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Volume 54, 2001

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Dr Alison Green

Australian Journal of Chemistry – an International Journal for Chemical Science

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10.1071/CH01161_AC

Accessory Publication: *Aust. J. Chem.*, 2001, **54**(11), 691-704.

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;
’ G. R. Clark ’
;
Department of Chemistry,
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Private Bag 92019,
Auckland, New Zealand.
;
’ D. C. R. Hockless ’
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Molecular Structure Corporation. (1992-1997). teXsan.
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_exptl_absorpt_coefficient_mu          0.684
_exptl_absorpt_correction_type         none
_exptl_special_details
;
The crystal was an extremely thin plate so data is very weak
  and precision therefore poor.

The scan width was (0.89+0.30tan\q)\% with an \w
scan speed of 2\% per minute
(up to 5 scans to achieve I/\s(I) > 10).
Stationary background counts were recorded at each end of the
```

```
scan, and the scan time:background time ratio was 2:1.
Data can only be collected to 2theta 120 deg on a AFC6R diffractometer
when the evacuated beam tunnel in used.
Mass attenuation coefficients for absorption from
International Tables for X-ray Crystallography, Vol IV (1974) Table 2.1C.
;
#-----------------------------------------------------------------------------
_diffrn_special_details
;
  ?
;
_diffrn_ambient_temperature            213.2
_diffrn_radiation_wavelength           1.5418
_diffrn_radiation_type                 'Cu K\a'
_diffrn_radiation_source               'Rigaku rotating anode'
_diffrn_radiation_monochromator        graphite
_diffrn_radiation_detector             'scintillation counter'
_diffrn_measurement_device_type        'Rigaku AFC6R'
_diffrn_measurement_method             \w-2\q
_diffrn_measurement_device_details
;
Rigaku AFC6R diffractometer with extended arm and
evacuated collimator and beam tunnel.
Data cannot be collected beyond \y 60 deg in this configuration.

The crystal was an extremely thin plate so data is very weak
and precision therefore poor.
;

_diffrn_standards_number               3
_diffrn_standards_interval_count       150
_diffrn_standards_decay_%              -11.83
loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
       2       0      0
       0       1      1
       0       0      4
_diffrn_reflns_number                   2916
_reflns_number_total                    1391
_reflns_number_gt                       891
_reflns_threshold_expression             I>3.00\s(I)
_diffrn_reflns_av_R_equivalents         0.00000
_diffrn_reflns_av_sigmaI/netI           0.110
_diffrn_reflns_limit_h_min              0
_diffrn_reflns_limit_h_max              8
_diffrn_reflns_limit_k_min              0
_diffrn_reflns_limit_k_max              23
_diffrn_reflns_limit_l_min              -11
_diffrn_reflns_limit_l_max              11
_diffrn_reflns_theta_min                2.09
_diffrn_reflns_theta_max                60.30
_diffrn_reflns_theta_full              60
_diffrn_measured_fraction_theta_max  1.
_diffrn_measured_fraction_theta_full 1.
_diffrn_reflns_reduction_process       'Lp corrections applied'
_diffrn_orient_matrix_UB_11            -0.09501
_diffrn_orient_matrix_UB_12             0.00423
_diffrn_orient_matrix_UB_13             0.00227
_diffrn_orient_matrix_UB_21             0.00467
```

