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_publ_contact_author_name      # Name of author for correspondence
;
Drs. A. Meetsma
;
_publ_contact_author_address    # Address of author for correspondence
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Crystal Structure Center,
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Materials Science Center,
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_publ_contact_author_fax        '+31 50 3634441'
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_publ_requested_journal         'Chem. Comm.'
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# FM, CM or EM for Metal-organic
# FO, CO or EO for Organic
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_publ_requested_coeditor_name   ?

_publ_contact_letter            # Include date of submission
;
Date of submission : 2007-08-06 11:58:08

Consider this CIF submission for deposition of the first
X-ray structure of a manuscript to be submitted to : Chem. Comm
(Our Compound_Identification_Code : Q1117)
;

loop_
_publ_author_name
```

B.Feringa
A.Meetsma
M.Pollard

_publ_section_exptl_refinement

;

The structure was solved by direct methods using the program SIR2004. The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined. A subsequent difference Fourier synthesis resulted in the location of all the hydrogen atoms, which coordinates and isotropic displacement parameters were refined.

;

Insert blank lines between references

_publ_section_references

;

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;

_publ_section_figure_captions

;

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

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

Fig. 3. Perspective ORTEP drawing of the title compound.
Displacement ellipsoids for non-H are represented at the 50% probability level.
The H-atoms are drawn with an arbitrary radius.

;

#=====

data_1

_database_code_depnum_ccdc_archive 'CCDC 666199'

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common

?

_chemical_melting_point

?

_chemical_formula_moiety

'C24 H28'

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

_chemical_formula_structural

?

_chemical_formula_sum

'C24 H28'

_chemical_formula_iupac

?

_chemical_formula_weight

316.48

_chemical_compound_source

'see text'

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_atom_type_description

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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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Triclinic

_symmetry_space_group_name_Hall '-P 1'

_symmetry_space_group_name_H-M 'P -1'

_symmetry_Int_Tables_number 2

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 -x,-y,-z

_cell_length_a 11.4202(7)

_cell_length_b 13.2038(8)

_cell_length_c 13.6607(8)

_cell_angle_alpha 106.538(1)

_cell_angle_beta 90.402(1)

_cell_angle_gamma 115.040(1)

_cell_volume 1769.71(19)

_cell_formula_units_Z 4

```

_cell_measurement_temperature      100(1)
_cell_measurement_reflns_used      6549
_cell_measurement_theta_min        2.35
_cell_measurement_theta_max        29.55
_cell_special_details

```

```

;
The final unit cell was obtained from the xyz centroids of
6549 reflections after integration using the SAINTPLUS
software package (Bruker, 2000).

```

```

Reduced cell calculations did not indicate any higher metric lattice symmetry
and examination of the final atomic coordinates of the structure did not
yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

```

```

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_exptl_crystal_size_mid            0.52
_exptl_crystal_size_min            0.44
_exptl_crystal_size_rad            ?
_exptl_crystal_density_meas        ?
_exptl_crystal_density_diffn       1.188
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_exptl_crystal_F_000               688
_exptl_absorpt_coefficient_mu       0.066
_exptl_absorpt_correction_type      Multi-Scan
_exptl_absorpt_process_details      '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min     0.959
_exptl_absorpt_correction_T_max     0.9714

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#=====

```

7. EXPERIMENTAL DATA

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_diffn_radiation_wavelength         0.71073
_diffn_radiation_type               MoK $\alpha$ 
_diffn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator       'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method            '\f and \w scans'
_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean      '4096x4096 / 62x62 (binned 512)'
_diffn_standards_number              0

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loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_av_sigmaI/netI 0.0365
_diffrn_reflns_limit_h_min -15
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_diffrn_reflns_limit_k_min -17
_diffrn_reflns_limit_k_max 17
_diffrn_reflns_limit_l_min -18
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_diffrn_reflns_theta_max   28.28
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_diffrn_reflns_theta_full  25.00
_diffrn_measured_fraction_theta_full 0.983

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total      8438
_reflns_number_gt         6985
_reflns_threshold_expression  $I > 2\sigma(I)$ 

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_computing_cell_refinement 'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction  'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on  $F^2$ , conventional R-factors R are based

```

on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

;

```
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0604P)^2^+0.7021P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    refall
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?
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_refine_ls_number_parameters      657
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_refine_ls_number_constraints     ?
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_refine_ls_R_factor_gt           0.0496
_refine_ls_wR_factor_ref         0.1240
_refine_ls_wR_factor_gt         0.1176
_refine_ls_goodness_of_fit_ref    1.033
_refine_ls_restrained_S_all      1.033
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean         0.000
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_vrn_publ_code_frame_time_sec    5.0
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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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C12 C Uani 0.08547(13) 0.27385(12) 0.44638(10) 1.000 0.0143(3) . .
C13 C Uani -0.01071(13) 0.17175(12) 0.35228(10) 1.000 0.0152(4) . .
```

