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Note

SUPPORTING INFORMATION

Synthesis and Crystal Structures of Cadmium(II) Complexes with 2-Acetylpyridine Schiff Bases of S-Methyldithiocarbazate or 4-Phenyl 3-thiosemicarbazide

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Table S1. CIF file for [Cd(acpy-mdtc)$_2$](1)

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 'C18 H20 Cd N6 S4'
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_shelx_space_group_comment
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The symmetry employed for this shelxl refinement is
uniquely defined by the following loop, which should always
be used as a source of symmetry information in preference to
the above space-group names.
They are only intended as comments.
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 '-x, -y, -z'

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_reflns_special_details
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Reflections were merged by SHELXL according to the crys-
tal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of
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Friedel pairs measured divided by the number that would
be possible theoretically, ignoring centric projections and
systematic absences.
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H4 H -0.1186 0.8014 0.5393 0.040 Uiso 1 1 calc R U . . .
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N3 N 0.35184(19) 0.69044(13) 0.34595(11) 0.0291(3) Uani
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C8 C 0.1587(3) 0.6921(2) 0.49777(16) 0.0485(5) Uani
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H8B H 0.1789 0.7515 0.5588 0.073 Uiso 1 1 calc R U . . .
H8C H 0.2630 0.6514 0.4890 0.073 Uiso 1 1 calc R U . . .
S2 S 0.61529(6) 0.60097(5) 0.26794(4) 0.03874(11) Uani
1 1 d . . . . .
C9 C 0.6225(3) 0.5409(2) 0.38075(18) 0.0497(5) Uani
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H9B H 0.7343 0.5099 0.3935 0.075 Uiso 1 1 calc R U . . .
H9C H 0.5258 0.4716 0.3764 0.075 Uiso 1 1 calc R U . . .
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C15 C -0.1385(2) 0.97602(17) 0.08098(12) 0.0287(3) Uani
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N6 N 0.01593(19) 1.14920(13) 0.18234(11) 0.0301(3) Uani
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S3 S 0.34087(6) 1.11434(4) 0.26806(4) 0.03651(10) Uani
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C17 C -0.2625(3) 1.0584(2) 0.04255(17) 0.0481(5) Uani
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H17B H -0.3030 1.0253 -0.0255 0.072 Uiso 1 1 calc R U . . .
H17C H -0.2014 1.1449 0.0492 0.072 Uiso 1 1 calc R U . . .
S4 S 0.19456(8) 1.35254(5) 0.29369(4) 0.04573(13) Uani
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0.01057(5)
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0.0096(6)
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0.0143(8)
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0.0188(9)
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C7 0.0266(8) 0.0231(8) 0.0341(9) 0.0030(7) 0.0003(7) 0.0071(6)
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C8 0.0599(14) 0.0598(13) 0.0409(11) 0.0305(10) 0.0175(10) 0.0293(11)
S2 0.0306(2) 0.0387(2) 0.0493(3) 0.0063(2) 0.0046(2) 0.01592(19)
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C10 0.0703(15) 0.0322(10) 0.0467(12) 0.0036(9) 0.0086(11) 0.0028(10)
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S3 0.0309(2) 0.0365(2) 0.0407(3) 0.0121(2) -0.00698(19) 0.00202(18)
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S4 0.0568(3) 0.0281(2) 0.0496(3) 0.0040(2) 0.0057(2) 0.0002(2)
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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.
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N5 N6 1.388(2) . ?
N6 C16 1.301(2) . ?
C16 S3 1.7282(18) . ?
C16 S4 1.7550(18) . ?
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C7 N3 N2 113.99(13) . . ?
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H8B C8 H8C 109.5 . . ?
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S2 C9 H9B 109.5 . . ?
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C13 C14 C15 122.75(18) . . ?
N5 C15 C14 116.13(15) . . ?
N5 C15 C17 123.32(17) . . ?
C14 C15 C17 120.49(16) . . ?
C15 N5 N6 116.17(14) . . ?
C15 N5 Cd1 122.04(12) . . ?
N6 N5 Cd1 120.36(10) . . ?
C16 N6 N5 113.63(14) . . ?
N6 C16 S3 130.37(14) . . ?
N6 C16 S4 116.43(13) . . ?
S3 C16 S4 113.19(10) . . ?
C16 S3 Cd1 94.99(6) . . ?
C15 C17 H17A 109.5 . . ?
C15 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
C15 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
C16 S4 C18 102.63(10) . . ?
S4 C18 H18A 109.5 . . ?
S4 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
S4 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?

