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_audit_conform_dict_name          cif_core.dic
_audit_conform_dict_version       2.2
_audit_conform_dict_location      ftp://ftp.iucr.org/pub/cif_core.dic

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

#1. SUBMISSION DETAILS
_publ_contact_author     # Name and address of author for correspondance
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_publ_contact_author_email          blackman@alkali.otago.ac.nz
_publ_author_name                   'Blackman, Allan G.'
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; These data are being deposited as part of a paper to be submitted to the
Australian Journal of Chemistry.

Sincerely
Allan Blackman
;

#==============================================================================
#------------------------------------------------------------------------------#
#                   CHEMICAL INFORMATION                                       #
#------------------------------------------------------------------------------#

_chemical_name_systematic
;
 'N,N,N-tris(2-aminoethyl)-N-methylammonium chloride trihydrochloride'
;
_chemical_formula_sum                    'C7 H24 Cl4 N4'
_chemical_formula_weight                 306.1

#------------------------------------------------------------------------------#
#                   UNIT CELL INFORMATION                                      #
#------------------------------------------------------------------------------#

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_symmetry_space_group_name_H-M           P6(3)
loop_
    _symmetry_equiv_pos_as_xyz
'x, y, z'
```

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

_cell_length_a                         10.625(3)
_cell_length_b                         10.625(3)
_cell_length_c                         7.466(4)
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_cell_volume                           729.9(5)
_cell_formula_units_Z                  2
_cell_measurement_temperature          158(2)
_cell_measurement_reflns_used          14
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#------------------------------------------------------------------------------#
#                   CRYSTAL INFORMATION                                        #
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_exptl_crystal_density_method          'not measured'
_exptl_crystal_F_000                   324
_exptl_special_details
;
 ?
;

#------------------------------------------------------------------------------#
#                   ABSORPTION CORRECTION                                      #
#------------------------------------------------------------------------------#

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_exptl-absorpt_process_details         'SHELXTL-Plus (Sheldrick, 1990)'
_exptl_absorpt_correction_T_min        0.5146
_exptl_absorpt_correction_T_max        0.5809

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#                   DATA COLLECTION                                            #
#------------------------------------------------------------------------------#

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_diffrn_radiation_type                 MoK\a
_diffrn_radiation_monochromator        graphite
_diffrn_measurement_device             'Siemens P4'
_diffrn_measurement_method             '\w scans'
_diffrn_standards_number               3
```

```
_diffrn_standards_interval_count        397
_diffrn_standards_decay_%               3.8
_diffrn_reflns_av_R_equivalents         0.0628
_diffrn_reflns_av_unetI/netI            0.0504
_diffrn_reflns_number                   2021
_diffrn_reflns_limit_h_min              -1
_diffrn_reflns_limit_h_max              14
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_diffrn_reflns_limit_l_min              -1
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                                        1
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                                        1
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_reflns_number_gt                       799
_reflns_threshold_expression            >2sigma(I)

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#                   COMPUTER PROGRAMS USED                                     #
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_computing_data_collection              'Siemens XSCANS'
_computing_cell_refinement              'Siemens XSCANS'
_computing_data_reduction               'Siemens SHELXTL'
_computing_structure_solution           'Siemens SHELXTL'
_computing_structure_refinement         'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics           'WinGX (Farrugia, 1999)'
