Uani	0.3328(5)	0.1639(11)	-0.0732(5)	1.000	0.057(4)
C18	C	Uani	0.3626(5)	0.2251(10)	0.0028(6)	1.000	0.061(4)
C19	C	Uani	0.3640(4)	0.1265(10)	0.0673(6)	1.000	0.051(4)
C20	C	Uani	0.4206(7)	0.3081(9)	0.0161(8)	1.000	0.068(5)
C21	C	Uani	0.4805(8)	0.3086(8)	0.0868(6)	1.000	0.079(5)
C22	C	Uani	0.5451(6)	0.3287(8)	0.0677(7)	1.000	0.066(5)
C23	C	Uani	0.6086(7)	0.2591(10)	0.1099(7)	1.000	0.080(5)
C24	C	Uani	0.6103(6)	0.1648(13)	0.1734(7)	1.000	0.103(6)
C25	C	Uani	0.6517(5)	0.0530(9)	0.1718(6)	1.000	0.060(4)
C26	C	Uani	0.6816(5)	0.0747(10)	0.1027(6)	1.000	0.065(4)
C27	C	Uani	0.6542(6)	0.2028(10)	0.0681(8)	1.000	0.091(6)
C28	C	Uani	0.6337(5)	-0.0777(11)	0.1856(5)	1.000	0.057(4)
C29	C	Uani	0.5686(5)	-0.1001(10)	0.2034(5)	1.000	0.049(3)
C30	C	Uani	0.6433(4)	-0.1826(10)	0.1333(5)	1.000	0.055(4)
C101	C	Uani	0.1348(4)	0.3759(7)	0.3532(4)	1.000	0.024(3)
C102	C	Uani	0.1429(4)	0.4441(7)	0.4237(4)	1.000	0.023(2)
C103	C	Uani	0.1438(4)	0.5828(7)	0.4256(4)	1.000	0.026(2)
C104	C	Uani	0.1379(3)	0.6538(7)	0.3551(4)	1.000	0.019(2)
C105	C	Uani	0.1299(4)	0.5849(7)	0.2852(4)	1.000	0.020(2)
C106	C	Uani	0.1285(4)	0.4449(6)	0.2844(4)	1.000	0.018(2)
C107	C	Uani	-0.0115(4)	0.3845(7)	0.0960(4)	1.000	0.023(2)
C108	C	Uani	-0.0696(4)	0.4566(8)	0.0457(4)	1.000	0.028(3)
C109	C	Uani	-0.0670(4)	0.5954(8)	0.0473(4)	1.000	0.032(3)
C110	C	Uani	-0.0083(4)	0.6643(7)	0.0979(4)	1.000	0.025(2)
C111	C	Uani	0.0497(4)	0.5899(7)	0.1468(4)	1.000	0.022(2)
C112	C	Uani	0.0476(4)	0.4498(6)	0.1462(4)	1.000	0.021(2)
C113	C	Uani	0.2218(4)	0.3737(7)	0.1463(4)	1.000	0.026(2)
C114	C	Uani	0.2703(4)	0.4408(7)	0.1180(4)	1.000	0.031(3)
C115	C	Uani	0.2729(4)	0.5796(7)	0.1192(4)	1.000	0.026(2)
C116	C	Uani	0.2262(4)	0.6514(7)	0.1468(4)	1.000	0.022(2)
C117	C	Uani	0.1788(4)	0.5836(7)	0.1750(4)	1.000	0.019(2)
C118	C	Uani	0.1754(4)	0.4449(6)	0.1735(4)	1.000	0.016(2)
C119	C	Uani	0.1175(4)	0.3865(7)	0.2012(4)	1.000	0.024(3)
C120	C	Uani	0.1204(3)	0.6465(6)	0.2040(4)	1.000	0.018(2)
C91	C	Uani	0.2227(3)	0.0117(8)	0.3683(3)	1.000	0.031(2)
C92	C	Uani	0.1753(3)	0.0130(7)	0.2807(3)	1.000	0.0191(17)
C93	C	Uani	0.1020(3)	0.0175(7)	0.2606(4)	1.000	0.027(2)
C94	C	Uani	0.0561(3)	0.0197(7)	0.1804(4)	1.000	0.030(2)
C95	C	Uani	0.0856(4)	0.0174(8)	0.1201(4)	1.000	0.034(2)
C96	C	Uani	0.1596(4)	0.0129(7)	0.1400(4)	1.000	0.027(2)
C97	C	Uani	0.2053(3)	0.0116(7)	0.2190(3)	1.000	0.0215(17)
C98	C	Uani	0.2854(3)	0.0080(8)	0.2375(4)	1.000	0.032(2)
H101	H	Uiso	0.13370	0.28090	0.35260	1.000	0.0290
H102	H	Uiso	0.14780	0.39550	0.47150	1.000	0.0280
H103	H	Uiso	0.14830	0.62920	0.47400	1.000	0.0310
H104	H	Uiso	0.13940	0.74880	0.35560	1.000	0.0230
H107	H	Uiso	-0.01280	0.28950	0.09550	1.000	0.0280
H108	H	Uiso	-0.11050	0.41140	0.01060	1.000	0.0340
H109	H	Uiso	-0.10660	0.64450	0.01270	1.000	0.0390
H110	H	Uiso	-0.00760	0.75930	0.09930	1.000	0.0300
H113	H	Uiso	0.22090	0.27870	0.14680	1.000	0.0320
H114	H	Uiso	0.30150	0.39150	0.09770	1.000	0.0370
H115	H	Uiso	0.30680	0.62520	0.10120	1.000	0.0310
H116	H	Uiso	0.22680	0.74650	0.14630	1.000	0.0270
H119	H	Uiso	0.11650	0.28650	0.20020	1.000	0.0280
H120	H	Uiso	0.12170	0.74650	0.20510	1.000	0.0220
H91A	H	Uiso	0.19300	0.02450	0.40220	1.000	0.0460
H91B	H	Uiso	0.25810	0.08410	0.37820	1.000	0.0460

H91C	H	Uiso	0.24780	-0.07440	0.38120	1.000	0.0460
H93	H	Uiso	0.08170	0.01920	0.30230	1.000	0.0330
H94	H	Uiso	0.00550	0.02280	0.16770	1.000	0.0360
H95	H	Uiso	0.05530	0.01880	0.06520	1.000	0.0410
H96	H	Uiso	0.17950	0.01060	0.09800	1.000	0.0330
H98A	H	Uiso	0.29620	0.02700	0.18830	1.000	0.0480
H98B	H	Uiso	0.30380	-0.08090	0.25770	1.000	0.0480
H98C	H	Uiso	0.30840	0.07540	0.27840	1.000	0.0480

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_atom_site_aniso_U_22

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_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