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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
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Cd1 N1 C1 C2 179.88(15) . . . . ?
N1 C1 C2 C3 1.6(3) . . . . ?
C1 C2 C3 C4 -1.1(3) . . . . ?
C2 C3 C4 C5 -0.8(3) . . . . ?
C1 N1 C5 C4 -2.0(3) . . . . ?
Cd1 N1 C5 C4 178.05(13) . . . . ?
C1 N1 C5 C6 176.68(16) . . . . ?
Cd1 N1 C5 C6 -3.26(19) . . . . ?
C3 C4 C5 N1 2.5(3) . . . . ?
C3 C4 C5 C6 -176.16(17) . . . . ?
N1 C5 C6 N2 -0.9(2) . . . . ?
C4 C5 C6 N2 177.84(16) . . . . ?
N1 C5 C6 C8 -179.51(17) . . . . ?
C4 C5 C6 C8 -0.8(3) . . . . ?
C5 C6 N2 N3 -178.65(14) . . . . ?
C8 C6 N2 N3 0.0(3) . . . . ?
C5 C6 N2 Cd1 4.9(2) . . . . ?
C8 C6 N2 Cd1 -176.51(15) . . . . ?
C6 N2 N3 C7 176.27(15) . . . . ?
Cd1 N2 N3 C7 -7.26(19) . . . . ?
N2 N3 C7 S1 -1.3(2) . . . . ?
N2 N3 C7 S2 178.31(11) . . . . ?
N3 C7 S1 Cd1 7.29(18) . . . . ?
S2 C7 S1 Cd1 -172.34(8) . . . . ?
N3 C7 S2 C9 1.28(17) . . . . ?
S1 C7 S2 C9 -179.04(11) . . . . ?
C14 N4 C10 C11 0.1(3) . . . . ?
Cd1 N4 C10 C11 179.43(17) . . . . ?
N4 C10 C11 C12 1.2(4) . . . . ?
C10 C11 C12 C13 -1.2(3) . . . . ?
C11 C12 C13 C14 0.0(3) . . . . ?
C10 N4 C14 C13 -1.3(3) . . . . ?
Cd1 N4 C14 C13 179.30(13) . . . . ?
C10 N4 C14 C15 177.83(17) . . . . ?
Cd1 N4 C14 C15 -1.58(19) . . . . ?
C12 C13 C14 N4 1.3(3) . . . . ?
C12 C13 C14 C15 -177.78(18) . . . . ?
N4 C14 C15 N5 5.5(2) . . . . ?
C13 C14 C15 N5 -175.40(17) . . . . ?
N4 C14 C15 C17 -171.66(17) . . . . ?
C13 C14 C15 C17 7.4(3) . . . . ?
C14 C15 N5 N6 -173.41(14) . . . . ?
C17 C15 N5 N6 3.7(2) . . . . ?
C14 C15 N5 Cd1 -7.0(2) . . . . ?
C17 C15 N5 Cd1 170.06(14) . . . . ?
C15 N5 N6 C16 -172.95(15) . . . . ?
Cd1 N5 N6 C16 20.40(18) . . . . ?
N5 N6 C16 S3 4.4(2) . . . . ?
N5 N6 C16 S4 -177.03(11) . . . . ?
N6 C16 S3 Cd1 -21.31(17) . . . . ?

S4 C16 S3 Cd1 160.10(8) . . . . ?
N6 C16 S4 C18 -2.47(17) . . . . ?
S3 C16 S4 C18 176.32(12) . . . . ?

_refine_diff_density_max 0.390
_refine_diff_density_min -0.337
_refine_diff_density_rms 0.061

Table S2. CIF file for [Cd(acpy-phTsc)2](2)
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_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety 'C28 H26 Cd N8 S2'
_chemical_formula_sum
'C28 H26 Cd N8 S2'
_chemical_formula_weight 651.09

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_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' 0.0000 0.0000
'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'
'S' 'S' 0.1246 0.1234
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Cd' 'Cd' -0.8075 1.2024
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_space_group_crystal_system triclinic
_space_group_IT_number 2
_space_group_name_H-M_alt 'P -1'
_space_group_name_Hall '-P 1'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names. They are only intended as comments.
;

loop_
_space_group_symop_operation_xyz
'x, y, z'
'-x, -y, -z'

