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Catalytic molecular motors

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data_c22.50h2
_database_code_depnum_ccdc_archive 'CCDC 268595'

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

?

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety 'C45 H41 Mn2 N6 O4, Cl O4'

_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 'C45 H41 Cl Mn2 N6 O8'

_chemical_formula_weight 939.18

_chemical_compound_source 'by syntheses'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

O O .0106 .0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

N N .0061 .0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

Mn Mn .3368 .7283 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

Cl Cl .1484 .1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

H H .0000 .0000 '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 2y'
 _symmetry_space_group_name_H-M 'C 2'

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

_cell_length_a 15.226(2)
 _cell_length_b 12.924(2)
 _cell_length_c 10.944(2)
 _cell_angle_alpha 90
 _cell_angle_beta 90.157(9)
 _cell_angle_gamma 90
 _cell_volume 2153.6(6)
 _cell_formula_units_Z 2
 _cell_measurement_temperature 130
 _cell_measurement_reflns_used 22
 _cell_measurement_theta_min 16.65
 _cell_measurement_theta_max 20.21
 _cell_special_details

;

Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting. 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 'cubic-shaped block'
 _exptl_crystal_colour 'light green transparent'
 _exptl_crystal_size_max 0.25
 _exptl_crystal_size_mid 0.25
 _exptl_crystal_size_min 0.25
 _exptl_crystal_size_rad ?
 _exptl_crystal_density_meas ?
 _exptl_crystal_density_diffn 1.448
 _exptl_crystal_density_method ?
 _exptl_crystal_F_000 968
 _exptl_absorpt_coefficient_mu .71
 _exptl_crystal_density_meas_temp ?
 _exptl_absorpt_correction_type none
 _exptl_absorpt_process_details ?
 _exptl_absorpt_correction_T_min ?
 _exptl_absorpt_correction_T_max ?

#=====

7. EXPERIMENTAL DATA

_exptl_special_details
 ;
 ?
 ;
 _diffn_ambient_temperature 130
 _diffn_radiation_wavelength .71073
 _diffn_radiation_type 'Mo K\alpha'

```

_diffrn_radiation_source 'fine focus sealed Philips Mo tube '
_diffrn_radiation_monochromator 'perpendicular mounted graphite'
_diffrn_radiation_detector
;
scintillation NaI crystal with photomultiplier
;
_diffrn_measurement_device_type
;
Enraf Nonius CAD-4F diffractometer
;

_diffrn_measurement_method \w/2\q

_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
Graphite-monochromated Mo K\alpha radiation,
\w/2\q scan, \D\w = (0.80 + 0.34 tg \q)\%.
;
_diffrn_detector_area_resol_mean ?

_diffrn_standards_number 3
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time 180
_diffrn_standards_decay_% 3.1

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
1 -1 -3
2 2 0
4 0 1

# number of measured reflections (redundant set)
_diffrn_reflns_number 5221
_diffrn_reflns_av_R_equivalents 0.0111
_diffrn_reflns_av_sigmaI/netI 0.0159
_diffrn_reflns_limit_h_min -19
_diffrn_reflns_limit_h_max 19
_diffrn_reflns_limit_k_min -16
_diffrn_reflns_limit_k_max 16
_diffrn_reflns_limit_l_min -13
_diffrn_reflns_limit_l_max 0
_diffrn_reflns_theta_min 1.86
_diffrn_reflns_theta_max 26.99
_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization effects, scale
variation, but not for absorption and reduced to  $F_o^2$ 
;

# number of unique reflections
_reflns_number_total 4691
_reflns_number_gt 4481
_reflns_threshold_expression >2sigma(I)

_computing_data_collection 'CAD4-UNIX Software Version 5.1, 1994'
_computing_cell_refinement 'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction 'HELENA (Spek, 1993)'
_computing_structure_solution
;
DIRDIF-97 (Beurskens et al., 1997)
;