C14 C Uani 0.06524(13) 0.18869(11) 0.26311(10) 1.000 0.0149(4) . .
 C15 C Uani 0.01551(13) 0.14088(12) 0.15831(11) 1.000 0.0170(4) . .
 C16 C Uani 0.10335(14) 0.17639(12) 0.08983(11) 1.000 0.0183(4) . .
 C17 C Uani 0.23303(14) 0.25834(13) 0.12604(11) 1.000 0.0182(4) . .
 C18 C Uani 0.28492(13) 0.30439(12) 0.23115(10) 1.000 0.0154(4) . .
 C19 C Uani 0.19931(13) 0.26419(11) 0.30001(10) 1.000 0.0141(3) . .
 C110 C Uani 0.06643(14) 0.38527(13) 0.45859(11) 1.000 0.0179(4) . .
 C111 C Uani -0.12661(15) 0.05567(13) 0.12031(12) 1.000 0.0213(4) . .
 C112 C Uani 0.42511(14) 0.39701(13) 0.26444(12) 1.000 0.0182(4) . .
 C113 C Uani 0.31358(12) 0.28509(11) 0.47139(10) 1.000 0.0133(3) . .
 C114 C Uani 0.42584(12) 0.26082(11) 0.42903(10) 1.000 0.0137(4) . .
 C115 C Uani 0.41536(13) 0.15965(12) 0.47056(11) 1.000 0.0147(4) . .
 C116 C Uani 0.36423(12) 0.18761(11) 0.57178(10) 1.000 0.0143(4) . .
 C117 C Uani 0.36881(13) 0.14537(12) 0.65364(11) 1.000 0.0169(4) . .
 C118 C Uani 0.32291(13) 0.18959(12) 0.74276(11) 1.000 0.0186(4) . .
 C119 C Uani 0.27902(13) 0.27450(13) 0.74982(11) 1.000 0.0182(4) . .
 C120 C Uani 0.27189(12) 0.31616(12) 0.66712(10) 1.000 0.0152(4) . .
 C121 C Uani 0.31097(12) 0.26756(11) 0.57516(10) 1.000 0.0133(3) . .
 C122 C Uani 0.55958(13) 0.36738(12) 0.47378(11) 1.000 0.0161(4) . .
 C123 C Uani 0.42461(15) 0.05886(13) 0.64839(13) 1.000 0.0221(4) . .
 C124 C Uani 0.23019(14) 0.41335(13) 0.68343(11) 1.000 0.0178(4) . .
 H12 H Uiso 0.0720(14) 0.2535(12) 0.5119(12) 1.000 0.010(3) . .
 H13 H Uiso -0.0301(16) 0.0936(15) 0.3606(13) 1.000 0.021(4) . .
 H13' H Uiso -0.0952(16) 0.1758(14) 0.3419(12) 1.000 0.017(4) . .
 H16 H Uiso 0.0713(16) 0.1431(15) 0.0133(14) 1.000 0.024(4) . .
 H17 H Uiso 0.2887(16) 0.2847(14) 0.0762(13) 1.000 0.022(4) . .
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 H111' H Uiso -0.1473(19) 0.0273(17) 0.0433(16) 1.000 0.037(5) . .
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 H112' H Uiso 0.4398(16) 0.4455(14) 0.3394(14) 1.000 0.022(4) . .
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 H119 H Uiso 0.2518(17) 0.3067(15) 0.8145(14) 1.000 0.024(4) . .
 H122 H Uiso 0.5650(15) 0.4408(14) 0.4630(12) 1.000 0.019(4) . .
 H122' H Uiso 0.6310(16) 0.3516(14) 0.4412(13) 1.000 0.022(4) . .
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 H123" H Uiso 0.401(2) 0.0241(19) 0.7039(17) 1.000 0.051(6) . .
 H124 H Uiso 0.2656(16) 0.4606(15) 0.6362(13) 1.000 0.023(4) . .
 H124' H Uiso 0.2628(18) 0.4686(16) 0.7568(15) 1.000 0.032(5) . .
 H124" H Uiso 0.1333(18) 0.3822(16) 0.6733(14) 1.000 0.029(5) . .
 C21 C Uani 0.27671(12) 0.71101(11) 0.02841(10) 1.000 0.0125(3) . .
 C22 C Uani 0.41188(12) 0.72836(11) 0.06756(10) 1.000 0.0133(3) . .
 C23 C Uani 0.50202(13) 0.83108(12) 0.02870(11) 1.000 0.0149(4) . .
 C24 C Uani 0.42211(12) 0.80839(11) -0.07105(10) 1.000 0.0139(4) . .
 C25 C Uani 0.46702(13) 0.85215(11) -0.15229(11) 1.000 0.0152(4) . .
 C26 C Uani 0.37672(13) 0.80918(12) -0.24129(11) 1.000 0.0161(4) . .
 C27 C Uani 0.24892(13) 0.72550(12) -0.24872(11) 1.000 0.0162(4) . .
 C28 C Uani 0.20117(12) 0.68486(11) -0.16579(10) 1.000 0.0137(3) . .
 C29 C Uani 0.28970(12) 0.73081(11) -0.07452(10) 1.000 0.0131(3) . .
 C210 C Uani 0.43476(14) 0.61931(12) 0.01835(11) 1.000 0.0175(4) . .
 C211 C Uani 0.60766(14) 0.93923(12) -0.14534(12) 1.000 0.0182(4) . .
 C212 C Uani 0.06155(13) 0.59188(12) -0.18105(11) 1.000 0.0165(4) . .