_cell_length_a 9.7622(4)
_cell_length_b 11.2798(3)
_cell_length_c 13.2904(5)
_cell_angle_alpha 88.4409(12)
_cell_angle_beta 86.0103(13)
_cell_angle_gamma 78.0000(13)
_cell_volume 1427.91(9)
_cell_formula_units_Z 2
_cell_measurement_temperature 223(2)
_cell_measurement_reflns_used 9926
_cell_measurement_theta_min 2.39
_cell_measurement_theta_max 28.29

_exptl_crystal_description Block
_exptl_crystal_colour yellow
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?
_exptl_crystal_density_diffrn 1.514
_exptl_crystal_F_000 660
_exptl_transmission_factor_min ?
_exptl_transmission_factor_max ?
_exptl_crystal_size_max 0.180
_exptl_crystal_size_mid 0.100
_exptl_crystal_size_min 0.080
_exptl_absorpt_coefficient_mu 0.944
_shelx_estimated_absorpt_T_min 0.848
_shelx_estimated_absorpt_T_max 0.928
_exptl_absorpt_correction_type Multi-scan
_exptl_absorpt_correction_T_min 0.6975
_exptl_absorpt_correction_T_max 0.7457
_exptl_absorpt_process_details 'Bruker SADABS'
_exptl_absorpt_special_details ?
_diffrn_ambient_temperature 223(2)
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type MoK\a
_diffrn_source ?
_diffrn_measurement_device_type 'PHOTON 100 CMOS'
_diffrn_measurement_method '\f and \w scans'
_diffrn_detector_area_resol_mean ?
_diffrn_reflns_number 47747

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_diffrn_reflns_av_unetI/netI 0.0482
_diffrn_reflns_av_R_equivalents 0.0809
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_diffrn_reflns_limit_h_max 13
_diffrn_reflns_limit_k_min -14
_diffrn_reflns_limit_k_max 15
_diffrn_reflns_limit_l_min -17
_diffrn_reflns_limit_l_max 17
_diffrn_reflns_theta_min 2.137
_diffrn_reflns_theta_max 28.336
_diffrn_reflns_theta_full 25.242
_diffrn_measured_fraction_theta_max 0.998
_diffrn_measured_fraction_theta_full 0.999
_diffrn_reflns_Laue_measured_fraction_max 0.998
_diffrn_reflns_Laue_measured_fraction_full 0.999
_diffrn_reflns_point_group_measured_fraction_max 0.998
_diffrn_reflns_point_group_measured_fraction_full 0.999
_reflns_number_total 7098
_reflns_number_gt 5694
_reflns_threshold_expression 'I > 2\s(I)'
_reflns_Friedel_coverage 0.000
_reflns_Friedel_fraction_max .
_reflns_Friedel_fraction_full .

_reflns_special_details
;
 Reflections were merged by SHELXL according to the
crystal class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of
unique
 Friedel pairs measured divided by the number that would
be possible theoretically, ignoring centric projections and
systematic absences.
;