C1	0.048(6)	0.037(5)	0.028(5)	-0.003(4)	0.026(4)	0.014(4)
C2	0.112(9)	0.021(5)	0.032(5)	-0.009(4)	0.045(6)	-0.002(5)
C3	0.045(6)	0.178(13)	0.031(6)	-0.082(7)	0.036(5)	-0.075(8)
C4	0.032(4)	0.062(5)	0.010(3)	0.003(4)	0.011(3)	0.003(5)
C5	0.031(4)	0.039(4)	0.019(3)	-0.001(4)	0.022(3)	-0.002(4)
C6	0.039(5)	0.038(5)	0.021(4)	0.004(3)	0.016(4)	-0.005(4)
C7	0.072(7)	0.025(4)	0.048(6)	0.016(4)	0.041(5)	0.001(4)
C8	0.052(6)	0.054(6)	0.043(6)	0.044(5)	0.028(5)	0.032(5)
C9	0.099(9)	0.034(6)	0.053(7)	0.015(5)	-0.006(7)	0.034(6)
C10	0.064(7)	0.022(5)	0.104(10)	0.024(5)	0.021(7)	0.008(5)
C11	0.091(8)	0.017(4)	0.068(7)	0.003(4)	0.051(6)	0.004(5)
C12	0.047(6)	0.022(4)	0.067(7)	0.015(4)	0.022(5)	-0.005(4)
C13	0.052(7)	0.090(8)	0.037(6)	0.007(6)	0.004(5)	-0.054(6)
C14	0.040(6)	0.082(7)	0.030(5)	0.006(5)	0.030(5)	-0.015(5)
C15	0.024(4)	0.126(10)	0.078(7)	0.002(9)	0.031(5)	-0.013(7)
C16	0.016(4)	0.116(10)	0.059(6)	-0.025(7)	-0.002(4)	0.010(6)
C17	0.031(5)	0.098(8)	0.045(6)	0.022(6)	0.015(5)	0.040(6)
C18	0.055(7)	0.085(8)	0.037(6)	0.001(6)	0.008(5)	0.061(6)
C19	0.008(4)	0.089(8)	0.053(7)	-0.010(6)	0.007(4)	0.015(5)
C20	0.091(9)	0.032(6)	0.104(10)	0.004(6)	0.062(8)	0.025(6)
C21	0.162(13)	0.024(5)	0.058(7)	-0.022(5)	0.048(8)	0.018(7)
C22	0.101(10)	0.016(5)	0.111(10)	-0.031(5)	0.076(9)	-0.027(5)
C23	0.114(11)	0.029(5)	0.053(7)	-0.002(5)	-0.027(7)	-0.045(6)
C24	0.088(10)	0.111(11)	0.062(8)	-0.053(8)	-0.038(8)	-0.022(9)
C25	0.057(7)	0.051(6)	0.040(6)	-0.005(5)	-0.027(5)	-0.004(5)
C26	0.024(5)	0.063(7)	0.079(8)	0.027(6)	-0.020(5)	-0.025(5)
C27	0.056(8)	0.054(7)	0.148(14)	-0.040(9)	0.014(9)	-0.047(6)
C28	0.037(5)	0.122(9)	0.007(4)	0.018(5)	0.000(4)	0.048(6)
C29	0.041(5)	0.083(7)	0.023(5)	0.013(5)	0.010(4)	0.018(5)
C30	0.031(5)	0.104(8)	0.038(5)	0.042(6)	0.022(4)	0.047(5)
C101	0.023(4)	0.019(4)	0.032(5)	0.001(3)	0.011(4)	-0.004(3)
C102	0.021(4)	0.033(4)	0.017(4)	0.005(3)	0.008(3)	-0.004(3)
C103	0.022(4)	0.033(4)	0.022(4)	-0.011(3)	0.006(4)	-0.001(3)
C104	0.015(4)	0.027(4)	0.014(4)	-0.005(3)	0.005(3)	-0.001(3)
C105	0.012(4)	0.024(4)	0.023(4)	0.001(3)	0.004(3)	0.000(3)
C106	0.019(4)	0.022(4)	0.014(4)	-0.004(3)	0.007(3)	-0.005(3)
C107	0.022(4)	0.031(4)	0.020(4)	-0.004(3)	0.011(3)	-0.009(3)
C108	0.011(4)	0.059(5)	0.012(4)	-0.013(3)	0.000(3)	-0.011(3)
C109	0.031(5)	0.050(5)	0.018(4)	0.008(4)	0.011(4)	0.008(4)
C110	0.032(4)	0.031(4)	0.015(4)	-0.002(3)	0.011(3)	0.007(4)
C111	0.024(4)	0.030(4)	0.014(4)	0.004(3)	0.011(3)	-0.004(3)
C112	0.019(4)	0.029(4)	0.018(4)	0.002(3)	0.009(3)	0.001(3)
C113	0.019(4)	0.034(4)	0.018(4)	-0.001(3)	-0.003(3)	0.005(3)
C114	0.032(5)	0.041(5)	0.030(5)	-0.003(3)	0.025(4)	0.002(4)
C115	0.018(4)	0.038(4)	0.022(4)	0.005(3)	0.008(4)	-0.003(3)
C116	0.024(4)	0.025(4)	0.025(4)	0.002(3)	0.017(4)	-0.002(3)
C117	0.019(4)	0.028(4)	0.009(4)	0.000(3)	0.003(3)	-0.002(3)
C118	0.014(4)	0.020(4)	0.013(4)	0.002(3)	0.003(3)	-0.004(3)
C119	0.032(5)	0.021(4)	0.019(4)	0.000(3)	0.009(3)	-0.002(3)
C120	0.015(4)	0.018(3)	0.021(4)	0.003(3)	0.005(3)	0.001(3)

C91	0.038(4)	0.037(4)	0.017(3)	-0.005(4)	0.010(3)	-0.001(4)
C92	0.023(3)	0.016(3)	0.017(3)	-0.004(3)	0.005(3)	-0.002(3)
C93	0.032(4)	0.025(4)	0.028(4)	-0.002(3)	0.014(3)	-0.001(4)
C94	0.018(3)	0.031(4)	0.038(4)	-0.004(4)	0.006(3)	-0.006(3)
C95	0.040(4)	0.034(4)	0.022(3)	-0.004(4)	0.002(3)	-0.005(4)
C96	0.035(4)	0.021(4)	0.029(3)	0.004(4)	0.015(3)	-0.001(4)
C97	0.027(3)	0.022(3)	0.014(3)	-0.005(3)	0.005(3)	0.002(3)
C98	0.032(4)	0.032(4)	0.035(4)	0.000(4)	0.015(3)	0.001(4)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

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C2	C21	1.368(13)	.	.	no
C3	C4	1.533(14)	.	.	no
C3	C24	1.332(16)	.	.	no
C4	C5	1.449(9)	.	.	no
C4	C29	1.371(13)	.	.	no
C5	C6	1.374(10)	.	.	no
C6	C7	1.436(11)	.	.	no
C6	C14	1.427(11)	.	.	no
C7	C8	1.358(14)	.	.	no
C7	C12	1.491(12)	.	.	no
C8	C9	1.494(15)	.	.	no
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C9	C10	1.265(15)	.	.	no
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C10	C11	1.424(17)	.	.	no
C10	C20	1.561(18)	.	3_655	no
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C11	C22	1.465(15)	.	3_655	no
C12	C13	1.447(14)	.	.	no
C13	C14	1.531(14)	.	.	no
C13	C27	1.308(17)	.	3_655	no
C14	C15	1.306(16)	.	.	no
C15	C16	1.522(14)	.	.	no
C15	C19	1.406(16)	.	.	no
C16	C17	1.424(16)	.	.	no
C16	C26	1.313(15)	.	3_655	no
C17	C18	1.409(13)	.	.	no
C17	C30	1.314(12)	.	3_655	no
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C20	C21	1.398(18)	.	.	no
C21	C22	1.44(2)	.	.	no
C22	C23	1.407(17)	.	.	no
C23	C24	1.457(17)	.	.	no

C23	C27	1.458(18)	.	.	no
C24	C25	1.391(16)	.	.	no
C25	C26	1.542(14)	.	.	no
C25	C28	1.397(14)	.	.	no
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C28	C29	1.442(15)	.	.	no
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C102	C103	1.387(10)	.	.	no
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C106	C119	1.526(9)	.	.	no
C107	C108	1.391(11)	.	.	no
C107	C112	1.368(10)	.	.	no
C108	C109	1.388(11)	.	.	no
C109	C110	1.383(11)	.	.	no
C110	C111	1.393(10)	.	.	no
C111	C112	1.401(9)	.	.	no
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C112	C119	1.530(11)	.	.	no
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C116	C117	1.379(11)	.	.	no
C117	C118	1.388(9)	.	.	no
C117	C120	1.547(10)	.	.	no
C118	C119	1.507(11)	.	.	no
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C102	H102	0.9500	.	.	no
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C104	H104	0.9500	.	.	no
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C108	H108	0.9493	.	.	no
C109	H109	0.9496	.	.	no
C110	H110	0.9499	.	.	no
C113	H113	0.9499	.	.	no
C114	H114	0.9498	.	.	no
C115	H115	0.9501	.	.	no
C116	H116	0.9508	.	.	no
C119	H119	0.9998	.	.	no
C120	H120	0.9999	.	.	no
C91	C92	1.512(7)	.	.	no
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C92	C97	1.407(8)	.	.	no
C93	C94	1.399(9)	.	.	no
C94	C95	1.377(10)	.	.	no
C95	C96	1.384(12)	.	.	no
C96	C97	1.380(9)	.	.	no
C97	C98	1.504(9)	.	.	no
C91	H91A	0.9791	.	.	no
C91	H91B	0.9802	.	.	no
C91	H91C	0.9808	.	.	no
C93	H93	0.9512	.	.	no
C94	H94	0.9482	.	.	no
C95	H95	0.9508	.	.	no
C96	H96	0.9508	.	.	no
C98	H98A	0.9812	.	.	no
C98	H98B	0.9803	.	.	no
C98	H98C	0.9793	.	.	no