```
_diffrn_orient_matrix_UB_22            0.00647
_diffrn_orient_matrix_UB_23            0.04715
_diffrn_orient_matrix_UB_31            0.00346
_diffrn_orient_matrix_UB_32            0.12689
_diffrn_orient_matrix_UB_33           -0.00250
#--------------------------------------------------------------------------
loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
   C  0    84 0.017 0.009
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
   H  0    84 0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
   N  0     4 0.029 0.018
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
   O  0    12 0.047 0.032
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
#--------------------------------------------------------------------------
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_refinement_flags
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
O(1') 0.7739(7) 0.3139(3) 0.0400 0.036(2) 1.000 . Uani d ?
O(2') 0.5037(7) 0.3210(2) -0.0510(7) 0.038(2) 1.000 . Uani d ?
O(3') 0.2577(8) 0.3521(3) -0.2330(8) 0.055(2) 1.000 . Uani d ?
N(12') 0.617(1) 0.4796(3) 0.004(1) 0.049(2) 1.000 . Uani d ?
C(1) 0.772(1) 0.2342(4) 0.272(1) 0.042(3) 1.000 . Uani d ?
C(1') 0.621(1) 0.2833(4) 0.009(1) 0.044(3) 1.000 . Uani d ?
C(2) 0.776(1) 0.2014(4) 0.385(1) 0.059(3) 1.000 . Uani d ?
C(2') 0.547(1) 0.3329(4) -0.182(1) 0.052(3) 1.000 . Uani d ?
C(3) 0.788(1) 0.2323(5) 0.500(1) 0.069(4) 1.000 . Uani d ?
C(3') 0.422(1) 0.3771(4) -0.233(1) 0.056(3) 1.000 . Uani d ?
C(4a) 0.796(1) 0.3323(4) 0.391(1) 0.037(3) 1.000 . Uani d ?
C(4) 0.799(1) 0.2995(4) 0.503(1) 0.050(3) 1.000 . Uani d ?
C(4') 0.137(1) 0.3933(6) -0.285(1) 0.084(4) 1.000 . Uani d ?
C(5) 1.080(1) 0.4600(4) 0.306(1) 0.046(3) 1.000 . Uani d ?
C(6) 1.198(1) 0.4692(4) 0.210(1) 0.050(3) 1.000 . Uani d ?
C(7) 1.185(1) 0.4382(5) 0.095(1) 0.051(3) 1.000 . Uani d ?
C(8) 1.050(1) 0.3951(4) 0.074(1) 0.041(3) 1.000 . Uani d ?
C(8a) 0.931(1) 0.3854(3) 0.169(1) 0.031(2) 1.000 . Uani d ?
C(9) 0.777(1) 0.3450(4) 0.160(1) 0.032(2) 1.000 . Uani d ?
C(9a) 0.779(1) 0.3019(3) 0.274(1) 0.032(2) 1.000 . Uani d ?
```

```
C(10) 0.806(1) 0.4030(4) 0.375(1) 0.042(3) 1.000 . Uani d ?
C(10a) 0.947(1) 0.4183(3) 0.286(1) 0.036(3) 1.000 . Uani d ?
C(11) 0.639(1) 0.4230(4) 0.3139(9) 0.037(3) 1.000 . Uani d ?
C(12) 0.622(1) 0.3906(3) 0.180(1) 0.032(2) 1.000 . Uani d ?
C(12') 0.619(1) 0.4403(4) 0.078(1) 0.038(3) 1.000 . Uani d ?
H(1) 0.7635 0.2123 0.1932 0.050 1.000 . Uiso c ?
H(1'a) 0.6461 0.2487 -0.0452 0.053 1.000 . Uiso c ?
H(1'b) 0.5712 0.2680 0.0857 0.053 1.000 . Uiso c ?
H(2) 0.7706 0.1565 0.3842 0.070 1.000 . Uiso c ?
H(2'a) 0.6575 0.3509 -0.1874 0.062 1.000 . Uiso c ?
H(2'b) 0.5442 0.2946 -0.2291 0.062 1.000 . Uiso c ?
H(3) 0.7877 0.2090 0.5772 0.083 1.000 . Uiso c ?
H(3'a) 0.4226 0.4142 -0.1820 0.067 1.000 . Uiso c ?
H(3'b) 0.4524 0.3875 -0.3177 0.067 1.000 . Uiso c ?
H(4) 0.8094 0.3213 0.5814 0.060 1.000 . Uiso c ?
H(4'a) 0.1502 0.4340 -0.2481 0.100 1.000 . Uiso c ?
H(4'b) 0.1526 0.3959 -0.3743 0.100 1.000 . Uiso c ?
H(4'c) 0.0260 0.3779 -0.2671 0.100 1.000 . Uiso c ?
H(5) 1.0895 0.4821 0.3839 0.055 1.000 . Uiso c ?
H(6) 1.2894 0.4975 0.2243 0.060 1.000 . Uiso c ?
H(7) 1.2666 0.4458 0.0305 0.061 1.000 . Uiso c ?
H(8) 1.0412 0.3733 -0.0052 0.049 1.000 . Uiso c ?
H(10) 0.8220 0.4233 0.4551 0.050 1.000 . Uiso c ?
H(11b) 0.6370 0.4676 0.3039 0.045 1.000 . Uiso c ?
H(11a) 0.5465 0.4104 0.3665 0.045 1.000 . Uiso c ?
H(12) 0.5194 0.3670 0.1771 0.038 1.000 . Uiso c ?