C213	C	Uani	0.18287(12)	0.71341(11)	0.08761(10)	1.000	0.0124(3)	. .
C214	C	Uani	0.06866(12)	0.73654(11)	0.05888(10)	1.000	0.0130(3)	. .
C215	C	Uani	0.07975(13)	0.83751(11)	0.15635(11)	1.000	0.0148(4)	. .
C216	C	Uani	0.13449(12)	0.81070(11)	0.24209(10)	1.000	0.0140(4)	. .
C217	C	Uani	0.13154(12)	0.85282(11)	0.34742(11)	1.000	0.0159(4)	. .
C218	C	Uani	0.17968(13)	0.80920(12)	0.41214(11)	1.000	0.0176(4)	. .
C219	C	Uani	0.22541(13)	0.72588(12)	0.37205(11)	1.000	0.0170(4)	. .
C220	C	Uani	0.23167(12)	0.68494(11)	0.26651(10)	1.000	0.0144(4)	. .
C221	C	Uani	0.18887(12)	0.73195(11)	0.20119(10)	1.000	0.0128(3)	. .
C222	C	Uani	-0.06498(13)	0.63026(12)	0.04484(11)	1.000	0.0162(4)	. .
C223	C	Uani	0.07618(14)	0.93946(13)	0.38895(12)	1.000	0.0208(4)	. .
C224	C	Uani	0.27735(14)	0.59024(12)	0.22956(11)	1.000	0.0165(4)	. .
H22	H	Uiso	0.4271(15)	0.7490(13)	0.1437(12)	1.000	0.014(4)	. .
H23	H	Uiso	0.5201(15)	0.9104(14)	0.0804(12)	1.000	0.016(4)	. .
H23'	H	Uiso	0.5879(16)	0.8310(14)	0.0170(13)	1.000	0.022(4)	. .
H26	H	Uiso	0.4043(17)	0.8363(15)	-0.3004(13)	1.000	0.025(4)	. .
H27	H	Uiso	0.1900(16)	0.6938(14)	-0.3154(13)	1.000	0.021(4)	. .
H210	H	Uiso	0.3698(18)	0.5474(16)	0.0318(14)	1.000	0.029(5)	. .
H210'	H	Uiso	0.5226(17)	0.6333(15)	0.0467(13)	1.000	0.023(4)	. .
H210"	H	Uiso	0.4325(17)	0.6033(15)	-0.0594(14)	1.000	0.026(4)	. .
H211	H	Uiso	0.6377(18)	1.0053(16)	-0.0788(15)	1.000	0.030(5)	. .
H211'	H	Uiso	0.6164(18)	0.9752(16)	-0.2018(14)	1.000	0.031(5)	. .
H211"	H	Uiso	0.6650(18)	0.9015(16)	-0.1513(14)	1.000	0.029(5)	. .
H212	H	Uiso	0.0003(17)	0.6280(15)	-0.1703(14)	1.000	0.028(5)	. .
H212'	H	Uiso	0.0499(16)	0.5470(14)	-0.1314(13)	1.000	0.021(4)	. .
H212"	H	Uiso	0.0367(16)	0.5365(15)	-0.2543(14)	1.000	0.024(4)	. .
H214	H	Uiso	0.0800(15)	0.7609(13)	-0.0030(12)	1.000	0.013(4)	. .
H215	H	Uiso	-0.0064(16)	0.8379(14)	0.1676(12)	1.000	0.016(4)	. .
H215'	H	Uiso	0.1418(15)	0.9170(14)	0.1519(12)	1.000	0.016(4)	. .
H218	H	Uiso	0.1796(16)	0.8374(15)	0.4875(14)	1.000	0.023(4)	. .
H219	H	Uiso	0.2526(16)	0.6926(14)	0.4199(12)	1.000	0.018(4)	. .
H222	H	Uiso	-0.0823(16)	0.6148(14)	0.1134(14)	1.000	0.023(4)	. .
H222'	H	Uiso	-0.0715(15)	0.5564(14)	-0.0068(13)	1.000	0.018(4)	. .
H222"	H	Uiso	-0.1357(17)	0.6472(15)	0.0203(13)	1.000	0.025(4)	. .
H223	H	Uiso	0.1123(18)	1.0057(16)	0.3620(14)	1.000	0.029(5)	. .
H223'	H	Uiso	0.0987(19)	0.9743(17)	0.4665(16)	1.000	0.037(5)	. .
H223"	H	Uiso	-0.0214(19)	0.9015(16)	0.3702(14)	1.000	0.033(5)	. .
H224	H	Uiso	0.3773(17)	0.6241(15)	0.2370(13)	1.000	0.024(4)	. .
H224'	H	Uiso	0.2434(16)	0.5454(14)	0.1551(13)	1.000	0.020(4)	. .
H224"	H	Uiso	0.2501(18)	0.5372(16)	0.2721(14)	1.000	0.031(5)	. .

