EJJ- Coden3:PDJ - Volume:26 - Issue:4 - Aip Id:006104 - File:/006104pdj_supplemental.txt

```
data_global

_publ_requested_journal   'Powder Diffraction'

_publ_contact_author_name         'Kenny Stahl'
_publ_contact_author_address
;
Department of Chemistry
Technical University of Denmark
Building 207
DK-2800 Lyngby
Denmark
;

_publ_contact_author_email       'kenny@kemi.dtu.dk'
_publ_contact_author_fax         '+45 45 88 31 36'
_publ_contact_author_phone       '+45 45 25 20 19'

_publ_section_title
;
Structure Determination of a novel Metal-Organic Compound
synthesized from Aluminum and 2,5-Pyridinedicarboxylic Acid.
;

loop_
   _publ_author_name
   _publ_author_address
'Kenny Stahl'
;
Department of Chemistry
Technical University of Denmark
Building 207
DK-2800 Lyngby
Denmark
;
'Bastian Brink'
;
Department of Chemistry
Technical University of Denmark
Building 207
DK-2800 Lyngby
Denmark
;
'Jonas Andersen'
;
Department of Chemistry
Technical University of Denmark
Building 207
DK-2800 Lyngby
Denmark
;

_publ_section_abstract
;
The structure of [Al2(pydc)2(?2-OH)2(H2O)2]n (pydc=2,5-pyridinedicarboxylate)
was determined from powder X-ray diffraction data.  The compound crystalizes
in the triclinic system (space group P -1) with a = 6.7813(1) \%A, b=7.4944(1)
\%A, c=8.5013(1) \%A, ? = 95.256(1)\%, ?=102.478(1)\%, ?=108.979(1)\%.
The structure consists of aluminum ions coordinating N and O in distorted
octahedra, sharing an edge through two hydroxide ions. These dinuclear
complexes are connected by pydc ions, which at one end coordinate by nitrogen
and oxygen and only by oxygen at the other end. The pydc orientation is
reversed in the neighboring pydc, forming double stranded chains
interconnected by the aluminum dinuclear complexes in a ladder-like arrangement
along (001).
;

_publ_section_references
;
Liang, Y., Hong, M., Cao, R., Weng, J. (2001).
?Hydrothermal Synthesis and Structure Characterization of Compound Zn(H2pydc)2
(H2O) (pydc=pyridine-2,5-dicarboxylate),? Chinese J. Struct. Chem, 20, 455-458.
;
data_alpyridine

loop_
   _atom_type_symbol
   _atom_type_description
   _atom_type_scat_dispersion_real
   _atom_type_scat_dispersion_imag
   _atom_type_scat_source
   H  H   0.0000  0.0000 'International Tables for Crystallography (Vol. IV)'
   C  C   0.0181  0.0091 'International Tables for Crystallography (Vol. IV)'
   N  N   0.0311  0.0180 'International Tables for Crystallography (Vol. IV)'
   O  O   0.0492  0.0322 'International Tables for Crystallography (Vol. IV)'
   Al Al  0.2130  0.2455 'International Tables for Crystallography (Vol. IV)'

_pd_spec_size_axial               6.0
_pd_spec_size_equat               6.0
_pd_spec_size_thick                0.01
_pd_spec_mounting             'scotch tape'
_pd_spec_mount_mode           'transmission'
_pd_spec_shape                'flat_sheet'
```

```
_pd_char_particle_morphology  ?
_pd_char_colour                'white'

_pd_prep_temperature          ?
_pd_prep_cool_rate            ?
_pd_prep_pressure             ?

_diffrn_ambient_temperature        295
_diffrn_source                     'sealed X-ray tube'
_diffrn_source_target              'Cu'
_diffrn_measurement_device_type   'Huber G670 Guinier camera'
_diffrn_detector                   'Imaging plate'
_diffrn_detector_type              'Huber G670 Guinier camera'
_diffrn_radiation_monochromator   'Quartz'
_diffrn_radiation_type             'CuK\a~1~'
_diffrn_radiation_wavelength      1.54056
_pd_instr_location
;
 Department of Chemistry
 Technical University of Denmark
 Lyngby, Denmark
;

_pd_meas_special_details
;
 Sample spinning by appr. 1 turn/sec during measurements
;

_pd_meas_scan_method              'step'
_pd_meas_number_of_points         19400
_pd_meas_2theta_range_min             3.000
_pd_meas_2theta_range_max           100.000
_pd_meas_2theta_range_inc             0.005
_pd_proc_ls_profile_function    'split pseudo-Voigt'
_pd_proc_ls_background_function 'Chebyshev'

_pd_proc_ls_special_details
;
 ?