_computing_publication_material         'WinGX (Farrugia, 1999)'

#------------------------------------------------------------------------------#
#                   REFINEMENT INFORMATION                                     #
#------------------------------------------------------------------------------#

_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^ > 2sigma(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^)+(0.0479P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary          difmap
_atom_sites_solution_hydrogens          geom
_refine_ls_hydrogen_treatment           constr
```

```
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_refine_ls_goodness_of_fit_ref          1.023
_refine_ls_restrained_S_all             1.022
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_refine_ls_shift/su_mean                0
_refine_ls_abs_structure_details
                                    'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack          -0.05(10)
_refine_diff_density_max                0.455
_refine_diff_density_min                -0.507
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#                   ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS            #
#-------------------------------------------------------------------------------#

loop_
    _atom_type_symbol
    _atom_type_description
    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
    _atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
    _atom_site_calc_flag
    _atom_site_refinement_flags
    _atom_site_disorder_assembly
    _atom_site_disorder_group
Cl1 Cl 0.38148(5) 0.11192(5) 0.06843(10) 0.01726(14) Uani 1 1 d . . .
Cl2 Cl 0 0 0.39913(14) 0.01492(17) Uani 1 3 d S . .
N1 N 0.3333 -0.3333 0.0709(5) 0.0106(4) Uani 1 3 d S . .
N2 N 0.06580(18) -0.20055(19) 0.1611(3) 0.0172(3) Uani 1 1 d . . .
H2A H -0.0261 -0.2306 0.1317 0.026 Uiso 1 1 calc R . .
H2B H 0.1223 -0.11 0.1224 0.026 Uiso 1 1 calc R . .
H2C H 0.0733 -0.2031 0.2796 0.026 Uiso 1 1 calc R . .
C1 C 0.26668(19) -0.24747(18) 0.1442(3) 0.0136(3) Uani 1 1 d . . .
H1A H 0.3286 -0.1461 0.1125 0.016 Uiso 1 1 calc R . .
```

```
H1B H 0.2645 -0.254 0.2739 0.016 Uiso 1 1 calc R . .
C2 C 0.11259(18) -0.2976(2) 0.0767(5) 0.0171(4) Uani 1 1 d . . .
H2D H 0.1121 -0.2903 -0.0528 0.021 Uiso 1 1 calc R . .
H2E H 0.0474 -0.3979 0.1106 0.021 Uiso 1 1 calc R . .
C3 C 0.3333 -0.3333 -0.1305(5) 0.0150(6) Uani 1 3 d S . .
H3A H 0.238 -0.4018 -0.1734 0.022 Uiso 0.33 1 calc PR . .
H3B H 0.4018 -0.3602 -0.1734 0.022 Uiso 0.33 1 calc PR . .
H3C H 0.3602 -0.238 -0.1734 0.022 Uiso 0.33 1 calc PR . .

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    _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
Cl1 0.0176(2) 0.0150(2) 0.0188(2) -0.0002(2) -0.0018(2) 0.00782(15)
Cl2 0.0146(2) 0.0146(2) 0.0155(3) 0 0 0.00732(11)
N1 0.0086(6) 0.0086(6) 0.0146(11) 0 0 0.0043(3)
N2 0.0189(7) 0.0203(8) 0.0189(7) 0.0009(7) 0.0016(8) 0.0146(7)
C1 0.0122(7) 0.0114(7) 0.0196(8) -0.0036(8) -0.0011(9) 0.0076(6)
C2 0.0139(8) 0.0177(8) 0.0231(11) -0.0047(13) -0.0034(9) 0.0104(6)
C3 0.0153(9) 0.0153(9) 0.0143(14) 0 0 0.0077(5)


#------------------------------------------------------------------------------#
#                    MOLECULAR GEOMETRY                                        #
#------------------------------------------------------------------------------#

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
;
loop_
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    _geom_bond_atom_site_label_2
    _geom_bond_distance
    _geom_bond_site_symmetry_2
    _geom_bond_publ_flag
N1 C3 1.504(5) . ?
N1 C1 1.510(2) . ?
N1 C1 1.510(2) 2_545 ?
N1 C1 1.510(2) 3_655 ?
N2 C2 1.491(3) . ?
N2 H2A 0.89 . ?
N2 H2B 0.89 . ?
N2 H2C 0.89 . ?
C1 C2 1.531(3) . ?
C1 H1A 0.97 . ?
C1 H1B 0.97 . ?
C2 H2D 0.97 . ?
```

```
C2 H2E 0.97 . ?
C3 H3A 0.96 . ?
C3 H3B 0.96 . ?
C3 H3C 0.96 . ?

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    _geom_angle_site_symmetry_3
    _geom_angle_publ_flag
C3 N1 C1 111.24(15) . . ?
C3 N1 C1 111.24(15) . 2_545 ?
C1 N1 C1 107.64(16) . 2_545 ?
C3 N1 C1 111.24(15) . 3_655 ?
C1 N1 C1 107.64(16) . 3_655 ?
C1 N1 C1 107.64(16) 2_545 3_655 ?
C2 N2 H2A 109.5 . . ?
C2 N2 H2B 109.5 . . ?
H2A N2 H2B 109.5 . . ?
C2 N2 H2C 109.5 . . ?
H2A N2 H2C 109.5 . . ?
H2B N2 H2C 109.5 . . ?
N1 C1 C2 114.41(18) . . ?
N1 C1 H1A 108.7 . . ?
C2 C1 H1A 108.7 . . ?
N1 C1 H1B 108.7 . . ?
C2 C1 H1B 108.7 . . ?
H1A C1 H1B 107.6 . . ?
N2 C2 C1 106.8(2) . . ?
N2 C2 H2D 110.4 . . ?
C1 C2 H2D 110.4 . . ?
N2 C2 H2E 110.4 . . ?
C1 C2 H2E 110.4 . . ?
H2D C2 H2E 108.6 . . ?
N1 C3 H3A 109.5 . . ?
N1 C3 H3B 109.5 . . ?
H3A C3 H3B 109.5 . . ?
N1 C3 H3C 109.5 . . ?
H3A C3 H3C 109.5 . . ?
H3B C3 H3C 109.5 . . ?
```