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
  O(1')  0.034(4)    0.034(3)    0.039(3)    -0.005(3)   0.005(3)    -0.009(3)
  O(2')  0.039(4)    0.041(3)    0.035(3)    0.001(3)    -0.005(3)   -0.002(3)
  O(3')  0.057(5)    0.053(4)    0.056(4)    0.012(4)    -0.022(4)   -0.008(4)
  N(12') 0.050(5)    0.040(4)    0.058(5)    -0.001(4)   -0.008(5)   0.019(4)
  C(1)   0.027(5)    0.041(5)    0.058(6)    0.000(4)    -0.001(5)   -0.001(5)
  C(1')  0.049(6)    0.037(5)    0.045(5)    0.000(5)    -0.010(5)   -0.010(5)
  C(2)   0.053(7)    0.047(5)    0.075(7)    -0.014(5)   -0.006(7)   0.033(6)
  C(2')  0.057(7)    0.055(6)    0.044(6)    -0.001(5)   0.000(6)    -0.002(5)
  C(3)   0.057(8)    0.09(1)     0.057(7)    -0.009(7)   -0.007(7)   0.035(7)
  C(3')  0.078(8)    0.060(6)    0.030(5)    -0.010(6)   -0.008(6)   -0.008(5)
  C(4a)  0.038(5)    0.032(4)    0.042(6)    -0.005(4)   0.000(5)    0.000(5)
  C(4)   0.047(7)    0.062(7)    0.040(6)    -0.009(5)   -0.005(5)   0.004(6)
  C(4')  0.067(8)    0.107(9)    0.077(9)    0.023(8)    -0.021(8)   -0.026(8)
  C(5)   0.037(5)    0.033(5)    0.068(7)    -0.003(4)   -0.012(6)   -0.004(5)
  C(6)   0.032(6)    0.037(5)    0.081(8)    -0.005(5)   -0.010(6)   0.003(6)
  C(7)   0.033(6)    0.054(6)    0.065(7)    0.002(5)    0.009(6)    0.018(6)
  C(8)   0.028(5)    0.043(5)    0.052(6)    -0.004(4)   0.003(5)    0.007(5)
  C(8a)  0.024(5)    0.034(4)    0.035(5)    0.004(4)    -0.005(4)   0.005(4)
  C(9)   0.027(5)    0.028(4)    0.040(5)    -0.002(4)   -0.004(5)   0.003(4)
  C(9a)  0.028(4)    0.027(4)    0.042(5)    0.000(4)    0.002(5)    0.006(4)
  C(10)  0.040(6)    0.048(5)    0.038(5)    -0.006(4)   0.001(5)    -0.015(5)
  C(10a) 0.027(5)    0.041(5)    0.041(6)    -0.003(4)   -0.010(5)   0.005(4)
  C(11)  0.035(5)    0.040(5)    0.037(5)    -0.004(4)   0.004(4)    -0.004(4)
  C(12)  0.028(5)    0.036(4)    0.031(5)    0.004(4)    0.004(4)    0.005(4)
  C(12') 0.021(5)    0.045(5)    0.047(6)    0.000(4)    0.000(5)    -0.017(5)
#-------------------------------------------------------------------------------
```