;

_pd_proc_ls_prof_R_factor         0.0416
_pd_proc_ls_prof_wR_factor        0.0577
_pd_proc_ls_prof_wR_expected      0.0184
_refine_special_details
;
Expected bond lengths of pydc (Liang et al., 2001) were used as restrains.
;

_pd_proc_2theta_range_min              8.003
_pd_proc_2theta_range_max             98.998
_pd_proc_2theta_range_inc              0.005
loop_
     _pd_proc_wavelength            1.540510  1.540510



_refine_ls_structure_factor_coef  'Inet'
_refine_ls_matrix_type            'full'
_refine_ls_weighting_scheme       'sigma'
_refine_ls_hydrogen_treatment     'noref'
_refine_ls_extinction_method      'none'
_refine_ls_extinction_coef        '?'
_refine_ls_number_parameters         80
_refine_ls_number_restraints         12
_refine_ls_number_constraints     0
_refine_ls_goodness_of_fit_all       3.14
_refine_ls_shift/su_max            0.0990
_refine_ls_shift/su_mean           0.0110

_computing_data_collection      'Huber G670'
_computing_cell_refinement      'WINPOW, local Rietveld program'
_computing_data_reduction       'WINPOW, local Rietveld program'
_computing_structure_solution
;
ITO, Visser, 1969 (j.appl.cryst.2,89(1969))
EXPO, Altomari et al., 1994, 1995
;
_computing_structure_refinement 'WINPOW, local Rietveld program'
_computing_molecular_graphics   'ATOMS 6.2, Shape Software, USA'
_computing_publication_material 'WINPOW, local Rietveld program'



_chemical_name_systematic
;
aqua-mu2-hydroxy-mu2-pyridine-2,5-dicarboxylato-aluminum(III)
;

_chemical_name_common
;
aqua-mu2-hydroxy-mu2-pyridine-2,5-dicarboxylato-aluminum(III)
;
_chemical_melting_point         ?
_chemical_formula_moiety        'C7 H6 Al N O6'
_chemical_formula_sum           'C7 H6 Al N O6'
_chemical_formula_weight            227.11
```

```
_symmetry_cell_setting             'Triclinic'
_symmetry_space_group_name_H-M     'P-1'
_symmetry_int_tables_number        ?
_symmetry_space_group_name_Hall    '-P 1'

loop_
 _symmetry_equiv_pos_as_xyz
  'x,y,z'
  '-x,-y,-z'

_cell_length_a                          6.78132(10)
_cell_length_b                          7.49436(13)
_cell_length_c                          8.50132(13)
_cell_angle_alpha                       95.2566(13)
_cell_angle_beta                        102.4778(10)
_cell_angle_gamma                       108.9790(9)
_cell_volume                            392.73(3)
_cell_formula_units_Z                   2
_cell_measurement_temperature        295.00
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn       1.895
_exptl_crystal_density_method     ?