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_geom_angle_site_symmetry_3							
_geom_angle_publ_flag							
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C5	C1	C19	118.1(7)	.	.	.	no
C1	C2	C3	107.3(7)	.	.	.	no
C1	C2	C21	123.2(9)	.	.	.	no
C3	C2	C21	117.5(11)	.	.	.	no
C2	C3	C4	105.4(7)	.	.	.	no
C2	C3	C24	123.2(10)	.	.	.	no
C4	C3	C24	119.9(10)	.	.	.	no
C3	C4	C5	107.8(7)	.	.	.	no
C3	C4	C29	119.7(7)	.	.	.	no
C5	C4	C29	119.2(8)	.	.	.	no
C1	C5	C4	109.2(7)	.	.	.	no
C1	C5	C6	118.3(6)	.	.	.	no
C4	C5	C6	120.0(7)	.	.	.	no
C5	C6	C7	119.2(7)	.	.	.	no
C5	C6	C14	119.3(7)	.	.	.	no
C7	C6	C14	110.8(7)	.	.	.	no
C6	C7	C8	120.8(7)	.	.	.	no
C6	C7	C12	108.4(7)	.	.	.	no
C8	C7	C12	118.6(8)	.	.	.	no
C7	C8	C9	120.5(8)	.	.	.	no
C7	C8	C29	120.1(9)	.	.	.	no
C9	C8	C29	106.1(9)	.	.	.	no
C8	C9	C10	118.3(11)	.	.	.	no
C8	C9	C30	109.1(8)	.	.	.	no
C10	C9	C30	122.7(10)	.	.	.	no
C9	C10	C11	122.7(11)	.	.	.	no
C9	C10	C20	118.2(11)	.	.	3_655	no
C11	C10	C20	106.3(10)	.	.	3_655	no
C10	C11	C12	122.7(9)	.	.	.	no
C10	C11	C22	108.3(10)	.	.	3_655	no
C12	C11	C22	117.0(10)	.	.	3_655	no
C7	C12	C11	117.0(9)	.	.	.	no
C7	C12	C13	106.8(7)	.	.	.	no
C11	C12	C13	123.3(9)	.	.	.	no
C12	C13	C14	108.2(8)	.	.	.	no
C12	C13	C27	121.7(10)	.	.	3_655	no
C14	C13	C27	120.6(9)	.	.	3_655	no
C6	C14	C13	105.9(8)	.	.	.	no
C6	C14	C15	123.6(9)	.	.	.	no
C13	C14	C15	116.1(8)	.	.	.	no
C14	C15	C16	124.5(10)	.	.	.	no
C14	C15	C19	117.7(9)	.	.	.	no
C16	C15	C19	107.5(10)	.	.	.	no
C15	C16	C17	107.6(9)	.	.	.	no
C15	C16	C26	114.0(10)	.	.	3_655	no
C17	C16	C26	125.8(9)	.	.	3_655	no
C16	C17	C18	108.6(8)	.	.	.	no
C16	C17	C30	116.7(9)	.	.	3_655	no
C18	C17	C30	124.0(10)	.	.	3_655	no
C17	C18	C19	109.4(9)	.	.	.	no
C17	C18	C20	118.7(10)	.	.	.	no
C19	C18	C20	118.0(9)	.	.	.	no
C1	C19	C15	122.7(9)	.	.	.	no
C1	C19	C18	118.8(8)	.	.	.	no
C15	C19	C18	106.9(9)	.	.	.	no
C18	C20	C21	124.1(11)	.	.	.	no
C10	C20	C18	118.2(10)	3_655	.	.	no
C10	C20	C21	106.7(12)	3_655	.	.	no
C2	C21	C20	117.4(12)	.	.	.	no

C2	C21	C22	120.2(11)	.	.	.	no
C20	C21	C22	109.9(10)	.	.	.	no
C21	C22	C23	120.6(10)	.	.	.	no
C11	C22	C21	108.8(10)	3_655	.	.	no
C11	C22	C23	118.9(11)	3_655	.	.	no
C22	C23	C24	120.7(12)	.	.	.	no
C22	C23	C27	121.1(11)	.	.	.	no
C24	C23	C27	106.5(10)	.	.	.	no
C3	C24	C23	117.8(11)	.	.	.	no
C3	C24	C25	118.9(11)	.	.	.	no
C23	C24	C25	111.3(10)	.	.	.	no
C24	C25	C26	106.8(9)	.	.	.	no
C24	C25	C28	124.1(10)	.	.	.	no
C26	C25	C28	117.3(8)	.	.	.	no
C25	C26	C27	105.7(9)	.	.	.	no
C16	C26	C25	117.3(9)	3_655	.	.	no
C16	C26	C27	125.2(10)	3_655	.	.	no
C23	C27	C26	109.6(10)	.	.	.	no
C13	C27	C23	117.9(11)	3_655	.	.	no
C13	C27	C26	119.4(10)	3_655	.	.	no
C25	C28	C29	118.8(9)	.	.	.	no
C25	C28	C30	117.9(8)	.	.	.	no
C29	C28	C30	110.2(9)	.	.	.	no
C4	C29	C8	120.6(9)	.	.	.	no
C4	C29	C28	118.5(9)	.	.	.	no
C8	C29	C28	109.7(9)	.	.	.	no
C9	C30	C28	104.8(8)	.	.	.	no
C9	C30	C17	118.2(9)	.	.	3_655	no
C17	C30	C28	124.9(10)	3_655	.	.	no
C102	C101	C106	120.0(6)	.	.	.	no
C101	C102	C103	120.8(6)	.	.	.	no
C102	C103	C104	119.2(6)	.	.	.	no
C103	C104	C105	119.5(6)	.	.	.	no
C104	C105	C106	120.4(6)	.	.	.	no
C104	C105	C120	125.9(6)	.	.	.	no
C106	C105	C120	113.7(6)	.	.	.	no
C101	C106	C105	120.0(6)	.	.	.	no
C101	C106	C119	127.1(6)	.	.	.	no
C105	C106	C119	112.8(6)	.	.	.	no
C108	C107	C112	120.3(7)	.	.	.	no
C107	C108	C109	119.2(7)	.	.	.	no
C108	C109	C110	121.9(7)	.	.	.	no
C109	C110	C111	117.9(7)	.	.	.	no
C110	C111	C112	120.9(7)	.	.	.	no
C110	C111	C120	126.0(6)	.	.	.	no
C112	C111	C120	113.2(6)	.	.	.	no
C107	C112	C111	119.9(7)	.	.	.	no
C107	C112	C119	127.0(6)	.	.	.	no
C111	C112	C119	113.0(6)	.	.	.	no
C114	C113	C118	120.0(6)	.	.	.	no
C113	C114	C115	120.1(7)	.	.	.	no
C114	C115	C116	119.9(7)	.	.	.	no
C115	C116	C117	119.3(7)	.	.	.	no
C116	C117	C118	121.2(7)	.	.	.	no
C116	C117	C120	126.5(6)	.	.	.	no
C118	C117	C120	112.1(7)	.	.	.	no
C113	C118	C117	119.4(7)	.	.	.	no
C113	C118	C119	125.8(6)	.	.	.	no
C117	C118	C119	114.7(7)	.	.	.	no
C106	C119	C112	104.8(6)	.	.	.	no
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C112	C119	C118	104.8(6)	.	.	.	no
C105	C120	C111	105.5(5)	.	.	.	no
C105	C120	C117	106.4(5)	.	.	.	no
C111	C120	C117	104.4(5)	.	.	.	no
C102	C101	H101	119.94	.	.	.	no
C106	C101	H101	120.01	.	.	.	no