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_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_23

_atom_site_aniso_U_13

_atom_site_aniso_U_12

C11	0.0136(6)	0.0132(6)	0.0150(6)	0.0053(5)	0.0039(5)	0.0066(5)
C12	0.0136(6)	0.0176(6)	0.0139(6)	0.0056(5)	0.0022(5)	0.0085(5)
C13	0.0134(6)	0.0175(6)	0.0159(7)	0.0058(5)	0.0014(5)	0.0076(5)
C14	0.0168(6)	0.0153(6)	0.0159(7)	0.0055(5)	0.0026(5)	0.0099(5)
C15	0.0200(7)	0.0164(6)	0.0174(7)	0.0038(5)	0.0002(5)	0.0118(5)
C16	0.0252(7)	0.0233(7)	0.0124(7)	0.0036(5)	0.0013(5)	0.0177(6)
C17	0.0238(7)	0.0245(7)	0.0152(7)	0.0089(5)	0.0072(5)	0.0171(6)
C18	0.0180(7)	0.0170(6)	0.0167(7)	0.0065(5)	0.0042(5)	0.0120(5)
C19	0.0165(6)	0.0157(6)	0.0136(6)	0.0048(5)	0.0021(5)	0.0103(5)
C110	0.0169(7)	0.0204(7)	0.0196(7)	0.0060(6)	0.0023(5)	0.0114(6)
C111	0.0206(7)	0.0208(7)	0.0198(8)	0.0011(6)	-0.0022(6)	0.0102(6)
C112	0.0180(7)	0.0207(7)	0.0201(7)	0.0100(6)	0.0066(5)	0.0101(6)

C113	0.0137(6)	0.0123(6)	0.0136(6)	0.0036(5)	0.0028(5)	0.0059(5)
C114	0.0136(6)	0.0152(6)	0.0137(7)	0.0045(5)	0.0023(5)	0.0078(5)
C115	0.0139(6)	0.0152(6)	0.0162(7)	0.0045(5)	0.0014(5)	0.0079(5)
C116	0.0102(6)	0.0138(6)	0.0159(7)	0.0043(5)	0.0001(5)	0.0030(5)
C117	0.0117(6)	0.0164(6)	0.0203(7)	0.0072(5)	-0.0026(5)	0.0034(5)
C118	0.0137(6)	0.0234(7)	0.0174(7)	0.0114(6)	-0.0002(5)	0.0040(5)
C119	0.0125(6)	0.0245(7)	0.0148(7)	0.0060(5)	0.0022(5)	0.0059(5)
C120	0.0099(6)	0.0173(6)	0.0162(7)	0.0046(5)	0.0008(5)	0.0044(5)
C121	0.0092(6)	0.0143(6)	0.0144(6)	0.0050(5)	0.0005(5)	0.0032(5)
C122	0.0132(6)	0.0171(6)	0.0180(7)	0.0048(5)	0.0034(5)	0.0071(5)
C123	0.0228(8)	0.0193(7)	0.0268(8)	0.0104(6)	-0.0012(6)	0.0098(6)
C124	0.0169(7)	0.0212(7)	0.0159(7)	0.0040(5)	0.0039(5)	0.0102(5)
C21	0.0111(6)	0.0118(6)	0.0138(6)	0.0032(5)	-0.0004(5)	0.0050(5)
C22	0.0103(6)	0.0168(6)	0.0127(6)	0.0037(5)	0.0008(5)	0.0066(5)
C23	0.0107(6)	0.0169(6)	0.0159(7)	0.0044(5)	0.0019(5)	0.0056(5)
C24	0.0140(6)	0.0140(6)	0.0148(7)	0.0029(5)	0.0023(5)	0.0083(5)
C25	0.0156(6)	0.0139(6)	0.0185(7)	0.0045(5)	0.0053(5)	0.0092(5)
C26	0.0200(7)	0.0176(6)	0.0164(7)	0.0080(5)	0.0064(5)	0.0118(5)
C27	0.0186(7)	0.0175(6)	0.0150(7)	0.0038(5)	0.0013(5)	0.0113(5)
C28	0.0143(6)	0.0138(6)	0.0147(6)	0.0039(5)	0.0024(5)	0.0081(5)
C29	0.0143(6)	0.0140(6)	0.0140(6)	0.0048(5)	0.0037(5)	0.0088(5)
C210	0.0161(7)	0.0194(7)	0.0204(7)	0.0057(5)	0.0035(5)	0.0114(5)
C211	0.0154(7)	0.0176(7)	0.0230(8)	0.0084(6)	0.0062(5)	0.0072(5)
C212	0.0143(6)	0.0178(6)	0.0156(7)	0.0041(5)	0.0001(5)	0.0062(5)
C213	0.0113(6)	0.0111(5)	0.0145(6)	0.0044(5)	0.0002(5)	0.0046(5)
C214	0.0117(6)	0.0150(6)	0.0145(6)	0.0062(5)	0.0029(5)	0.0070(5)
C215	0.0120(6)	0.0140(6)	0.0192(7)	0.0058(5)	0.0034(5)	0.0062(5)
C216	0.0092(6)	0.0126(6)	0.0178(7)	0.0045(5)	0.0026(5)	0.0030(5)
C217	0.0109(6)	0.0149(6)	0.0176(7)	0.0024(5)	0.0027(5)	0.0036(5)
C218	0.0129(6)	0.0211(7)	0.0135(7)	0.0028(5)	0.0025(5)	0.0045(5)
C219	0.0123(6)	0.0214(7)	0.0160(7)	0.0076(5)	0.0008(5)	0.0054(5)
C220	0.0100(6)	0.0155(6)	0.0159(7)	0.0051(5)	0.0012(5)	0.0040(5)
C221	0.0088(6)	0.0135(6)	0.0136(6)	0.0035(5)	0.0013(4)	0.0032(5)
C222	0.0114(6)	0.0167(6)	0.0196(7)	0.0059(5)	0.0013(5)	0.0054(5)
C223	0.0169(7)	0.0197(7)	0.0221(8)	0.0006(6)	0.0037(6)	0.0087(6)
C224	0.0168(7)	0.0186(6)	0.0176(7)	0.0073(5)	0.0021(5)	0.0100(5)

