SUPPORTING INFORMATION

```
# Ms.No. JA012136I-26-209
# CIF-file generated for   2-Azido-2-methylpropanoic acid

#==============================================================================
data_global
#==============================================================================

# 0. AUDIT DETAILS

_audit_creation_date                    'Aug 23 11:20:44 2001'
_audit_creation_method                  'PLATON <TABLE ACC> option'
_audit_update_record
;
 ?
;

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

# 1. SUBMISSION DETAILS

_publ_contact_author_name            # Name of author for correspondence
;
 Morten Meldal
;
_publ_contact_author_address         # address of author for correspondence
;
Department of Chemistry
Gamle Carlsberg Vej 10
DK-2500 Valby
Denmark
;

_publ_contact_author_email             mpm@crc.dk
_publ_contact_author_fax               +4533274708
_publ_contact_author_phone             +4533275301

_publ_requested_journal                'Acta Crystallographica C'
# Publication choise FI FM FO CI CM CO
_publ_requested_category               ?
_publ_requested_coeditor_name          ?

_publ_contact_letter                 # Include date of submission
;
Date of submission ?

Please consider this CIF submission for publication as a
Regular Structural Paper in Acta Crystallographica C.
;

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

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic          ?

_journal_date_to_coeditor              ?
_journal_date_from_coeditor            ?
_journal_date_accepted                 ?

_journal_date_printers_first           ?
_journal_date_printers_final           ?
```

```
_journal_date_proofs_out              ?
_journal_date_proofs_in               ?

_journal_coeditor_name                ?
_journal_coeditor_code                ?
_journal_coeditor_notes
; ?
;

_journal_techeditor_code              ?
_journal_techeditor_notes
; ?
;

_journal_coden_ASTM                   ?
_journal_name_full                    ?
_journal_year                         ?
_journal_volume                       ?
_journal_issue                        ?
_journal_page_first                   ?
_journal_page_last                    ?


_journal_suppl_publ_number            ?
_journal_suppl_publ_pages             ?

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

# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
 ?
;
_publ_section_title_footnote
;
 ?
;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
; ?  # author related footnote
;
; ?  # Address of this author
;

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

# 4. TEXT

_publ_section_synopsis
;
 ?
```

```
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
 ?
;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
 ?
;

# Insert blank lines between references

_publ_section_references
;.
```

```
;
_publ_section_figure_captions
;
 ?
;
_publ_section_acknowledgements
; ?
;
_publ_section_figure_captions
; View of the title compound with the atom numbering scheme.
Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.
;

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

data_n3aiboh

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

# 5. CHEMICAL DATA

_chemical_name_systematic
;
 2-Azido-2-methylpropionic acid
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
'C4 H7 N3 O2'
_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
'C4 H7 N3 O2'
_chemical_formula_weight                 129.13
_chemical_compound_source             'see text'
```

```
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 O   O    0.0492    0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N    0.0311    0.0180
 '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    0.0181    0.0091
 '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'

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

_cell_length_a                       10.7302(12)
_cell_length_b                       11.9893(11)
_cell_length_c                       10.8108(13)
_cell_angle_alpha                          90
_cell_angle_beta                     114.095(9)
_cell_angle_gamma                          90
_cell_volume                         1269.6(3)
_cell_formula_units_Z                8
_cell_measurement_temperature        0
_cell_measurement_reflns_used        ?
_cell_measurement_theta_min          ?
_cell_measurement_theta_max          ?
_cell_special_details
; ?
;

_exptl_crystal_description           ' ?                '
_exptl_crystal_colour                ' ?                '

_exptl_crystal_size_max              ?
_exptl_crystal_size_mid              ?
_exptl_crystal_size_min              ?
_exptl_crystal_size_rad              ?
_exptl_crystal_density_meas          ?
_exptl_crystal_density_diffrn        1.351
_exptl_crystal_density_method        'Not Measured'
```

```
_exptl_crystal_F_000                          544
_exptl_absorpt_coefficient_mu                0.940
_exptl_crystal_density_meas_temp      ?

# Permitted for _exptl_absorpt_correction_type :
# analytical      'analytical from crystal shape'
# cylinder        'cylindrical'
# empirical       'empirical from intensities'
# gaussian        'Gaussian from crystal shape'
# integration     'integration from crystal shape'
# multi-scan      'symmetry-related measurements'
# none            'no absorption corr. applied'
# numerical       'numerical from crystal shape'
# psi-scan        'psi-scan corrections'
# refdelf         'refined from delta-F'
# sphere          'spherical'
_exptl_absorpt_correction_type       ' ?
# Example: '(North, Phillips & Mathews, 1968)'
_exptl_absorpt_process_details        ?
_exptl_absorpt_correction_T_min      ?
_exptl_absorpt_correction_T_max      ?

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

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature          ?
_diffrn_radiation_wavelength           1.54184
_diffrn_radiation_type               'CuKa'
_diffrn_radiation_source              ?
_diffrn_radiation_monochromator       ?

_diffrn_measurement_device_type       ?
_diffrn_measurement_method            ?
_diffrn_detector_area_resol_mean      ?

_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?
_diffrn_standards_decay_%             ?

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                 ?
_diffrn_reflns_av_R_equivalents       ?
_diffrn_reflns_av_sigmaI/netI         ?
_diffrn_reflns_limit_h_min            ?
_diffrn_reflns_limit_h_max            ?
_diffrn_reflns_limit_k_min            ?
_diffrn_reflns_limit_k_max            ?
_diffrn_reflns_limit_l_min            ?
_diffrn_reflns_limit_l_max            ?
_diffrn_reflns_theta_min              ?
```

```
_diffrn_reflns_theta_max            ?
_diffrn_reflns_theta_full           ?
_diffrn_measured_fraction_theta_max ?
_diffrn_measured_fraction_theta_full?
_diffrn_reflns_reduction_process
;
 ?
;

# number of unique reflections
_reflns_number_total                ?
# number of observed reflections (> n sig(I))
_reflns_number_gt                   ?
_reflns_threshold_expression          ?

_computing_data_collection           ?
_computing_cell_refinement           ?
_computing_data_reduction.           ?
_computing_structure_solution        ?
_computing_structure_refinement      ?
_computing_molecular_graphics        ?
_computing_publication_material      'PLATON (Spek, 1990)'

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

#'8. REFINEMENT DATA

_refine_special_details              ?
_refine_ls_structure_factor_coef      ?
_refine_ls_matrix_type                ?
_refine_ls_weighting_scheme          ' ?                '
_refine_ls_weighting_details
 ?
_atom_sites_solution_primary        ' ?                '
_atom_sites_solution_secondary      ' ?                '
_atom_sites_solution_hydrogens      ' ?                '
_refine_ls_hydrogen_treatment       'see text          '

_refine_ls_extinction_method          ?
_refine_ls_extinction_coef                      0
_refine_ls_extinction_expression
 ?
_refine_ls_abs_structure_details     ?
_refine_ls_abs_structure_Flack       none
_refine_ls_number_reflns            ?
_refine_ls_number_parameters        ?
_refine_ls_number_restraints                0
_refine_ls_number_constraints        ?
_refine_ls_R_factor_all             ?
_refine_ls_R_factor_gt              ?
_refine_ls_wR_factor_ref            ?
_refine_ls_wR_factor_gt             ?
_refine_ls_goodness_of_fit_ref      ?
_refine_ls_restrained_S_all         ?
_refine_ls_shift/su_max             ?
_refine_ls_shift/su_mean            ?
_refine_diff_density_max            ?
_refine_diff_density_min            ?
_refine_diff_density_rms            ?

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