```
_refine_special_details
;
Origin assigned in z direction by fixing z coordinate of one non-H atom.
;
_refine_ls_structure_factor_coef       F
_refine_ls_matrix_type                 full
_refine_ls_weighting_scheme            sigma
_refine_ls_weighting_details
;
w = 1/[\s^2^(Fo) + 0.00006|Fo|^2^]
;
_refine_ls_hydrogen_treatment          noref
_refine_ls_extinction_method           none
_refine_ls_extinction_coef             ?
_refine_ls_abs_structure_details
;
Absolute structure arbitarily assigned.
;
_refine_ls_abs_structure_Flack         ?
_refine_ls_number_reflns               891
_refine_ls_number_parameters           225
_refine_ls_number_restraints           0
_refine_ls_number_constraints          0
_refine_ls_R_factor_all                0.0984
_refine_ls_R_factor_gt                 0.0463
_refine_ls_wR_factor_all               0.0547
_refine_ls_wR_factor_ref               0.0489
_refine_ls_goodness_of_fit_all         1.733
_refine_ls_goodness_of_fit_ref         2.047
_refine_ls_shift/su_max               0.0047
_refine_ls_shift/su_mean              0.0046
_refine_diff_density_min               -0.17
_refine_diff_density_max               0.18
#-------------------------------------------------------------------------------
_geom_special_details
;
  ?
;
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
  O(1')  C(1')  1.41(1)  .  .  yes
  O(1')  C(9)  1.42(1)  .  .  yes
  O(2')  C(1')  1.373(9)  .  .  yes
  O(2')  C(2')  1.44(1)  .  .  yes
  O(3')  C(3')  1.40(1)  .  .  yes
  O(3')  C(4')  1.40(1)  .  .  yes
  N(12')  C(12')  1.14(1)  .  .  yes
  C(1)  C(2)  1.38(1)  .  .  yes
  C(1)  C(9a)  1.43(1)  .  .  yes
  C(1)  H(1)  0.95  .  .  no
  C(1')  H(1'a)  0.95  .  .  no
  C(1')  H(1'b)  0.95  .  .  no
  C(2)  C(3)  1.37(2)  .  .  yes
  C(2)  H(2)  0.95  .  .  no
  C(2')  C(3')  1.46(1)  .  .  yes
  C(2')  H(2'a)  0.95  .  .  no
```