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10. MOLECULAR GEOMETRY

_geom_special_details

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

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loop_

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_geom_bond_atom_site_label_2

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H214 H16 2.56(3) . 2_565 no
H215 C223 2.900(16) . . no
H215 H222" 2.55(2) . . no
H215 H222 2.56(2) . . no
H218 H123' 2.47(3) . 1_565 no
H218 H223' 2.43(3) . . no
H218 C12 3.03(2) . 2_566 no
H218 C13 2.922(19) . 2_566 no
H218 H13' 2.55(2) . 2_566 no
H219 H224" 2.43(3) . . no
H219 C122 3.064(19) . 2_666 no
H222 C216 2.800(18) . . no
H222 C221 2.874(19) . . no
H222 H215 2.56(2) . . no
H222 H212' 2.39(3) . 2_565 no
H223 C13 3.09(2) . 1_565 no
H223 C215 2.949(19) . . no
H223 H13 2.37(3) . 1_565 no
H223 H115 2.53(3) . 1_565 no
H224 C22 2.962(18) . . no
H224 C210 3.051(17) . . no
H224 H22 2.25(2) . . no

```

Loop Mechanism for Extra Tables(s)

```

#loop_
#_publ_manuscript_incl_extra_item
#'_geom_extra_tableA_col_1'
#'_geom_extra_tableA_col_2'
#'_geom_extra_tableA_col_3'
#'_geom_extra_table_head_A'
#'_geom_table_footnote_A'
#'_geom_extra_tableB_col_1'
#'_geom_extra_tableB_col_2'
#'_geom_extra_tableB_col_3'
#'_geom_extra_table_head_B'
#'_geom_table_footnote_B'

#
#loop_
#_geom_extra_tableA_col_1
#_geom_extra_tableA_col_2
#_geom_extra_tableA_col_3

```

```

# ? ? ?

#
#loop_
#_geom_extra_tableB_col_1
#_geom_extra_tableB_col_2
#_geom_extra_tableB_col_3
# ? ? ?

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#
#_geom_table_footnote_A
#;
# ?
#;

#
#_geom_table_footnote_B
#;
# ?
#;

#===END of Crystallographic Information File

# Attachment 'q1118.cif'

# CIF-file generated for C24H28 C2/c q1118
#=====
data_2
_database_code_depnum_ccdc_archive 'CCDC 666200'

# 5. CHEMICAL DATA

_chemical_name_systematic
;
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety 'C24 H28'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural ?
_chemical_formula_sum 'C24 H28'
_chemical_formula_iupac ?
_chemical_formula_weight 316.48
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real

```



```

_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```

```

#=====

```

``` # 6. CRYSTAL DATA ```

```

_symmetry_cell_setting      Monoclinic
_symmetry_space_group_name_Hall '-C 2yc'
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15

```

```

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z

```

```

_cell_length_a      38.531(9)
_cell_length_b      5.981(1)
_cell_length_c      16.016(4)
_cell_angle_alpha    90
_cell_angle_beta     93.416(4)
_cell_angle_gamma    90
_cell_volume         3684.4(14)
_cell_formula_units_Z 8

```