```

```

_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 1997)
ORTEP (Burnett et al., 1996)
PLATON (Spek, 1994, 1996)
;
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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 w=1/[s2(Fo2)+(0.0422P)2+2.3179P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack 0.428(15)
_refine_ls_number_reflns 4691
_refine_ls_number_parameters 375
_refine_ls_number_restraints 1
_refine_ls_R_factor_all 0.0329
_refine_ls_R_factor_gt 0.0303
_refine_ls_wR_factor_ref 0.0778
_refine_ls_wR_factor_gt 0.0760
_refine_ls_goodness_of_fit_ref 1.027
_refine_ls_restrained_S_all 1.026
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

_refine_diff_density_max .551
_refine_diff_density_min -.520
_refine_diff_density_rms .051

#=====

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_
_atom_site_label
_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
Mn Uani .07875(2) .00111(2) .41011(3) 1.000 .0241(1)
O1 Uani .05356(11) -.04469(14) .59691(14) 1.000 .0301(5)

```

```

O2 Uani .04933(13) .16203(14) .42542(18) 1.000 .0368(6)
N1 Uani .22262(11) -.00802(18) .46914(15) 1.000 .0248(5)
N2 Uani .16141(14) .07360(16) .24962(17) 1.000 .0289(6)
N3 Uani .13522(15) -.14282(15) .31559(18) 1.000 .0305(6)
C1 Uani .10637(15) -.04535(18) .6956(2) 1.000 .0259(6)
C2 Uani .07153(17) -.02851(19) .8126(2) 1.000 .0311(7)
C3 Uani .12479(18) -.03113(19) .9157(2) 1.000 .0327(7)
C4 Uani .21384(18) -.04843(19) .9051(2) 1.000 .0313(7)
C5 Uani .24910(16) -.06486(18) .7896(2) 1.000 .0279(7)
C6 Uani .19682(15) -.06438(17) .68488(19) 1.000 .0248(6)
C7 Uani .23652(17) -.09017(19) .5627(2) 1.000 .0272(7)
C8 Uani .25689(18) .0923(2) .5127(2) 1.000 .0314(8)
C9 Uani .26415(17) -.03766(18) .3515(2) 1.000 .0283(7)
C10 Uani .24612(17) .04740(19) .2596(2) 1.000 .0290(7)
C11 Uani .3115(2) .0945(2) .1919(2) 1.000 .0353(8)
C12 Uani .2879(2) .1746(2) .1141(2) 1.000 .0418(9)
C13 Uani .2009(2) .2028(2) .1043(2) 1.000 .0385(8)
C14 Uani .1392(2) .15075(19) .1740(2) 1.000 .0346(8)
C15 Uani .22261(18) -.13645(18) .3031(2) 1.000 .0299(7)
C16 Uani .2720(2) -.2106(2) .2432(2) 1.000 .0394(9)
C17 Uani .2290(3) -.2947(2) .1941(2) 1.000 .0479(11)
C18 Uani .1395(3) -.3023(2) .2053(2) 1.000 .0485(12)
C19 Uani .0944(2) -.2250(2) .2670(2) 1.000 .0402(9)
C20 Uani .00000 .2060(3) .50000 1.000 .0305(10)
C21 Uani .00000 .3227(3) .50000 1.000 .0416(13)
C22 Uani .01555(18) .3763(3) .3925(4) 1.000 .0535(12)
C23 Uani .0147(2) .4842(3) .3941(6) 1.000 .0804(19)
C24 Uani .00000 .5373(4) .50000 1.000 .100(3)
C1 Uani .00000 .42958(9) .00000 1.000 .0390(3)
O3 Uani .0701(4) .3798(6) -.0492(7) 1.000 .195(3)
O42 Uani .0385(7) .4529(11) .1085(11) .605(17) .161(5)
O41 Uani .0200(11) .5295(11) .0434(11) .395(17) .115(6)
H2 Uiso .009(2) -.010(3) .821(3) 1.000 .056(9)
H3 Uiso .093(2) -.018(3) 1.000(3) 1.000 .069(11)
H4 Uiso .257(2) -.046(3) .984(3) 1.000 .046(9)
H5 Uiso .311(2) -.080(3) .782(3) 1.000 .037(8)
H7 Uiso .2993(18) -.101(2) .577(2) 1.000 .020(6)
H7' Uiso .2100(18) -.152(2) .527(3) 1.000 .024(6)
H8 Uiso .2441(19) .150(3) .458(3) 1.000 .033(7)
H8' Uiso .324(2) .089(3) .524(3) 1.000 .044(9)
H8" Uiso .228(2) .102(3) .600(3) 1.000 .045(9)
H9 Uiso .3258(19) -.047(2) .364(2) 1.000 .029(7)
H11 Uiso .374(2) .071(3) .201(3) 1.000 .047(9)
H12 Uiso .331(3) .204(3) .074(4) 1.000 .062(11)
H13 Uiso .184(2) .259(3) .055(3) 1.000 .046(9)
H14 Uiso .071(2) .172(3) .172(3) 1.000 .042(8)
H16 Uiso .330(3) -.201(4) .227(4) 1.000 .077(14)
H17 Uiso .258(3) -.348(4) .152(4) 1.000 .073(12)
H18 Uiso .108(3) -.351(4) .178(4) 1.000 .066(12)
H19 Uiso .031(2) -.227(2) .276(3) 1.000 .033(7)
H22 Uiso .029(2) .342(3) .334(3) 1.000 .049(11)
H23 Uiso .023(3) .513(4) .329(4) 1.000 .065(12)
H24 Uiso .00000 .616(7) .50000 1.000 .11(3)

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
Mn .0288(2) .0259(2) .0177(1) -.0006(1) -.0019(1) .0006(2)
O1 .0312(8) .0421(9) .0170(7) .0003(6) -.0034(6) .0072(7)
O2 .0407(10) .0274(9) .0424(10) .0026(8) .0084(8) .0040(7)
N1 .0321(8) .0225(9) .0197(7) -.0030(8) .0001(6) .0014(9)