```
# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
O1 O Uani 0.09098 0.02169 0.17035 1.000 0.0231 . .
O2 O Uani 0.04377 0.13799 -0.00470 1.000 0.0270 . .
N1 N Uani 0.17196 0.19692 0.34879 1.000 0.0207 . .
N2 N Uani 0.22889 0.11645 0.42143 1.000 0.0218 . .
N3 N Uani 0.27609 0.04801 0.49879 1.000 0.0318 . .
C1 C Uani 0.09794 0.11552 0.12041 1.000 0.0177 . .
C2 C Uani 0.18564 0.20535 0.21724 1.000 0.0200 . .
C3 C Uani 0.13626 0.32200 0.16415 1.000 0.0273 . .
C4 C Uani 0.33317 0.18563 0.23543 1.000 0.0303 . .
H1 H Uiso 0.03645 -0.03994 0.09764 1.000 0.0277 . .
H3A H Uiso 0.04010 0.32966 0.15303 1.000 0.0345 . .
H3B H Uiso 0.18824 0.37568 0.23021 1.000 0.0396 . .
H3C H Uiso 0.14146 0.33780 0.07393 1.000 0.0388 . .
H4A H Uiso 0.39003 0.23601 0.30041 1.000 0.0369 . .
H4B H Uiso 0.36622 0.11108 0.27046 1.000 0.0398 . .
H4C H Uiso 0.34197 0.19839 0.15005 1.000 0.0393 . .