C101	C102	H102	119.64	.	.	.	no
C103	C102	H102	119.55	.	.	.	no
C102	C103	H103	120.43	.	.	.	no
C104	C103	H103	120.38	.	.	.	no
C103	C104	H104	120.29	.	.	.	no
C105	C104	H104	120.18	.	.	.	no
C108	C107	H107	119.89	.	.	.	no
C112	C107	H107	119.82	.	.	.	no
C107	C108	H108	120.36	.	.	.	no
C109	C108	H108	120.42	.	.	.	no
C108	C109	H109	119.13	.	.	.	no
C110	C109	H109	119.02	.	.	.	no
C109	C110	H110	121.07	.	.	.	no
C111	C110	H110	121.07	.	.	.	no
C114	C113	H113	120.10	.	.	.	no
C118	C113	H113	119.94	.	.	.	no
C113	C114	H114	119.97	.	.	.	no
C115	C114	H114	119.92	.	.	.	no
C114	C115	H115	120.07	.	.	.	no
C116	C115	H115	120.03	.	.	.	no
C115	C116	H116	120.26	.	.	.	no
C117	C116	H116	120.45	.	.	.	no
C106	C119	H119	113.26	.	.	.	no
C112	C119	H119	113.21	.	.	.	no
C118	C119	H119	113.22	.	.	.	no
C105	C120	H120	113.23	.	.	.	no
C111	C120	H120	113.25	.	.	.	no
C117	C120	H120	113.31	.	.	.	no
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C93	C92	C97	119.1(5)	.	.	.	no
C92	C93	C94	121.8(6)	.	.	.	no
C93	C94	C95	118.9(6)	.	.	.	no
C94	C95	C96	119.5(6)	.	.	.	no
C95	C96	C97	121.9(7)	.	.	.	no
C92	C97	C96	118.7(6)	.	.	.	no
C92	C97	C98	121.5(5)	.	.	.	no
C96	C97	C98	119.9(6)	.	.	.	no
C92	C91	H91A	109.44	.	.	.	no
C92	C91	H91B	109.43	.	.	.	no
C92	C91	H91C	109.50	.	.	.	no
H91A	C91	H91B	109.55	.	.	.	no
H91A	C91	H91C	109.50	.	.	.	no
H91B	C91	H91C	109.41	.	.	.	no
C92	C93	H93	119.17	.	.	.	no
C94	C93	H93	118.99	.	.	.	no
C93	C94	H94	120.59	.	.	.	no
C95	C94	H94	120.50	.	.	.	no
C94	C95	H95	120.18	.	.	.	no
C96	C95	H95	120.28	.	.	.	no
C95	C96	H96	118.99	.	.	.	no
C97	C96	H96	119.09	.	.	.	no
C97	C98	H98A	109.45	.	.	.	no
C97	C98	H98B	109.48	.	.	.	no
C97	C98	H98C	109.52	.	.	.	no
H98A	C98	H98B	109.40	.	.	.	no
H98A	C98	H98C	109.50	.	.	.	no
H98B	C98	H98C	109.48	.	.	.	no

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C19	C1	C2	C21	0.4(14)	.	.	.	.	no
C2	C1	C5	C4	1.4(8)	.	.	.	.	no
C2	C1	C5	C6	-140.9(7)	.	.	.	.	no
C19	C1	C5	C4	141.9(7)	.	.	.	.	no
C19	C1	C5	C6	-0.3(11)	.	.	.	.	no
C2	C1	C19	C15	136.2(9)	.	.	.	.	no
C2	C1	C19	C18	-2.3(13)	.	.	.	.	no
C5	C1	C19	C15	-1.2(13)	.	.	.	.	no
C5	C1	C19	C18	-139.7(8)	.	.	.	.	no
C1	C2	C3	C4	-0.4(9)	.	.	.	.	no
C1	C2	C3	C24	142.4(11)	.	.	.	.	no
C21	C2	C3	C4	-144.4(7)	.	.	.	.	no
C21	C2	C3	C24	-1.6(14)	.	.	.	.	no
C1	C2	C21	C20	1.0(16)	.	.	.	.	no
C1	C2	C21	C22	-137.1(10)	.	.	.	.	no
C3	C2	C21	C20	138.8(11)	.	.	.	.	no
C3	C2	C21	C22	0.8(12)	.	.	.	.	no
C2	C3	C4	C5	1.3(8)	.	.	.	.	no
C2	C3	C4	C29	142.0(7)	.	.	.	.	no
C24	C3	C4	C5	-143.1(9)	.	.	.	.	no
C24	C3	C4	C29	-2.4(12)	.	.	.	.	no
C2	C3	C24	C23	1.7(16)	.	.	.	.	no
C2	C3	C24	C25	-137.9(11)	.	.	.	.	no
C4	C3	C24	C23	139.5(10)	.	.	.	.	no
C4	C3	C24	C25	-0.1(15)	.	.	.	.	no
C3	C4	C5	C1	-1.6(7)	.	.	.	.	no
C3	C4	C5	C6	139.9(7)	.	.	.	.	no
C29	C4	C5	C1	-142.5(7)	.	.	.	.	no
C29	C4	C5	C6	-1.1(9)	.	.	.	.	no
C3	C4	C29	C8	-136.7(8)	.	.	.	.	no
C3	C4	C29	C28	3.3(10)	.	.	.	.	no
C5	C4	C29	C8	-0.4(11)	.	.	.	.	no
C5	C4	C29	C28	139.6(7)	.	.	.	.	no
C1	C5	C6	C7	140.0(7)	.	.	.	.	no
C1	C5	C6	C14	-1.2(11)	.	.	.	.	no
C4	C5	C6	C7	2.0(10)	.	.	.	.	no
C4	C5	C6	C14	-139.3(7)	.	.	.	.	no
C5	C6	C7	C8	-1.5(12)	.	.	.	.	no
C5	C6	C7	C12	-143.2(7)	.	.	.	.	no
C14	C6	C7	C8	142.7(9)	.	.	.	.	no
C14	C6	C7	C12	1.1(10)	.	.	.	.	no
C5	C6	C14	C13	142.1(8)	.	.	.	.	no
C5	C6	C14	C15	4.6(14)	.	.	.	.	no
C7	C6	C14	C13	-2.1(10)	.	.	.	.	no
C7	C6	C14	C15	-139.6(10)	.	.	.	.	no
C6	C7	C8	C9	-135.4(9)	.	.	.	.	no
C6	C7	C8	C29	0.1(12)	.	.	.	.	no
C12	C7	C8	C9	2.6(12)	.	.	.	.	no
C12	C7	C8	C29	138.1(8)	.	.	.	.	no
C6	C7	C12	C11	143.5(8)	.	.	.	.	no
C6	C7	C12	C13	0.6(11)	.	.	.	.	no
C8	C7	C12	C11	0.8(11)	.	.	.	.	no
C8	C7	C12	C13	-142.1(8)	.	.	.	.	no
C7	C8	C9	C10	-5.1(13)	.	.	.	.	no
C7	C8	C9	C30	141.5(9)	.	.	.	.	no
C29	C8	C9	C10	-146.0(9)	.	.	.	.	no
C29	C8	C9	C30	0.7(10)	.	.	.	.	no
C7	C8	C29	C4	0.8(13)	.	.	.	.	no
C7	C8	C29	C28	-142.3(9)	.	.	.	.	no
C9	C8	C29	C4	141.9(8)	.	.	.	.	no
C9	C8	C29	C28	-1.3(10)	.	.	.	.	no