```

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 7794
_cell_measurement_theta_min 2.55
_cell_measurement_theta_max 29.50
_cell_special_details

```

```

;
```

The final unit cell was obtained from the xyz centroids of 7794 reflections after integration using the SAINTPLUS software package (Bruker, 2000).

Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

```

;
```

```

_exptl_crystal_description      needle
_exptl_crystal_colour           colorless
_exptl_crystal_size_max         0.57
_exptl_crystal_size_mid         0.17
_exptl_crystal_size_min         0.15
_exptl_crystal_size_rad         ?
_exptl_crystal_density_meas     ?
_exptl_crystal_density_diffn    1.141
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            1376
_exptl_absorpt_coefficient_mu   0.064

```

```
_exptl_absorpt_correction_type    Multi-Scan
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min  0.9616
_exptl_absorpt_correction_T_max  0.9905
```

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

``` # 7. EXPERIMENTAL DATA ```

```
_exptl_special_details
;
;
_diffn_ambient_temperature      100(1)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK\alpha
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'

_diffn_standards_number         0
_diffn_standards_interval_count ?
_diffn_standards_interval_time  ?
_diffn_standards_decay_%        0

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number            12897
_diffn_reflns_av_R_equivalents  0.0375
_diffn_reflns_av_sigmaI/netI    0.0397
_diffn_reflns_limit_h_min       -47
_diffn_reflns_limit_h_max       47
_diffn_reflns_limit_k_min       -7
_diffn_reflns_limit_k_max       7
_diffn_reflns_limit_l_min       -19
_diffn_reflns_limit_l_max       19
_diffn_reflns_theta_min         2.55
_diffn_reflns_theta_max         26.02
_diffn_measured_fraction_theta_max 0.999
_diffn_reflns_theta_full        25.00
_diffn_measured_fraction_theta_full 0.999

_diffn_reflns_reduction_process
```

```

;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total      3628
_reflns_number_gt         2970
_reflns_threshold_expression  I>2\|s(I)

_computing_data_collection 'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement 'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction  'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
PLATON (Spek, 2003)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on  $F^2$ , conventional R-factors R are based
on F, with F set to zero for negative  $F^2$ . The threshold expression of
 $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on  $F^2$  are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\|s^2(Fo^2)+(0.0674P)^2+2.0136P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment refall
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 3628
_refine_ls_number_parameters 329
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0566

```

_refine_ls_R_factor_gt	0.0451
_refine_ls_wR_factor_ref	0.1211
_refine_ls_wR_factor_gt	0.1137
_refine_ls_goodness_of_fit_ref	1.020
_refine_ls_restrained_S_all	1.020
_refine_ls_shift/su_max	0.000
_refine_ls_shift/su_mean	0.000
_refine_diff_density_max	0.262
_refine_diff_density_min	-0.195
_refine_diff_density_rms	0.044
_vrn_publ_code_frame_time_sec	20.0
_vrn_publ_code_meas_time_hour	16.3

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```

H10" H Uiso 0.1507(4) 0.130(3) 0.1242(10) 1.000 0.029(4) . .
H11 H Uiso 0.2412(5) 0.821(3) 0.2478(13) 1.000 0.048(5) . .
H11' H Uiso 0.2530(6) 0.903(4) 0.3459(13) 1.000 0.061(6) . .
H11" H Uiso 0.2175(5) 0.987(3) 0.2975(11) 1.000 0.039(5) . .
H12 H Uiso 0.1460(4) 0.090(3) 0.4798(11) 1.000 0.032(4) . .
H12' H Uiso 0.1830(5) -0.030(3) 0.4680(10) 1.000 0.033(4) . .
H12" H Uiso 0.1527(5) -0.030(3) 0.3916(11) 1.000 0.036(5) . .
H14 H Uiso 0.0904(4) 0.129(3) 0.1676(10) 1.000 0.020(4) . .
H15 H Uiso 0.0408(5) -0.102(3) 0.2317(11) 1.000 0.035(5) . .
H15' H Uiso 0.0809(4) -0.190(3) 0.2513(10) 1.000 0.030(4) . .
H18 H Uiso 0.0340(5) -0.050(3) 0.5357(11) 1.000 0.035(5) . .
H19 H Uiso 0.0684(4) 0.275(3) 0.5626(11) 1.000 0.030(4) . .
H22 H Uiso 0.0364(4) 0.362(3) 0.2486(10) 1.000 0.026(4) . .
H22' H Uiso 0.0322(4) 0.259(3) 0.1553(11) 1.000 0.032(4) . .
H22" H Uiso 0.0571(4) 0.471(3) 0.1718(11) 1.000 0.035(5) . .
H23 H Uiso 0.0352(5) -0.426(3) 0.3845(11) 1.000 0.040(5) . .
H23' H Uiso 0.0046(6) -0.271(4) 0.3444(15) 1.000 0.066(7) . .
H23" H Uiso 0.0069(6) -0.323(4) 0.4393(14) 1.000 0.057(6) . .
H24 H Uiso 0.0967(4) 0.601(3) 0.5066(11) 1.000 0.031(4) . .
H24' H Uiso 0.1086(4) 0.603(3) 0.4113(11) 1.000 0.034(5) . .
H24" H Uiso 0.1315(5) 0.476(3) 0.4870(11) 1.000 0.039(5) . .

```