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

# 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
 O1      C1          1.2631                .     .     yes
 O2      C1          1.2641                .     .     yes
 O1      H1          1.0633                .     .     no
 N1      C2          1.4915                .     .     yes
 N1      N2          1.2365                .     .     yes
 N2      N3          1.1329                .     .     yes
 C1      C2          1.5287                .     .     no
 C2      C3          1.5224                .     .     no
 C2      C4          1.5318                .     .     no
 C3      H3A         0.9932                .     .     no
```

```
C3    H3B    0.9540    .    .    no
C3    H3C    1.0172    .    .    no
C4    H4A    0.9384    .    .    no
C4    H4B    0.9790    .    .    no
C4    H4C    0.9775    .    .    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
C1    O1    H1     114.43    .    .    .    no
N2    N1    C2     116.30    .    .    .    yes
N1    N2    N3     171.91    .    .    .    yes
O1    C1    O2     124.44    .    .    .    yes
O1    C1    C2     117.52    .    .    .    yes
O2    C1    C2     117.92    .    .    .    yes
N1    C2    C3     105.50    .    .    .    yes
N1    C2    C4     111.47    .    .    .    yes
N1    C2    C1     109.42    .    .    .    yes
C1    C2    C4     107.10    .    .    .    no
C3    C2    C4     111.87    .    .    .    no
C1    C2    C3     111.52    .    .    .    no
C2    C3    H3A    108.36    .    .    .    no
C2    C3    H3B    109.29    .    .    .    no
C2    C3    H3C    112.69    .    .    .    no
H3A   C3    H3B    106.81    .    .    .    no
H3A   C3    H3C    109.13    .    .    .    no
H3B   C3    H3C    110.36    .    .    .    no
C2    C4    H4A    108.59    .    .    .    no
C2    C4    H4B    112.50    .    .    .    no
C2    C4    H4C    110.35    .    .    .    no
H4A   C4    H4B    106.02    .    .    .    no
H4A   C4    H4C    108.80    .    .    .    no
H4B   C4    H4C    110.41    .    .    .    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
N2    N1    C2    C4     -45.88    .    .    .    .    no
N2    N1    C2    C3    -167.51    .    .    .    .    no
N2    N1    C2    C1      72.40    .    .    .    .    no
O2    C1    C2    C3      30.51    .    .    .    .    no
O2    C1    C2    C4     -92.19    .    .    .    .    no
O1    C1    C2    N1     -37.05    .    .    .    .    no
O1    C1    C2    C3    -153.38    .    .    .    .    no
O1    C1    C2    C4      83.91    .    .    .    .    no
O2    C1    C2    N1     146.85    .    .    .    .    no
```

```
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 O1      N1          2.7425                .      .          no
 O1      N2          2.7511                .      .          no
 O1      C1          3.3902                .      3_555      no
 O1      O1          3.0861                .      2_555      no
 O1      O2          2.6170                .      3_555      no
 O2      C1          3.4003                .      3_555      no
 O2      O1          2.6170                .      3_555      no
 O1      H1          2.6601                .      3_555      no
 O1      H4B         2.9038                .      .          no
 O1      H3B         2.7844                .      6_545      no
 O2      H3C         2.6140                .      .          no
 O2      H3A         2.8713                .      .          no
 O2      H1          1.5576                .      3_555      no
 O2      H4A         2.5699                .      8_454      no
 N1      O1          2.7425                .      .          no
 N1      C1          3.1997                .      2_555      no
 N1      N1          3.2624                .      7_556      no
 N1      N2          3.1862                .      7_556      no
 N2      N1          3.1862                .      7_556      no
 N2      O1          2.7511                .      .          no
 N2      C1          3.3479                .      2_555      no
 N3      C1          3.3585                .      4_555      no
 N1      H3A         2.7702                .      2_555      no
 N2      H4A         2.9332                .      .          no
 N2      H4B         2.6083                .      .          no
 N3      H3C         2.8845                .      6_545      no
 N3      H3B         2.9413                .      7_556      no
 C1      N1          3.1997                .      2_555      no
 C1      N2          3.3479                .      2_555      no
 C1      O1          3.3902                .      3_555      no
 C1      O2          3.4003                .      3_555      no
 C1      N3          3.3585                .      4_554      no
 C4      C4          3.4636                .      2_655      no
 C1      H1          2.3837                .      3_555      no
 H1      O1          2.6601                .      3_555      no
 H1      O2          1.5576                .      3_555      no
 H1      C1          2.3837                .      3_555      no
 H1      H1          2.1534                .      3_555      no
 H3A     O2          2.8713                .      .          no
 H3A     N1          2.7702                .      2_555      no
 H3A     H3A         2.5709                .      2_555      no
 H3B     H4A         2.5935                .      .          no
 H3B     O1          2.7844                .      6_555      no
 H3B     N3          2.9413                .      7_556      no
 H3C     O2          2.6140                .      .          no
 H3C     H4C         2.5797                .      .          no
 H3C     N3          2.8845                .      6_555      no
 H3C     H4C         2.5366                .      7_555      no
 H4A     N2          2.9332                .      .          no
 H4A     H3B         2.5935                .      .          no
 H4A     O2          2.5699                .      8_555      no
 H4B     O1          2.9038                .      .          no
 H4B     N2          2.6083                .      .          no
 H4C     H3C         2.5797                .      .          no
```

```
 H4C     H3C          2.5366                    .     7_555                 no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
O1      H1      O2          1.0633     1.5576     2.6170     173.55   3_555 yes
C4      H4A     O2          0.9384     2.5699     3.5053     174.64   8_555 yes

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