```

```

N2 .0424(12) .0230(9) .0212(9) -.0008(7) .0022(8) .0002(8)
N3 .0459(12) .0250(10) .0206(9) -.0031(7) -.0011(8) -.0025(9)
C1 .0339(12) .0251(10) .0187(10) .0008(8) -.0040(9) .0043(9)
C2 .0355(12) .0388(14) .0189(10) -.0001(9) -.0003(9) .0055(9)
C3 .0478(14) .0324(12) .0179(10) -.0023(8) -.0023(9) .0023(10)
C4 .0459(14) .0264(12) .0216(11) .0022(9) -.0108(10) -.0019(10)
C5 .0343(12) .0254(11) .0241(11) .0051(9) -.0040(9) .0012(9)
C6 .0324(11) .0221(10) .0198(10) .0006(8) -.0041(8) .0035(9)
C7 .0317(12) .0275(12) .0225(12) .0006(9) -.0013(9) .0070(9)
C8 .0373(14) .0289(13) .0281(13) -.0059(10) -.0029(10) -.0019(10)
C9 .0332(12) .0253(10) .0263(12) -.0026(9) .0024(9) .0011(9)
C10 .0434(14) .0251(11) .0185(10) -.0051(9) .0002(9) -.0024(10)
C11 .0450(15) .0388(14) .0222(11) -.0040(10) .0068(10) -.0068(11)
C12 .0619(18) .0391(15) .0243(12) .0007(11) .0082(12) -.0155(13)
C13 .0663(19) .0265(12) .0228(11) .0016(10) -.0011(12) -.0052(12)
C14 .0583(17) .0259(11) .0197(11) -.0025(9) -.0022(10) .0012(11)
C15 .0478(14) .0248(11) .0170(10) .0008(8) .0033(9) .0043(10)
C16 .0666(19) .0269(13) .0248(12) .0046(9) .0117(12) .0100(12)
C17 .097(3) .0239(12) .0229(12) .0010(10) .0154(14) .0052(14)
C18 .100(3) .0222(12) .0232(13) -.0031(10) -.0009(14) -.0128(14)
C19 .067(2) .0298(13) .0237(12) .0012(10) -.0031(12) -.0129(13)
C20 .0212(15) .0259(16) .0444(19) .0000 -.0022(13) .0000
C21 .0155(15) .0252(17) .084(3) .0000 .0082(17) .0000
C22 .0198(12) .0357(15) .105(3) .0176(18) .0148(15) .0023(11)
C23 .0304(14) .036(2) .175(5) .038(2) .037(2) .0064(13)
C24 .030(2) .025(2) .246(10) .0000 .053(4) .0000
C1 .0301(4) .0532(6) .0337(5) .0000 .0001(3) .0000
O3 .138(4) .220(7) .226(6) .006(5) .028(4) .131(5)
O42 .166(7) .158(11) .158(8) -.039(8) -.127(7) .012(7)
O41 .157(14) .104(9) .084(8) -.049(6) .024(7) -.098(10)