```

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C1 0.0170(6) 0.0169(7) 0.0203(7) -0.0009(5) 0.0004(5) 0.0025(5)
C2 0.0180(7) 0.0232(8) 0.0221(7) 0.0035(6) -0.0003(5) 0.0014(6)
C3 0.0196(7) 0.0220(8) 0.0301(8) 0.0042(6) 0.0048(6) 0.0010(6)
C4 0.0154(6) 0.0197(7) 0.0279(7) -0.0031(6) 0.0039(5) 0.0029(5)
C5 0.0137(6) 0.0219(8) 0.0362(8) -0.0076(6) 0.0043(6) 0.0016(6)
C6 0.0128(7) 0.0328(9) 0.0359(9) -0.0113(7) -0.0013(6) 0.0023(6)
C7 0.0162(7) 0.0327(9) 0.0267(8) -0.0029(6) -0.0017(6) 0.0083(6)
C8 0.0155(6) 0.0235(8) 0.0234(7) -0.0020(6) 0.0021(5) 0.0057(6)
C9 0.0137(6) 0.0198(7) 0.0228(7) -0.0036(5) 0.0014(5) 0.0022(5)
C10 0.0229(7) 0.0295(9) 0.0229(8) 0.0009(6) 0.0031(6) 0.0024(7)
C11 0.0181(7) 0.0256(9) 0.0522(11) -0.0054(8) 0.0068(7) -0.0035(7)
C12 0.0206(7) 0.0267(8) 0.0278(8) 0.0058(7) 0.0021(6) 0.0068(6)
C13 0.0173(7) 0.0165(7) 0.0208(7) -0.0012(5) -0.0003(5) 0.0026(5)
C14 0.0169(7) 0.0240(8) 0.0221(7) -0.0039(6) 0.0006(5) -0.0010(6)
C15 0.0184(7) 0.0215(8) 0.0321(8) -0.0048(6) -0.0002(6) -0.0018(6)
C16 0.0140(6) 0.0186(7) 0.0278(7) -0.0006(6) -0.0006(5) 0.0035(5)
C17 0.0137(6) 0.0214(8) 0.0355(8) 0.0058(6) 0.0017(6) 0.0041(6)
C18 0.0193(7) 0.0301(9) 0.0310(8) 0.0091(7) 0.0066(6) 0.0057(6)
C19 0.0212(7) 0.0300(9) 0.0233(8) 0.0009(6) 0.0021(6) 0.0073(6)
C20 0.0144(6) 0.0230(8) 0.0229(7) 0.0003(6) -0.0013(5) 0.0056(5)
C21 0.0123(6) 0.0193(7) 0.0243(7) 0.0025(6) -0.0005(5) 0.0035(5)
C22 0.0209(7) 0.0281(9) 0.0255(8) -0.0041(7) -0.0046(6) 0.0002(6)
C23 0.0191(8) 0.0241(9) 0.0454(10) 0.0053(7) 0.0047(7) -0.0008(6)
C24 0.0196(7) 0.0250(8) 0.0237(8) -0.0062(6) -0.0016(6) 0.0037(6)

```

```

#=====

```

```

# 10. MOLECULAR GEOMETRY

```

```

_geom_special_details
;

```

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

;