_exptl_crystal_F_000                226.0
_exptl_absorpt_coefficient_mu        2.30
_exptl_absorpt_correction_type    none


loop_
     _atom_site_label
     _atom_site_fract_x
     _atom_site_fract_y
     _atom_site_fract_z
     _atom_site_occupancy
     _atom_site_U_iso_or_equiv
     _atom_site_adp_type
     _atom_site_type_symbol
Al1    .2013(4)   .1529(4)   .5291(3)   1.0000   .0515(9) Uiso   Al
C1     .2500(8)   .1244(8)   .8971(6)   1.0000   .0206(5) Uiso   C
C2     .2458(9)   .1989(9)  1.0622(8)   1.0000   .0217(5) Uiso   C
C3     .2225(8)   .3740(8)  1.0812(7)   1.0000   .0206(5) Uiso   C
C4     .2407(7)   .4843(7)   .9628(7)   1.0000   .0206(5) Uiso   C
C5     .2313(9)   .4219(10)  .8040(8)   1.0000   .0206(5) Uiso   C
C6     .2550(10)  .0619(8)  1.1882(8)   1.0000   .0206(5) Uiso   C
C7     .2512(9)   .5323(8)   .6600(7)   1.0000   .0206(5) Uiso   C
N1     .2421(7)   .2354(6)   .7843(6)   1.0000   .0206(5) Uiso   N
O1     .3082(5)  -.0704(5)  1.1760(5)   1.0000   .0206(5) Uiso   O
O2     .2212(6)   .1511(5)  1.3129(4)   1.0000   .0206(5) Uiso   O
O3     .2742(6)   .6932(5)   .6970(4)   1.0000   .0206(5) Uiso   O
O4     .2571(5)   .4251(5)   .5405(4)   1.0000   .0206(5) Uiso   O
O5     .8944(5)   .1041(6)   .4704(4)   1.0000   .0206(5) Uiso   O
O6     .5202(5)   .2048(4)   .5903(4)   1.0000   .0206(5) Uiso   O
H1     .2649(8)   .0035(8)   .8732(6)   1.0000   .0380 Uiso   H
H3     .1935(8)   .4213(8)  1.1784(7)   1.0000   .0380 Uiso   H
H4     .2662(7)   .6175(7)   .9966(7)   1.0000   .0380 Uiso   H

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_3
_geom_angle_publ_flag
N1 Al1 O2 163.7(2) . 1_554 ?
N1 Al1 O4 79.94(18) . . ?
N1 Al1 O5 94.54(19) . 1_455 ?
N1 Al1 O5 95.5(2) . 2_656 ?
N1 Al1 O6 85.36(18) . . ?
O2 Al1 O4 86.05(19) 1_554 . ?
O2 Al1 O5 93.59(19) 1_554 1_455 ?
O2 Al1 O5 99.6(2) 1_554 2_656 ?
O2 Al1 O6 86.45(18) 1_554 . ?
O4 Al1 O5 89.62(19) . 1_455 ?
O4 Al1 O5 169.8(2) . 2_656 ?
O4 Al1 O6 90.12(17) . . ?
O5 Al1 O5 81.6(2) 1_455 2_656 ?
O5 Al1 O6 179.7(2) 1_455 . ?
O5 Al1 O6 98.67(18) 2_656 . ?
C2 C1 N1 117.7(5) . . ?
C2 C1 H1 121.2(6) . . ?
N1 C1 H1 121.1(6) . . ?
C1 C2 C3 115.8(5) . . ?
C1 C2 C6 115.1(5) . . ?
C3 C2 C6 129.0(5) . . ?
C2 C3 C4 121.0(5) . . ?
C2 C3 H3 120.4(6) . . ?
C4 C3 H3 118.5(6) . . ?
C3 C4 C5 125.5(5) . . ?
C3 C4 H4 115.9(6) . . ?
C5 C4 H4 118.6(6) . . ?
C4 C5 C7 130.3(6) . . ?
C4 C5 N1 111.0(5) . . ?
C7 C5 N1 117.7(5) . . ?
C2 C6 O1 126.4(6) . . ?
```

```
 C2 C6 O2 101.9(4) . . ?
 O1 C6 O2 130.9(6) . . ?
 C5 C7 O3 112.2(5) . . ?
 C5 C7 O4 109.2(5) . . ?
 O3 C7 O4 138.2(6) . . ?
 C1 N1 C5 127.5(5) . . ?

 loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
 Al1 O5 1.822(5) 2_656 y
 Al1 O2 1.871(4) 1_554 y
 Al1 O5 1.933(4) 1_455 y
 Al1 O4 1.939(5) . y
 Al1 O6 2.007(4) . y
 Al1 N1 2.133(5) . y
 C1 H1 .952(8) . ?
 C1 N1 1.329(7) . ?
 C1 C2 1.472(8) . ?
 C2 C3 1.371(8) . ?
 C2 C6 1.556(9) . ?
 C3 H3 .953(8) . ?
 C3 C4 1.361(8) . ?
 C4 H4 .961(7) . ?
 C4 C5 1.369(8) . ?
 C5 N1 1.419(8) . ?
 C5 C7 1.544(9) . ?
 C6 O1 1.163(7) . ?
 C6 O2 1.303(7) . ?
 C7 O3 1.168(7) . ?
 C7 O4 1.252(7) . ?
 O1 O6 2.539(5) 2_657 y
 O3 O5 2.542(5) 2_666 y
```