```

#=====

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

Mn O1 2.1636(16) . . yes

Mn O2 2.1341(19) . . yes

Mn N1 2.2852(17) . . yes

Mn N2 2.358(2) . . yes

Mn N3 2.297(2) . . yes

Mn O1 2.1009(18) . 2_556 yes

C1 O41 1.409(14) . . yes

C1 O3 1.359(7) . . yes

C1 O42 1.357(12) . . yes

O1 C1 1.345(3) . . yes

O2 C20 1.248(3) . . yes

O41 O41 1.127(19) . 2_555 yes

N1 C8 1.476(3) . . yes

N1 C9 1.486(3) . . yes

N1 C7 1.490(3) . . yes

N2 C10 1.338(3) . . yes
 N2 C14 1.339(3) . . yes
 N3 C19 1.340(3) . . yes
 N3 C15 1.341(4) . . yes
 C1 C6 1.404(3) . . no
 C1 C2 1.404(3) . . no
 C2 C3 1.388(3) . . no
 C3 C4 1.379(4) . . no
 C4 C5 1.391(3) . . no
 C5 C6 1.394(3) . . no
 C6 C7 1.506(3) . . no
 C9 C15 1.520(3) . . no
 C9 C10 1.515(3) . . no
 C10 C11 1.384(4) . . no
 C11 C12 1.387(4) . . no
 C12 C13 1.378(4) . . no
 C13 C14 1.386(4) . . no
 C15 C16 1.384(4) . . no
 C16 C17 1.377(4) . . no
 C17 C18 1.372(6) . . no
 C18 C19 1.389(4) . . no
 C20 C21 1.508(5) . . no
 C21 C22 1.386(5) . . no
 C22 C23 1.395(5) . . no
 C23 C24 1.366(6) . . no
 C2 H2 .99(3) . . no
 C3 H3 1.06(3) . . no
 C4 H4 1.08(3) . . no
 C5 H5 .97(3) . . no
 C7 H7 .98(3) . . no
 C7 H7' .98(3) . . no
 C8 H8" 1.06(3) . . no
 C8 H8 .98(4) . . no
 C8 H8' 1.03(3) . . no
 C9 H9 .96(3) . . no
 C11 H11 1.00(3) . . no
 C12 H12 .88(4) . . no
 C13 H13 .94(4) . . no
 C14 H14 1.07(3) . . no
 C16 H16 .91(5) . . no
 C17 H17 .94(5) . . no
 C18 H18 .85(5) . . no
 C19 H19 .97(3) . . no
 C22 H22 .81(3) . . no
 C23 H23 .81(5) . . no
 C24 H24 1.02(9) . . no

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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
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 O1 Mn O2 98.90(7) . . . yes
 O1 Mn N1 83.74(6) . . . yes
 O1 Mn N2 155.37(7) . . . yes
 O1 Mn N3 105.76(7) . . . yes
 O1 Mn O1 77.59(6) . . 2_556 yes
 O2 Mn N1 103.26(8) . . . yes
 O2 Mn N2 77.52(7) . . . yes
 O2 Mn N3 154.64(7) . . . yes
 O1 Mn O2 94.36(7) 2_556 . . yes
 N1 Mn N2 73.61(7) . . . yes

N1 Mn N3 74.08(8) . . . yes
 O1 Mn N1 156.08(7) 2_556 . . yes
 N2 Mn N3 77.59(7) . . . yes
 O1 Mn N2 126.76(7) 2_556 . . yes
 O1 Mn N3 96.63(7) 2_556 . . yes
 O3 C1 O41 118.0(7) . . 2_555 yes
 O3 C1 O42 95.5(6) 2_555 . . yes
 O42 C1 O42 154.3(9) . . 2_555 yes
 O3 C1 O42 96.5(6) . . . yes
 O3 C1 O41 113.5(7) . . . yes
 O3 C1 O3 123.5(5) . . 2_555 yes
 O3 C1 O42 95.5(6) . . 2_555 yes
 O3 C1 O41 118.0(7) 2_555 . . yes
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