```
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
C1 C2 1.5318(19) . . no
C1 C9 1.4870(17) . . no
C1 C13 1.3551(17) . . no
C2 C3 1.559(2) . . no
C2 C10 1.538(2) . . no
C3 C4 1.511(2) . . no
C4 C5 1.4006(18) . . no
C4 C9 1.4111(17) . . no
C5 C6 1.396(2) . . no
C5 C11 1.512(2) . . no
C6 C7 1.393(2) . . no
C7 C8 1.409(2) . . no
C8 C9 1.4080(19) . . no
C8 C12 1.510(2) . . no
C13 C14 1.5362(18) . . no
C13 C21 1.4807(18) . . no
C14 C15 1.555(2) . . no
C14 C22 1.538(2) . . no
C15 C16 1.511(2) . . no
C16 C17 1.3986(19) . . no
C16 C21 1.4113(17) . . no
C17 C18 1.398(2) . . no
C17 C23 1.512(2) . . no
C18 C19 1.393(2) . . no
C19 C20 1.406(2) . . no
C20 C21 1.4084(18) . . no
C20 C24 1.509(2) . . no
C2 H2 0.983(15) . . no
C3 H3 1.001(16) . . no
C3 H3' 1.025(17) . . no
C6 H6 0.983(19) . . no
C7 H7 1.005(16) . . no
C10 H10 0.977(19) . . no
C10 H10' 1.017(18) . . no
C10 H10" 1.015(17) . . no
C11 H11 1.01(2) . . no
C11 H11' 1.02(2) . . no
C11 H11" 0.998(18) . . no
C12 H12 1.005(17) . . no
C12 H12' 1.016(18) . . no
C12 H12" 0.998(18) . . no
C14 H14 0.984(16) . . no
C15 H15 1.030(19) . . no
C15 H15' 1.030(17) . . no
C18 H18 0.990(18) . . no
C19 H19 0.999(18) . . no
C22 H22 0.993(16) . . no
```

C22 H22' 0.976(17) . . no
 C22 H22" 1.030(18) . . no
 C23 H23 0.994(18) . . no
 C23 H23' 1.00(2) . . no
 C23 H23" 0.97(2) . . no
 C24 H24 0.988(17) . . no
 C24 H24' 1.003(18) . . no
 C24 H24" 0.987(19) . . 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
 C2 C1 C9 105.25(10) . . . no
 C2 C1 C13 123.19(12) . . . no
 C9 C1 C13 131.44(12) . . . no
 C1 C2 C3 101.88(11) . . . no
 C1 C2 C10 112.30(11) . . . no
 C3 C2 C10 111.21(13) . . . no
 C2 C3 C4 102.80(12) . . . no
 C3 C4 C5 127.49(12) . . . no
 C3 C4 C9 110.18(11) . . . no
 C5 C4 C9 122.32(12) . . . no
 C4 C5 C6 116.42(12) . . . no
 C4 C5 C11 121.41(13) . . . no
 C6 C5 C11 122.17(13) . . . no
 C5 C6 C7 121.77(14) . . . no
 C6 C7 C8 122.31(14) . . . no
 C7 C8 C9 116.24(12) . . . no
 C7 C8 C12 119.43(13) . . . no
 C9 C8 C12 124.20(12) . . . no
 C1 C9 C4 108.32(11) . . . no
 C1 C9 C8 130.62(11) . . . no
 C4 C9 C8 120.67(11) . . . no
 C1 C13 C14 123.50(11) . . . no
 C1 C13 C21 131.57(12) . . . no
 C14 C13 C21 104.72(10) . . . no
 C13 C14 C15 101.31(11) . . . no
 C13 C14 C22 112.42(11) . . . no
 C15 C14 C22 110.68(11) . . . no
 C14 C15 C16 102.51(12) . . . no
 C15 C16 C17 128.02(12) . . . no
 C15 C16 C21 109.79(12) . . . no
 C17 C16 C21 122.15(12) . . . no
 C16 C17 C18 116.30(12) . . . no
 C16 C17 C23 121.86(13) . . . no
 C18 C17 C23 121.83(13) . . . no
 C17 C18 C19 121.91(14) . . . no
 C18 C19 C20 122.31(14) . . . no
 C19 C20 C21 116.02(12) . . . no
 C19 C20 C24 120.07(12) . . . no
 C21 C20 C24 123.75(11) . . . no
 C13 C21 C16 108.41(11) . . . no
 C13 C21 C20 130.13(11) . . . no
 C16 C21 C20 121.03(11) . . . no
 C1 C2 H2 112.7(9) . . . no

C3 C2 H2 110.3(10) . . . no
C10 C2 H2 108.3(9) . . . no
C2 C3 H3 111.9(10) . . . no
C2 C3 H3' 113.1(9) . . . no
C4 C3 H3 114.5(9) . . . no
C4 C3 H3' 109.1(9) . . . no
H3 C3 H3' 105.7(14) . . . no
C5 C6 H6 118.2(10) . . . no
C7 C6 H6 120.1(10) . . . no
C6 C7 H7 121.6(10) . . . no
C8 C7 H7 116.1(10) . . . no
C2 C10 H10 109.2(11) . . . no
C2 C10 H10' 111.0(10) . . . no
C2 C10 H10" 112.2(9) . . . no
H10 C10 H10' 111.0(14) . . . no
H10 C10 H10" 105.3(14) . . . no
H10' C10 H10" 107.9(13) . . . no
C5 C11 H11 111.4(10) . . . no
C5 C11 H11' 110.2(13) . . . no
C5 C11 H11" 112.2(11) . . . no
H11 C11 H11' 111.9(16) . . . no
H11 C11 H11" 104.8(15) . . . no
H11' C11 H11" 106.2(17) . . . no
C8 C12 H12 112.1(10) . . . no
C8 C12 H12' 109.7(11) . . . no
C8 C12 H12" 111.7(10) . . . no
H12 C12 H12' 106.3(14) . . . no
H12 C12 H12" 107.8(15) . . . no
H12' C12 H12" 109.0(15) . . . no
C13 C14 H14 111.9(9) . . . no
C15 C14 H14 112.0(10) . . . no
C22 C14 H14 108.5(10) . . . no
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# Loop Mechanism for Extra Tables(s)

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#;
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