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_computing_cell_refinement 'Bruker SAINT'
_computing_data_reduction 'Bruker SAINT'
_computing_structure_solution 'Bruker SHELXTL'
_computing_structure_refinement 'SHELXL-2014/7
(Sheldrick, 2014)'
_computing_molecular_graphics 'Bruker SHELXTL'
_computing_publication_material 'Bruker SHELXTL'
_refine_special_details ?
_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary ?
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_refine_ls_extinction_method none
_refine_ls_extinction_coef .
_refine_ls_number_reflns 7098
_refine_ls_number_parameters 354
_refine_ls_number_restraints 0
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 _atom_site_disorder_group
Cd1 Cd 0.65377(2) 0.72100(2) 0.74009(2) 0.02424(6)
Uani 1 1 d . . . . .
N1 N 0.6146(2) 0.91777(19) 0.65937(16) 0.0286(5) Uani
1 1 d . . . . .
C1 C 0.6744(3) 0.9416(3) 0.5697(2) 0.0354(7) Uani
1 1 d . . . . .
H1 H 0.7344 0.8777 0.5347 0.043 Uiso 1 1 calc R U . . .
C2 C 0.6519(3) 1.0561(3) 0.5260(2) 0.0402(7) Uani
1 1 d . . . . .
H2 H 0.6962 1.0697 0.4630 0.048 Uiso 1 1 calc R U . . .
C3 C 0.5642(4) 1.1486(3) 0.5763(2) 0.0442(8) Uani
1 1 d . . . . .
H3 H 0.5472 1.2273 0.5483 0.053 Uiso 1 1 calc R U . . .
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C4 C 0.5004(3) 1.1257(2) 0.6685(2) 0.0382(7) Uani
1 1 d . . . . .
H4 H 0.4392 1.1886 0.7038 0.046 Uiso 1 1 calc R U . . .
C5 C 0.5274(3) 1.0091(2) 0.7090(2) 0.0278(6) Uani
1 1 d . . . . .
C6 C 0.4622(3) 0.9794(2) 0.8084(2) 0.0273(6) Uani
1 1 d . . . . .
N2 N 0.4972(2) 0.86845(18) 0.83994(15) 0.0241(5) Uani
1 1 d . . . . .
N3 N 0.4365(2) 0.84174(19) 0.93231(16) 0.0261(5) Uani
1 1 d . . . . .
C7 C 0.4715(3) 0.7277(2) 0.95990(18) 0.0234(5) Uani
1 1 d . . . . .
S1 S 0.58235(8) 0.60762(6) 0.89694(5) 0.03275(17) Uani
1 1 d . . . . .
C8 C 0.3630(4) 1.0756(3) 0.8677(2) 0.0465(8) Uani
1 1 d . . . . .
H8A H 0.2671 1.0711 0.8562 0.070 Uiso 1 1 calc R U . . .
H8B H 0.3794 1.1546 0.8463 0.070 Uiso 1 1 calc R U . . .
H8C H 0.3781 1.0634 0.9389 0.070 Uiso 1 1 calc R U . . .
N4 N 0.4153(3) 0.6925(2) 1.04996(16) 0.0308(5) Uani
1 1 d . . . . .
H4N H 0.4431 0.6158 1.0639 0.037 Uiso 1 1 calc R U . . .
C9 C 0.3214(3) 0.7559(2) 1.12469(19) 0.0285(6) Uani
1 1 d . . . . .
C10 C 0.2516(3) 0.8750(3) 1.1184(2) 0.0378(7) Uani
1 1 d . . . . .
H10 H 0.2670 0.9225 1.0611 0.045 Uiso 1 1 calc R U . . .
C11 C 0.1586(4) 0.9241(3) 1.1973(2) 0.0479(8) Uani
1 1 d . . . . .
H11 H 0.1103 1.0051 1.1925 0.057 Uiso 1 1 calc R U . . .
C12 C 0.1353(4) 0.8575(3) 1.2820(2) 0.0486(8) Uani
1 1 d . . . . .
H12 H 0.0713 0.8921 1.3346 0.058 Uiso 1 1 calc R U . . .
C13 C 0.2066(4) 0.7394(3) 1.2891(2) 0.0457(8) Uani
1 1 d . . . . .
H13 H 0.1923 0.6931 1.3473 0.055 Uiso 1 1 calc R U . . .
C14 C 0.2987(3) 0.6887(3) 1.2118(2) 0.0359(7) Uani
1 1 d . . . . .
H14 H 0.3472 0.6078 1.2175 0.043 Uiso 1 1 calc R U . . .
N5 N 0.8678(2) 0.74299(19) 0.80506(16) 0.0288(5) Uani
1 1 d . . . . .
C15 C 0.8787(3) 0.7682(3) 0.9010(2) 0.0372(7) Uani
1 1 d . . . . .
H15 H 0.7997 0.7720 0.9463 0.045 Uiso 1 1 calc R U . . .
C16 C 1.0004(4) 0.7890(3) 0.9369(2) 0.0448(8) Uani
1 1 d . . . . .
H16 H 1.0050 0.8061 1.0052 0.054 Uiso 1 1 calc R U . . .
C17 C 1.1148(4) 0.7842(3) 0.8698(3) 0.0479(8) Uani
1 1 d . . . . .
H17 H 1.1993 0.7989 0.8917 0.058 Uiso 1 1 calc R U . . .
C18 C 1.1051(3) 0.7576(3) 0.7700(2) 0.0393(7) Uani
1 1 d . . . . .
H18 H 1.1826 0.7545 0.7233 0.047 Uiso 1 1 calc R U . . .
C19 C 0.9799(3) 0.7354(2) 0.7394(2) 0.0277(6) Uani
1 1 d . . . . .
C20 C 0.9630(3) 0.7012(2) 0.6345(2) 0.0287(6) Uani
1 1 d . . . . .
N6 N 0.8456(2) 0.67273(19) 0.61859(15) 0.0264(5) Uani
1 1 d . . . . .
N7 N 0.8275(2) 0.6412(2) 0.52136(16) 0.0294(5) Uani
1 1 d . . . . .
C21 C 0.7090(3) 0.6060(2) 0.51201(19) 0.0281(6) Uani
1 1 d . . . . .
S2 S 0.57633(9) 0.59405(7) 0.60506(5) 0.03629(18) Uani
1 1 d . . . . .
C22 C 1.0770(3) 0.7001(3) 0.5533(2) 0.0485(8) Uani
1 1 d . . . . .
H22A H 1.0815 0.6319 0.5095 0.073 Uiso 1 1 calc R U . . .
H22B H 1.1661 0.6929 0.5835 0.073 Uiso 1 1 calc R U . . .
H22C H 1.0574 0.7750 0.5143 0.073 Uiso 1 1 calc R U . . .
N8 N 0.6800(3) 0.5739(2) 0.41869(16) 0.0315(5) Uani
1 1 d . . . . .
H8N H 0.6018 0.5486 0.4178 0.038 Uiso 1 1 calc R U . . .
C23 C 0.7535(3) 0.5740(2) 0.32336(19) 0.0301(6) Uani
1 1 d . . . . .
C24 C 0.8819(4) 0.6038(4) 0.3049(2) 0.0588(10) Uani
1 1 d . . . . .
H24 H 0.9289 0.6268 0.3581 0.071 Uiso 1 1 calc R U . . .
C25 C 0.9424(4) 0.5999(4) 0.2068(3) 0.0699(12) Uani
1 1 d . . . . .
H25 H 1.0307 0.6204 0.1943 0.084 Uiso 1 1 calc R U . . .
C26 C 0.8760(4) 0.5668(3) 0.1281(2) 0.0500(9) Uani
1 1 d . . . . .
H26 H 0.9176 0.5653 0.0620 0.060 Uiso 1 1 calc R U . . .
C27 C 0.7491(4) 0.5362(3) 0.1467(2) 0.0438(8) Uani
1 1 d . . . . .
H27 H 0.7029 0.5125 0.0933 0.053 Uiso 1 1 calc R U . . .
C28 C 0.6879(3) 0.5397(3) 0.2432(2) 0.0369(7) Uani
1 1 d . . . . .
H28 H 0.5999 0.5184 0.2550 0.044 Uiso 1 1 calc R U . . .