C8	C9	C10	C11	4.1(15)	.	.	.	.	no
C8	C9	C10	C20	140.4(10)	.	.	.	3_655	no
C30	C9	C10	C11	-137.8(11)	.	.	.	.	no
C30	C9	C10	C20	-1.5(16)	.	.	.	3_655	no
C8	C9	C30	C28	0.2(12)	.	.	.	.	no
C8	C9	C30	C17	-144.3(9)	.	.	.	3_655	no
C10	C9	C30	C28	145.1(10)	.	.	.	.	no
C10	C9	C30	C17	0.6(15)	.	.	.	3_655	no
C9	C10	C11	C12	-0.7(15)	.	.	.	.	no
C9	C10	C11	C22	140.6(10)	.	.	.	3_655	no
C20	C10	C11	C12	-141.3(9)	3_655	.	.	.	no
C20	C10	C11	C22	0.0(9)	3_655	.	.	3_655	no
C9	C10	C20	C18	2.0(16)	.	.	3_655	3_655	no
C9	C10	C20	C21	-143.5(10)	.	.	3_655	3_655	no
C11	C10	C20	C18	144.7(10)	.	.	3_655	3_655	no
C11	C10	C20	C21	-0.8(10)	.	.	3_655	3_655	no
C10	C11	C12	C7	-1.9(12)	.	.	.	.	no
C10	C11	C12	C13	134.4(10)	.	.	.	.	no
C22	C11	C12	C7	-140.1(8)	3_655	.	.	.	no
C22	C11	C12	C13	-3.8(13)	3_655	.	.	.	no
C10	C11	C22	C21	0.9(10)	.	.	3_655	3_655	no
C10	C11	C22	C23	-142.5(9)	.	.	3_655	3_655	no
C12	C11	C22	C21	144.6(8)	.	.	3_655	3_655	no
C12	C11	C22	C23	1.3(13)	.	.	3_655	3_655	no
C7	C12	C13	C14	-1.8(10)	.	.	.	.	no
C7	C12	C13	C27	144.6(10)	.	.	.	3_655	no
C11	C12	C13	C14	-141.9(9)	.	.	.	.	no
C11	C12	C13	C27	4.5(15)	.	.	.	3_655	no
C12	C13	C14	C6	2.5(11)	.	.	.	.	no
C12	C13	C14	C15	143.7(9)	.	.	.	.	no
C27	C13	C14	C6	-144.4(10)	3_655	.	.	.	no
C27	C13	C14	C15	-3.2(15)	3_655	.	.	.	no
C12	C13	C27	C23	-2.4(16)	.	.	3_655	3_655	no
C12	C13	C27	C26	-139.7(11)	.	.	3_655	3_655	no
C14	C13	C27	C23	139.9(10)	.	.	3_655	3_655	no
C14	C13	C27	C26	2.6(17)	.	.	3_655	3_655	no
C6	C14	C15	C16	134.5(10)	.	.	.	.	no
C6	C14	C15	C19	-6.0(14)	.	.	.	.	no
C13	C14	C15	C16	0.9(15)	.	.	.	.	no
C13	C14	C15	C19	-139.6(9)	.	.	.	.	no
C14	C15	C16	C17	-142.6(10)	.	.	.	.	no
C14	C15	C16	C26	1.8(14)	.	.	.	3_655	no
C19	C15	C16	C17	1.2(11)	.	.	.	.	no
C19	C15	C16	C26	145.6(9)	.	.	.	3_655	no
C14	C15	C19	C1	4.3(14)	.	.	.	.	no
C14	C15	C19	C18	146.9(9)	.	.	.	.	no
C16	C15	C19	C1	-142.4(9)	.	.	.	.	no
C16	C15	C19	C18	0.2(11)	.	.	.	.	no
C15	C16	C17	C18	-2.3(11)	.	.	.	.	no
C15	C16	C17	C30	143.7(9)	.	.	.	3_655	no
C26	C16	C17	C18	-141.2(11)	3_655	.	.	.	no
C26	C16	C17	C30	4.7(15)	3_655	.	.	3_655	no
C15	C16	C26	C25	-140.0(9)	.	.	3_655	3_655	no
C15	C16	C26	C27	-2.5(15)	.	.	3_655	3_655	no
C17	C16	C26	C25	-3.2(15)	.	.	3_655	3_655	no
C17	C16	C26	C27	134.3(12)	.	.	3_655	3_655	no
C16	C17	C18	C19	2.4(12)	.	.	.	.	no
C16	C17	C18	C20	142.0(10)	.	.	.	.	no
C30	C17	C18	C19	-140.4(10)	3_655	.	.	.	no
C30	C17	C18	C20	-0.9(16)	3_655	.	.	.	no
C16	C17	C30	C9	-140.0(9)	.	.	3_655	3_655	no
C16	C17	C30	C28	-3.2(14)	.	.	3_655	3_655	no
C18	C17	C30	C9	0.2(15)	.	.	3_655	3_655	no
C18	C17	C30	C28	137.0(11)	.	.	3_655	3_655	no
C17	C18	C19	C1	142.7(9)	.	.	.	.	no
C17	C18	C19	C15	-1.6(11)	.	.	.	.	no
C20	C18	C19	C1	2.8(14)	.	.	.	.	no

C20	C18	C19	C15	-141.5(10)	.	.	.	.	no
C17	C18	C20	C21	-137.5(12)	.	.	.	.	no
C17	C18	C20	C10	1.7(15)	.	.	.	3_655	no
C19	C18	C20	C21	-1.4(17)	.	.	.	.	no
C19	C18	C20	C10	137.8(10)	.	.	.	3_655	no
C18	C20	C21	C2	-0.5(18)	.	.	.	.	no
C18	C20	C21	C22	141.6(11)	.	.	.	.	no
C10	C20	C21	C2	-143.5(10)	3_655	.	.	.	no
C10	C20	C21	C22	-1.4(10)	3_655	.	.	.	no
C2	C21	C22	C23	-0.2(14)	.	.	.	.	no
C2	C21	C22	C11	142.3(8)	.	.	.	3_655	no
C20	C21	C22	C23	-141.1(10)	.	.	.	.	no
C20	C21	C22	C11	1.4(10)	.	.	.	3_655	no
C21	C22	C23	C24	0.4(15)	.	.	.	.	no
C21	C22	C23	C27	138.4(11)	.	.	.	.	no
C11	C22	C23	C24	-138.6(11)	3_655	.	.	.	no
C11	C22	C23	C27	-0.5(15)	3_655	.	.	.	no
C22	C23	C24	C3	-1.1(17)	.	.	.	.	no
C22	C23	C24	C25	141.4(11)	.	.	.	.	no
C27	C23	C24	C3	-144.4(12)	.	.	.	.	no
C27	C23	C24	C25	-1.9(14)	.	.	.	.	no
C22	C23	C27	C26	-141.2(11)	.	.	.	.	no
C22	C23	C27	C13	0.0(16)	.	.	.	3_655	no
C24	C23	C27	C26	1.9(14)	.	.	.	.	no
C24	C23	C27	C13	143.1(11)	.	.	.	3_655	no
C3	C24	C25	C26	143.2(10)	.	.	.	.	no
C3	C24	C25	C28	1.5(16)	.	.	.	.	no
C23	C24	C25	C26	1.2(13)	.	.	.	.	no
C23	C24	C25	C28	-140.5(11)	.	.	.	.	no
C24	C25	C26	C27	0.1(12)	.	.	.	.	no
C24	C25	C26	C16	-145.0(10)	.	.	.	3_655	no
C28	C25	C26	C27	144.8(10)	.	.	.	.	no
C28	C25	C26	C16	-0.3(14)	.	.	.	3_655	no
C24	C25	C28	C29	-0.5(15)	.	.	.	.	no
C24	C25	C28	C30	137.1(11)	.	.	.	.	no
C26	C25	C28	C29	-138.6(9)	.	.	.	.	no
C26	C25	C28	C30	-1.0(13)	.	.	.	.	no
C25	C26	C27	C23	-1.3(12)	.	.	.	.	no
C25	C26	C27	C13	-141.8(11)	.	.	.	3_655	no
C16	C26	C27	C23	140.1(11)	3_655	.	.	.	no
C16	C26	C27	C13	-0.4(18)	3_655	.	.	3_655	no
C25	C28	C29	C4	-2.0(12)	.	.	.	.	no
C25	C28	C29	C8	142.0(9)	.	.	.	.	no
C30	C28	C29	C4	-142.6(8)	.	.	.	.	no
C30	C28	C29	C8	1.4(11)	.	.	.	.	no
C25	C28	C30	C9	-141.9(9)	.	.	.	.	no
C25	C28	C30	C17	-0.6(14)	.	.	.	3_655	no
C29	C28	C30	C9	-0.9(10)	.	.	.	.	no
C29	C28	C30	C17	140.4(9)	.	.	.	3_655	no
C106	C101	C102	H102	-179.29	.	.	.	.	no
H101	C101	C102	C103	-179.25	.	.	.	.	no
H101	C101	C102	H102	0.59	.	.	.	.	no
H101	C101	C106	C105	179.81	.	.	.	.	no
H101	C101	C106	C119	1.66	.	.	.	.	no
C101	C102	C103	H103	178.57	.	.	.	.	no
H102	C102	C103	C104	178.80	.	.	.	.	no
H102	C102	C103	H103	-1.27	.	.	.	.	no
C102	C103	C104	H104	-178.72	.	.	.	.	no
H103	C103	C104	C105	-178.63	.	.	.	.	no
H103	C103	C104	H104	1.35	.	.	.	.	no
H104	C104	C105	C106	179.26	.	.	.	.	no
H104	C104	C105	C120	-2.13	.	.	.	.	no
C104	C105	C120	H120	1.59	.	.	.	.	no
C106	C105	C120	H120	-179.72	.	.	.	.	no
C101	C106	C119	H119	-1.80	.	.	.	.	no
C105	C106	C119	H119	179.94	.	.	.	.	no
C112	C107	C108	H108	179.60	.	.	.	.	no