```
  C(2′) H(2′b) 0.95 . . no
  C(3) C(4) 1.43(1) . . yes
  C(3) H(3) 0.95 . . no
  C(3′) H(3′a) 0.95 . . no
  C(3′) H(3′b) 0.95 . . no
  C(4a) C(4) 1.37(1) . . yes
  C(4a) C(9a) 1.39(1) . . yes
  C(4a) C(10) 1.51(1) . . yes
  C(4) H(4) 0.95 . . no
  C(4′) H(4′a) 0.95 . . no
  C(4′) H(4′b) 0.95 . . no
  C(4′) H(4′c) 0.95 . . no
  C(5) C(6) 1.38(1) . . yes
  C(5) C(10a) 1.38(1) . . yes
  C(5) H(5) 0.95 . . no
  C(6) C(7) 1.38(1) . . yes
  C(6) H(6) 0.95 . . no
  C(7) C(8) 1.42(1) . . yes
  C(7) H(7) 0.95 . . no
  C(8) C(8a) 1.39(1) . . yes
  C(8) H(8) 0.95 . . no
  C(8a) C(9) 1.48(1) . . yes
  C(8a) C(10a) 1.41(1) . . yes
  C(9) C(9a) 1.51(1) . . yes
  C(9) C(12) 1.57(1) . . yes
  C(10) C(10a) 1.49(1) . . yes
  C(10) C(11) 1.53(1) . . yes
  C(10) H(10) 0.95 . . no
  C(11) C(12) 1.57(1) . . yes
  C(11) H(11b) 0.95 . . no
  C(11) H(11a) 0.95 . . no
  C(12) C(12′) 1.50(1) . . yes
  C(12) H(12) 0.95 . . 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
  C(1′) O(1′)  C(9) 115.6(6) . . . yes
  C(1′) O(2′)  C(2′) 112.5(7) . . . yes
  C(3′) O(3′)  C(4′) 113.1(8) . . . yes
  C(2) C(1)  C(9a) 119.2(9) . . . yes
  C(2) C(1)  H(1) 120.4 . . . no
  C(9a) C(1)  H(1) 120.4 . . . no
  O(1′) C(1′)  O(2′) 114.4(6) . . . yes
  O(1′) C(1′)  H(1′a) 108.2 . . . no
  O(1′) C(1′)  H(1′b) 108.3 . . . no
  O(2′) C(1′)  H(1′a) 108.2 . . . no
  O(2′) C(1′)  H(1′b) 108.2 . . . no
  H(1′a) C(1′)  H(1′b) 109.5 . . . no
  C(1) C(2)  C(3) 121.3(9) . . . yes
  C(1) C(2)  H(2) 119.4 . . . no
  C(3) C(2)  H(2) 119.4 . . . no
  O(2′) C(2′)  C(3′) 107.5(8) . . . yes
  O(2′) C(2′)  H(2′a) 110.0 . . . no
  O(2′) C(2′)  H(2′b) 110.0 . . . no
```

C(3′) C(2′) H(2′a) 110.0 . . . no
C(3′) C(2′) H(2′b) 110.0 . . . no
H(2′a) C(2′) H(2′b) 109.5 . . . no
C(2) C(3) C(4) 119.8(9) . . . yes
C(2) C(3) H(3) 120.1 . . . no
C(4) C(3) H(3) 120.1 . . . no
O(3′) C(3′) C(2′) 112.5(8) . . . yes
O(3′) C(3′) H(3′a) 108.7 . . . no
O(3′) C(3′) H(3′b) 108.7 . . . no
C(2′) C(3′) H(3′a) 108.7 . . . no
C(2′) C(3′) H(3′b) 108.7 . . . no
H(3′a) C(3′) H(3′b) 109.4 . . . no
C(4) C(4a) C(9a) 121.8(7) . . . yes
C(4) C(4a) C(10) 126.4(9) . . . yes
C(9a) C(4a) C(10) 111.9(8) . . . yes
C(3) C(4) C(4a) 119.1(9) . . . yes
C(3) C(4) H(4) 120.4 . . . no
C(4a) C(4) H(4) 120.4 . . . no
O(3′) C(4′) H(4′a) 109.5 . . . no
O(3′) C(4′) H(4′b) 109.5 . . . no
O(3′) C(4′) H(4′c) 109.5 . . . no
H(4′a) C(4′) H(4′b) 109.4 . . . no
H(4′a) C(4′) H(4′c) 109.5 . . . no
H(4′b) C(4′) H(4′c) 109.5 . . . no
C(6) C(5) C(10a) 119.2(9) . . . yes
C(6) C(5) H(5) 120.4 . . . no