H107	C107	C108	C109	179.79	.	.	.	.	no
H107	C107	C108	H108	-0.35	.	.	.	.	no
H107	C107	C112	C111	179.78	.	.	.	.	no
H107	C107	C112	C119	3.99	.	.	.	.	no
C107	C108	C109	H109	179.65	.	.	.	.	no
H108	C108	C109	C110	179.81	.	.	.	.	no
H108	C108	C109	H109	-0.20	.	.	.	.	no
C108	C109	C110	H110	-178.60	.	.	.	.	no
H109	C109	C110	C111	-178.67	.	.	.	.	no
H109	C109	C110	H110	1.42	.	.	.	.	no
H110	C110	C111	C112	178.18	.	.	.	.	no
H110	C110	C111	C120	-2.73	.	.	.	.	no
C110	C111	C120	H120	1.69	.	.	.	.	no
C112	C111	C120	H120	-179.15	.	.	.	.	no
C107	C112	C119	H119	-2.98	.	.	.	.	no
C111	C112	C119	H119	-179.01	.	.	.	.	no
C118	C113	C114	H114	-178.18	.	.	.	.	no
H113	C113	C114	C115	-178.33	.	.	.	.	no
H113	C113	C114	H114	1.88	.	.	.	.	no
H113	C113	C118	C117	177.87	.	.	.	.	no
H113	C113	C118	C119	-3.78	.	.	.	.	no
C113	C114	C115	H115	178.38	.	.	.	.	no
H114	C114	C115	C116	178.32	.	.	.	.	no
H114	C114	C115	H115	-1.83	.	.	.	.	no
C114	C115	C116	H116	-178.18	.	.	.	.	no
H115	C115	C116	C117	-178.04	.	.	.	.	no
H115	C115	C116	H116	1.97	.	.	.	.	no
H116	C116	C117	C118	177.67	.	.	.	.	no
H116	C116	C117	C120	3.30	.	.	.	.	no
C116	C117	C120	H120	-4.75	.	.	.	.	no
C118	C117	C120	H120	-179.55	.	.	.	.	no
C113	C118	C119	H119	2.27	.	.	.	.	no
C117	C118	C119	H119	-179.32	.	.	.	.	no
C91	C92	C93	C94	179.6(7)	.	.	.	.	no
C97	C92	C93	C94	0.5(11)	.	.	.	.	no
C91	C92	C97	C96	-180.0(7)	.	.	.	.	no
C91	C92	C97	C98	0.3(11)	.	.	.	.	no
C93	C92	C97	C96	-0.9(10)	.	.	.	.	no
C93	C92	C97	C98	179.4(7)	.	.	.	.	no
C92	C93	C94	C95	-0.1(11)	.	.	.	.	no
C93	C94	C95	C96	0.0(11)	.	.	.	.	no
C94	C95	C96	C97	-0.5(11)	.	.	.	.	no
C95	C96	C97	C92	0.9(11)	.	.	.	.	no
C95	C96	C97	C98	-179.4(7)	.	.	.	.	no

#---END

CIF-file generated for s1561a - Complex # 2

data_s1561a

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

?

;

_chemical_name_common

?

_chemical_melting_point

?

_chemical_formula_moiety

'C60, C19 H13 N'

_chemical_formula_structural

?

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

_chemical_formula_sum

'C79 H13 N'

_chemical_formula_weight

975.90

_chemical_compound_source

'see text'

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loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
N N 0.0061 0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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6. CRYSTAL DATA

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_symmetry_cell_setting          Hexagonal
_symmetry_space_group_name_Hall 'P 6c -2c'
_symmetry_space_group_name_H-M  'P 63 m c'

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loop_
_symmetry_equiv_pos_as_xyz
x,y,z
x-y,x,1/2+z
-y,x-y,z
-x,-y,1/2+z
-x+y,-x,z
y,-x+y,1/2+z
y,x,1/2+z
-x+y,y,z
-x,-x+y,1/2+z
-y,-x,z
x-y,-y,1/2+z
x,x-y,z

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_cell_length_a          13.4643(11)
_cell_length_b          13.4643(11)
_cell_length_c          12.6983(9)
_cell_angle_alpha       90
_cell_angle_beta        90
_cell_angle_gamma       120
_cell_volume            1993.6(3)
_cell_formula_units_Z    2
_cell_measurement_temperature 150

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_exptl_crystal_description      block
_exptl_crystal_colour          'dark-red'
_exptl_crystal_size_max        0.75
_exptl_crystal_size_mid        0.60
_exptl_crystal_size_min        0.50
_exptl_crystal_density_diffrn  1.626
_exptl_crystal_density_method  'Not Measured'
_exptl_crystal_F_000          988
_exptl_absorpt_coefficient_mu  0.09

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#####

7. EXPERIMENTAL DATA

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_diffraction_ambient_temperature 150
_diffraction_radiation_wavelength 0.71073
_diffraction_radiation_type       'Mo K\alpha'
_diffraction_radiation_source     'Rotating-Anode'
_diffraction_radiation_monochromator 'graphite'

_diffraction_measurement_device_type 'Nonius CAD4-T'

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_diffrn_measurement_method      'Omega-scan'

# number of measured reflections (redundant set)
_diffrn_reflms_number           6587
_diffrn_reflms_av_R_equivalents 0.0694
_diffrn_reflms_av_sigmaI/netI   0.0301
_diffrn_reflms_limit_h_min      -17
_diffrn_reflms_limit_h_max      17
_diffrn_reflms_limit_k_min      -17
_diffrn_reflms_limit_k_max      17
_diffrn_reflms_limit_l_min      0
_diffrn_reflms_limit_l_max      16
_diffrn_reflms_theta_min        1.75
_diffrn_reflms_theta_max        27.52

# number of unique reflections
_reflms_number_total            909
# number of observed reflections (> n sig(I))
_reflms_number_gt               711
_reflms_threshold_expression     'I>2sigma(I)'

_computing_data_collection      'Locally modified CAD4-Version 5 Software'
_computing_cell_refinement      'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction       'HELENA (Spek, 1997)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement on F^2 for ALL reflections except those
flagged by the user for potential systematic errors.
Weighted R-factors wR and all goodnesses 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
observed criterion of F^2 > 2sigma(F^2) is used only
for calculating -R-factor-obs 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/[^2^(FO^2^)+(0.1351P)^2^+4.0391P] WHERE P=(FO^2^+2FC^2^)/3'
_refine_ls_hydrogen_treatment    'H-atom refinement: see text '
_refine_ls_extinction_method      none
_refine_ls_abs_structure_details
'Flack H.D. (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    8(10)
_refine_ls_number_reflms          909
_refine_ls_number_parameters      143
_refine_ls_number_restraints      24
_refine_ls_R_factor_all           0.1080
_refine_ls_R_factor_gt            0.0861
_refine_ls_wR_factor_ref          0.2717
_refine_ls_wR_factor_gt           0.2438
_refine_ls_goodness_of_fit_ref    1.051
_refine_ls_restrained_S_all       1.044
_refine_ls_shift/su_max           0.113
_refine_ls_shift/su_mean          0.037
_refine_diff_density_max          0.651

```

_refine_diff_density_min -0.603
_refine_diff_density_rms 0.078

#=====

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

```
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_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
C1      C  Uani    0.1327(11)  0.4851(13)  0.4348(8)  1.000  0.144(6)
C2      C  Uani    0.2322(7)   0.5612(6)  0.5026(7)  1.000  0.189(14)
C5      C  Uani    0.0683(15)  0.5342(7)  0.380(2)   1.000  0.170(11)
C6      C  Uani    0.1189(14)  0.3842(11) 0.2699(17) 1.000  0.251(15)
C7      C  Uani    0.1916(6)   0.3831(12) 0.183(3)   1.000  0.28(3)
C9      C  Uani    0.1537(7)   0.4167(13) 0.3803(16) 1.000  0.246(11)
C11     C  Uani    0.0607(8)   0.4304(12) 0.2395(14) 1.000  0.212(9)
C12     C  Uani    0.0736(12)  0.4819(7)  0.1344(15) 1.000  0.241(16)
C14     C  Uani    0.0363(14)  0.5181(7)  0.284(3)   1.000  0.36(4)
C16     C  Uani    0.2279(6)   0.5659(7) -0.0027(7) 1.000  0.129(7)
C17     C  Uani    0.1392(12)  0.4752(12) 0.0630(8)  1.000  0.155(9)
C19     C  Uani    0.2155(11)  0.431(2)   0.092(2)   1.000  0.35(4)
N1      N  Uani    0.00000      0.00000    0.3505(10) 1.000  0.032(3)
C101    C  Uani    0.00000      0.00000    0.1465(12) 1.000  0.021(3)
C102    C  Uani    0.1176(6)   0.0588(3)  0.3056(8)  1.000  0.023(2)
C103    C  Uani    0.2199(8)   0.1100(4)  0.3603(9)  1.000  0.029(3)
C104    C  Uani    0.3220(7)   0.1610(4)  0.3049(9)  1.000  0.029(2)
C105    C  Uani    0.3209(7)   0.1605(4) 0.1960(10) 1.000  0.033(2)
C106    C  Uani    0.2181(8)   0.1091(4)  0.1388(8)  1.000  0.027(2)
C107    C  Uani    0.1176(6)   0.0588(3)  0.1949(9)  1.000  0.025(2)
H101    H  Uiso    0.00000      0.00000    0.06770    1.000  0.0250
H103    H  Uiso    0.22020      0.11010    0.43510    1.000  0.0350
H104    H  Uiso    0.39300      0.19650    0.34160    1.000  0.0340
H105    H  Uiso    0.39170      0.19585    0.15900    1.000  0.0390
H106    H  Uiso    0.21800      0.10900    0.06400    1.000  0.0330
```