C(10a) C(5) H(5) 120.4 . . . no
C(5) C(6) C(7) 121.4(8) . . . yes
C(5) C(6) H(6) 119.3 . . . no
C(7) C(6) H(6) 119.3 . . . no
C(6) C(7) C(8) 120.1(9) . . . yes
C(6) C(7) H(7) 120.0 . . . no
C(8) C(7) H(7) 119.9 . . . no
C(7) C(8) C(8a) 118.9(8) . . . yes
C(7) C(8) H(8) 120.5 . . . no
C(8a) C(8) H(8) 120.5 . . . no
C(8) C(8a) C(9) 126.0(8) . . . yes
C(8) C(8a) C(10a) 119.4(7) . . . yes
C(9) C(8a) C(10a) 114.5(7) . . . yes
O(1′) C(9) C(8a) 109.8(7) . . . yes
O(1′) C(9) C(9a) 115.2(6) . . . yes
O(1′) C(9) C(12) 113.1(7) . . . yes
C(8a) C(9) C(9a) 106.6(7) . . . yes
C(8a) C(9) C(12) 105.7(6) . . . yes
C(9a) C(9) C(12) 105.8(7) . . . yes
C(1) C(9a) C(4a) 118.8(8) . . . yes
C(1) C(9a) C(9) 126.2(9) . . . yes
C(4a) C(9a) C(9) 115.0(7) . . . yes
C(4a) C(10) C(10a) 108.8(7) . . . yes
C(4a) C(10) C(11) 105.9(7) . . . yes
C(4a) C(10) H(10) 111.2 . . . no
C(10a) C(10) C(11) 108.4(7) . . . yes
C(10a) C(10) H(10) 111.2 . . . no
C(11) C(10) H(10) 111.2 . . . no
C(5) C(10a) C(8a) 121.0(8) . . . yes
C(5) C(10a) C(10) 127.2(8) . . . yes
C(8a) C(10a) C(10) 111.8(7) . . . yes
C(10) C(11) C(12) 109.2(7) . . . yes
C(10) C(11) H(11b) 109.5 . . . no
C(10) C(11) H(11a) 109.5 . . . no
C(12) C(11) H(11b) 109.5 . . . no

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  C(12) C(11)  H(11a) 109.5 . . . no
  H(11b) C(11)  H(11a) 109.5 . . . no
  C(9) C(12)  C(11) 109.1(7) . . . yes
  C(9) C(12)  C(12') 110.1(7) . . . yes
  C(9) C(12)  H(12) 109.4 . . . no
  C(11) C(12)  C(12') 109.5(6) . . . yes
  C(11) C(12)  H(12) 109.4 . . . no
  C(12') C(12)  H(12) 109.4 . . . no
  N(12') C(12')  C(12) 177.5(9) . . . yes
#-------------------------------------------------------------------------------
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
  O(1')     C(1')     3.43(1)    . 4 no
  O(1')     O(2')     3.511(7)   . 4 no
  O(3')     C(3)      3.33(1)    . 4_454 no
  N(12')    C(5)      3.42(1)    . 2_764 no
  N(12')    C(11)     3.51(1)    . 2_664 no
  N(12')    C(6)      3.58(1)    . 2_764 no
  C(7)      C(12')    3.42(1)    . 1_655 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_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag
  O(1') C(1') O(2') C(2') . . . . 74.7(9) no
  O(1') C(9) C(8a) C(8) . . . . 4(1) no
  O(1') C(9) C(8a) C(10a) . . . . -179.4(7) no
  O(1') C(9) C(9a) C(1) . . . . -3(1) no
  O(1') C(9) C(9a) C(4a) . . . . 175.3(8) no
  O(1') C(9) C(12) C(11) . . . . -179.3(6) no
  O(1') C(9) C(12) C(12') . . . . -59.1(8) no
  O(2') C(1') O(1') C(9) . . . . 88.0(9) no
  O(2') C(2') C(3') O(3') . . . . -63(1) no