```
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_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C1      0.122(13)  0.110(10)  0.071(7)  0.025(8)  0.050(8) -0.039(10)
C2      0.29(3)   0.31(3)   0.061(9)  0.108(12) 0.102(12) 0.22(2)
C5      0.023(7)   0.29(3)  0.107(15) 0.017(4)  0.033(9) 0.011(4)
C6      0.142(16)  0.049(8)  0.39(4)  -0.024(17) 0.10(2) -0.081(10)
C7      0.30(5)   0.004(6)  0.45(8)  -0.08(2)  -0.038(10) 0.002(3)
C9      0.28(3)   0.074(9)  0.156(14) 0.060(11) 0.077(19) -0.082(15)
C11     0.021(4)   0.23(2)  0.211(17) -0.147(17) 0.028(9) -0.068(8)
C12     0.117(15) 0.25(4)  0.187(19) -0.076(19) -0.114(16) -0.036(17)
C14     0.011(7)   0.54(10)  0.34(7)  0.044(11) 0.09(2) 0.006(3)
C16     0.164(13) 0.154(14) 0.039(6)  -0.046(7) -0.054(7) 0.058(11)
C17     0.143(17) 0.190(18) 0.105(12) -0.118(13) -0.093(12) 0.063(14)
C19     0.40(7)   0.25(5)  0.33(7)  -0.29(6)  -0.14(3) 0.12(3)
N1      0.038(5)   0.038(5)  0.019(6)  0.0000  0.0000 0.019(2)
C101    0.014(3)   0.014(3)  0.034(8)  0.0000  0.0000 0.0071(17)
C102    0.026(4)   0.018(2)  0.027(4)  0.0003(15) 0.001(3) 0.0132(19)
C103    0.034(5)   0.023(3)  0.034(5) -0.0019(18) -0.004(4) 0.017(2)
C104    0.029(4)   0.018(3)  0.043(5) -0.003(2)  -0.006(4) 0.014(2)
```

C105	0.023(4)	0.026(3)	0.048(5)	0.005(2)	0.010(4)	0.0117(18)
C106	0.035(5)	0.029(3)	0.021(4)	0.0046(17)	0.009(3)	0.018(2)
C107	0.025(4)	0.021(3)	0.032(4)	-0.0017(16)	-0.003(3)	0.013(2)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds 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

N1	C102	1.485(9)	.	5_555	yes
N1	C102	1.485(9)	.	.	yes
N1	C102	1.485(9)	.	3_555	yes
C1	C2	1.488(17)	.	.	no
C1	C5	1.50(3)	.	.	no
C1	C9	1.29(2)	.	.	no
C2	C2	1.303(16)	.	8_555	no
C2	C2	1.478(13)	.	12_565	no
C5	C14	1.27(4)	.	.	no
C6	C11	1.28(2)	.	.	no
C6	C9	1.47(3)	.	.	no
C6	C7	1.48(4)	.	.	no
C7	C19	1.28(4)	.	.	no
C9	C9	1.47(3)	.	8_555	no
C11	C12	1.47(2)	.	.	no
C11	C14	1.49(2)	.	.	no
C12	C12	1.48(2)	.	12_565	no
C12	C17	1.30(2)	.	.	no
C16	C17	1.468(16)	.	.	no
C16	C16	1.482(16)	.	8_555	no
C16	C16	1.294(13)	.	12_565	no
C17	C19	1.47(3)	.	.	no
C101	C107	1.503(10)	.	.	no
C101	C107	1.503(10)	.	3_555	no
C101	C107	1.503(10)	.	5_555	no
C102	C103	1.380(13)	.	.	no
C102	C107	1.406(15)	.	.	no
C103	C104	1.383(14)	.	.	no
C104	C105	1.383(17)	.	.	no
C105	C106	1.402(14)	.	.	no
C106	C107	1.371(13)	.	.	no
C101	H101	1.001(15)	.	.	no
C103	H103	0.950(11)	.	.	no
C104	H104	0.950(9)	.	.	no
C105	H105	0.950(10)	.	.	no
C106	H106	0.950(10)	.	.	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

C102	N1	C102	106.2(7)	3_555	.	5_555	yes
C102	N1	C102	106.2(7)	.	.	3_555	yes
C102	N1	C102	106.2(7)	.	.	5_555	yes
C2	C1	C9	111.0(14)	.	.	.	no
C2	C1	C5	119.0(12)	.	.	.	no
C5	C1	C9	116.6(14)	.	.	.	no
C1	C2	C2	123.8(9)	.	.	8_555	no
C1	C2	C2	103.8(9)	.	.	12_565	no
C2	C2	C2	120.0(8)	8_555	.	12_565	no
C1	C5	C1	93.8(15)	.	.	12_565	no
C1	C5	C14	126.3(13)	12_565	.	.	no
C1	C5	C14	126.1(17)	.	.	.	no
C7	C6	C11	110.4(19)	.	.	.	no
C7	C6	C9	126.8(18)	.	.	.	no
C9	C6	C11	108.9(16)	.	.	.	no
C6	C7	C19	131.8(16)	.	.	.	no
C6	C7	C6	84(2)	.	.	8_555	no
C6	C7	C19	131.9(16)	8_555	.	.	no
C6	C9	C9	99.8(15)	.	.	8_555	no
C1	C9	C6	124.8(15)	.	.	.	no
C1	C9	C9	125.1(16)	.	.	8_555	no
C6	C11	C12	123.0(16)	.	.	.	no
C6	C11	C14	135(2)	.	.	.	no
C12	C11	C14	89.5(16)	.	.	.	no
C12	C12	C17	114.1(13)	12_565	.	.	no
C11	C12	C17	121.6(14)	.	.	.	no
C11	C12	C12	114.3(15)	.	.	12_565	no
C5	C14	C11	107.8(15)	.	.	12_565	no
C5	C14	C11	108.0(18)	.	.	.	no
C11	C14	C11	130(3)	.	.	12_565	no
C16	C16	C17	113.4(9)	8_555	.	.	no
C16	C16	C17	115.2(10)	12_565	.	.	no
C16	C16	C16	120.0(8)	8_555	.	12_565	no
C16	C17	C19	92.1(14)	.	.	.	no
C12	C17	C16	129.6(12)	.	.	.	no
C12	C17	C19	119.4(15)	.	.	.	no
C7	C19	C17	112.3(17)	.	.	.	no
C7	C19	C17	112.2(17)	.	.	8_555	no
C17	C19	C17	128.9(19)	.	.	8_555	no
C107	C101	C107	104.4(8)	.	.	3_555	no
C107	C101	C107	104.4(8)	.	.	5_555	no
C107	C101	C107	104.4(8)	3_555	.	5_555	no
N1	C102	C103	127.2(10)	.	.	.	yes
N1	C102	C107	112.6(8)	.	.	.	yes
C103	C102	C107	120.2(8)	.	.	.	no
C102	C103	C104	119.2(10)	.	.	.	no
C103	C104	C105	120.0(9)	.	.	.	no
C104	C105	C106	121.7(9)	.	.	.	no
C105	C106	C107	117.5(10)	.	.	.	no
C101	C107	C102	114.1(8)	.	.	.	no
C101	C107	C106	124.6(11)	.	.	.	no
C102	C107	C106	121.3(8)	.	.	.	no
C107	C101	H101	114.1(7)	.	.	.	no
C107	C101	H101	114.1(7)	3_555	.	.	no
C107	C101	H101	114.1(7)	5_555	.	.	no
C102	C103	H103	120.4(10)	.	.	.	no
C104	C103	H103	120.4(10)	.	.	.	no
C103	C104	H104	120.0(11)	.	.	.	no
C105	C104	H104	119.9(9)	.	.	.	no
C104	C105	H105	119.1(10)	.	.	.	no
C106	C105	H105	119.1(12)	.	.	.	no
C105	C106	H106	121.3(10)	.	.	.	no
C107	C106	H106	121.2(10)	.	.	.	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
C5      C1      C2      C2      -136.7(14)      .      .      .      8_555 no
C5      C1      C2      C2      4.9(16)      .      .      .      12_565 no
C9      C1      C2      C2      2.8(17)      .      .      .      8_555 no
C9      C1      C2      C2      144.4(12)      .      .      .      12_565 no
C2      C1      C5      C14      134.6(14)      .      .      .      . no
C2      C1      C5      C1      -6.9(18)      .      .      .      12_565 no
C9      C1      C5      C14      -3(2)      .      .      .      . no
C9      C1      C5      C1      -144.3(16)      .      .      .      12_565 no
C2      C1      C9      C6      -140.8(14)      .      .      .      . no
C2      C1      C9      C9      -3(2)      .      .      .      8_555 no
C5      C1      C9      C6      0(2)      .      .      .      . no
C5      C1      C9      C9      137.8(18)      .      .      .      8_555 no
C1      C2      C2      C2      135.9(10)      .      .      8_555      3_665 no
C1      C2      C2      C1      0.0(15)      .      .      8_555      8_555 no
C1      C2      C2      C2      -143.4(10)      .      .      12_565      5_565 no
C1      C2      C2      C1      0.0(11)      .      .      12_565      12_565 no
C1      C5      C14      C11      7(2)      .      .      .      . no
C1      C5      C14      C11      -136.9(15)      .      .      .      12_565 no
C1      C5      C14      C11      136.8(19)      12_565      .      .      . no
C9      C6      C7      C19      -125(3)      .      .      .      . no
C9      C6      C7      C6      17.9(16)      .      .      .      8_555 no
C11      C6      C7      C19      10(3)      .      .      .      . no
C11      C6      C7      C6      153.1(13)      .      .      .      8_555 no
C7      C6      C9      C1      132.8(18)      .      .      .      . no
C7      C6      C9      C9      -13.4(19)      .      .      .      8_555 no
C11      C6      C9      C1      -3(2)      .      .      .      . no
C11      C6      C9      C9      -149.2(14)      .      .      .      8_555 no
C7      C6      C11      C12      -4(2)      .      .      .      . no
C7      C6      C11      C14      -133(2)      .      .      .      . no
C9      C6      C11      C12      139.2(15)      .      .      .      . no
C9      C6      C11      C14      10(3)      .      .      .      . no
C6      C7      C19      C17      -14(3)      .      .      .      . no
C6      C7      C19      C17      141(2)      .      .      .      8_555 no
C6      C7      C19      C17      -141(2)      8_555      .      .      . no
C1      C9      C9      C1      0(3)      .      .      8_555      8_555 no
C1      C9      C9      C6      -146.1(17)      .      .      8_555      8_555 no
C6      C9      C9      C1      146.1(17)      .      .      8_555      8_555 no
C6      C9      C9      C6      0.0(14)      .      .      8_555      8_555 no
C6      C11      C12      C17      6(2)      .      .      .      . no
C6      C11      C12      C12      -138.0(17)      .      .      .      12_565 no
C14      C11      C12      C17      152.0(14)      .      .      .      . no
C14      C11      C12      C12      8.5(16)      .      .      .      12_565 no
C6      C11      C14      C5      -12(3)      .      .      .      . no
C6      C11      C14      C11      121(3)      .      .      .      12_565 no
C12      C11      C14      C5      -151.8(15)      .      .      .      . no
C12      C11      C14      C11      -18(2)      .      .      .      12_565 no
C11      C12      C17      C16      -130.7(14)      .      .      .      . no
C11      C12      C17      C19      -9(2)      .      .      .      . no
C12      C12      C17      C16      13(2)      12_565      .      .      . no
C12      C12      C17      C19      134.2(18)      12_565      .      .      . no
C11      C12      C12      C11      0(2)      .      .      12_565      12_565 no
C11      C12      C12      C17      146.3(16)      .      .      12_565      12_565 no
C17      C12      C12      C11      -146.3(16)      .      .      12_565      12_565 no
C17      C12      C12      C17      0(2)      .      .      12_565      12_565 no
C16      C16      C17      C12      130.7(17)      8_555      .      .      . no
C16      C16      C17      C19      -1.2(13)      8_555      .      .      . no

```

C16	C16	C17	C12	-13(2)	12_565	.	.	.	no
C16	C16	C17	C19	-144.8(13)	12_565	.	.	.	no
C17	C16	C16	C16	-141.7(9)	.	.	8_555	3_665	no
C17	C16	C16	C17	0.0(12)	.	.	8_555	8_555	no
C17	C16	C16	C16	141.1(10)	.	.	12_565	5_565	no
C17	C16	C16	C17	0.0(14)	.	.	12_565	12_565	no
C12	C17	C19	C7	13(3)	.	.	.	.	no
C12	C17	C19	C17	-136(2)	.	.	.	8_555	no
C16	C17	C19	C7	151.3(18)	.	.	.	.	no
C16	C17	C19	C17	2(2)	.	.	.	8_555	no
H101	C101	C107	C102	-180.0(3)	.	.	.	.	no
H101	C101	C107	C106	0.0(6)	.	.	.	.	no
N1	C102	C103	H103	0.1(10)	.	.	.	.	no
C107	C102	C103	H103	-180.0(6)	.	.	.	.	no
C102	C103	C104	H104	-180.0(6)	.	.	.	.	no
H103	C103	C104	C105	180(4)	.	.	.	.	no
H103	C103	C104	H104	-0.1(11)	.	.	.	.	no
C103	C104	C105	H105	-180.0(6)	.	.	.	.	no
H104	C104	C105	C106	180(3)	.	.	.	.	no
H104	C104	C105	H105	0.1(11)	.	.	.	.	no
C104	C105	C106	H106	-179.9(7)	.	.	.	.	no
H105	C105	C106	C107	179.9(15)	.	.	.	.	no
H105	C105	C106	H106	0.0(11)	.	.	.	.	no
H106	C106	C107	C101	-0.1(10)	.	.	.	.	no
H106	C106	C107	C102	180.0(5)	.	.	.	.	no

End of Crystallographic Information File