  N(12') C(12') C(12) C(9) . . . . -124.2(2) no
  N(12') C(12') C(12) C(11) . . . . -4.3(2) no
  C(1) C(2) C(3) C(4) . . . . -1(2) no
  C(1) C(9a) C(4a) C(4) . . . . -2(1) no
  C(1) C(9a) C(4a) C(10) . . . . 178.7(8) no
  C(1) C(9a) C(9) C(8a) . . . . -125.0(9) no
  C(1) C(9a) C(9) C(12) . . . . 122.9(9) no
  C(1') O(1') C(9) C(8a) . . . . -168.9(7) no
  C(1') O(1') C(9) C(9a) . . . . 70.8(9) no
  C(1') O(1') C(9) C(12) . . . . -51.1(9) no
  C(1') O(2') C(2') C(3') . . . . -175.7(7) no
  C(2) C(1) C(9a) C(4a) . . . . 2(1) no
  C(2) C(1) C(9a) C(9) . . . . 179.7(9) no
  C(2) C(3) C(4) C(4a) . . . . 1(2) no
  C(2') C(3') O(3') C(4') . . . . -178.3(8) no
  C(3) C(2) C(1) C(9a) . . . . 0(2) no
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  C(3) C(4) C(4a) C(9a) . . . . 1(2) no
  C(3) C(4) C(4a) C(10) . . . . 179.8(9) no
  C(4a) C(9a) C(9) C(8a) . . . . 53(1) no
  C(4a) C(9a) C(9) C(12) . . . . -59.0(9) no
  C(4a) C(10) C(10a) C(5) . . . . -128.1(9) no
  C(4a) C(10) C(10a) C(8a) . . . . 54(1) no
  C(4a) C(10) C(11) C(12) . . . . -61.4(9) no
  C(4) C(4a) C(9a) C(9) . . . . 179.8(9) no
  C(4) C(4a) C(10) C(10a) . . . . 126(1) no
  C(4) C(4a) C(10) C(11) . . . . -118(1) no
  C(5) C(6) C(7) C(8) . . . . -1(2) no
  C(5) C(10a) C(8a) C(8) . . . . 0(1) no
  C(5) C(10a) C(8a) C(9) . . . . -176.8(7) no
  C(5) C(10a) C(10) C(11) . . . . 117.3(9) no
  C(6) C(5) C(10a) C(8a) . . . . 0(1) no
  C(6) C(5) C(10a) C(10) . . . . -178.6(8) no
  C(6) C(7) C(8) C(8a) . . . . 1(1) no
  C(7) C(6) C(5) C(10a) . . . . 1(1) no
  C(7) C(8) C(8a) C(9) . . . . 176.3(8) no
  C(7) C(8) C(8a) C(10a) . . . . 0(1) no
  C(8) C(8a) C(9) C(9a) . . . . 129.1(8) no
  C(8) C(8a) C(9) C(12) . . . . -118.7(9) no
  C(8) C(8a) C(10a) C(10) . . . . 178.7(7) no
  C(8a) C(9) C(12) C(11) . . . . -59.1(8) no
  C(8a) C(9) C(12) C(12') . . . . 61.1(9) no
  C(8a) C(10a) C(10) C(11) . . . . -61.0(8) no
  C(9) C(8a) C(10a) C(10) . . . . 2(1) no
  C(9) C(9a) C(4a) C(10) . . . . 0(1) no
  C(9) C(12) C(11) C(10) . . . . 4.0(9) no
  C(9a) C(4a) C(10) C(10a) . . . . -55(1) no
  C(9a) C(4a) C(10) C(11) . . . . 62(1) no
  C(9a) C(9) C(8a) C(10a) . . . . -54.0(9) no
  C(9a) C(9) C(12) C(11) . . . . 53.7(8) no
  C(9a) C(9) C(12) C(12') . . . . 173.9(7) no
  C(10) C(11) C(12) C(12') . . . . -116.6(7) no
  C(10a) C(8a) C(9) C(12) . . . . 58.2(9) no
  C(10a) C(10) C(11) C(12) . . . . 55.1(8) no
#------------------------------------------------------------------------------
#===END
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