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_atom_site_aniso_U_22
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_atom_site_aniso_U_23

_atom_site_aniso_U_13
_atom_site_aniso_U_12
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N1 0.0358(14) 0.0268(12) 0.0233(11) 0.0034(9) -0.0017(10) -0.0072(10)
C1 0.0441(19) 0.0347(15) 0.0270(15) 0.0019(12) 0.0015(13) -0.0087(13)
C2 0.049(2) 0.0440(18) 0.0300(16) 0.0136(13) -0.0022(14) -0.0173(15)
C3 0.059(2) 0.0335(16) 0.0392(18) 0.0151(13) -0.0054(16) -0.0094(15)
C4 0.0448(19) 0.0256(14) 0.0422(18) 0.0047(12) -0.0019(14) -0.0034(13)
C5 0.0305(15) 0.0282(14) 0.0264(14) 0.0027(11) -0.0060(11) -0.0092(12)
C6 0.0283(15) 0.0276(14) 0.0273(14) -0.0004(11) -0.0022(11) -0.0084(11)
N2 0.0255(12) 0.0267(11) 0.0212(11) 0.0003(8) 0.0011(9) -0.0090(9)
N3 0.0297(13) 0.0269(11) 0.0213(11) 0.0003(9) 0.0047(9) -0.0069(9)
C7 0.0265(14) 0.0275(13) 0.0171(12) -0.0023(10) 0.0015(10) -0.0083(11)
S1 0.0504(5) 0.0242(3) 0.0210(3) -0.0002(3) 0.0112(3) -0.0061(3)
C8 0.053(2) 0.0342(16) 0.0458(19) -0.0008(14) 0.0118(16) 0.0005(15)
N4 0.0409(15) 0.0262(11) 0.0231(12) -0.0003(9) 0.0089(10) -0.0056(10)
C9 0.0296(15) 0.0335(14) 0.0236(13) -0.0048(11) 0.0045(11) -0.0110(12)
C10 0.0440(19) 0.0364(16) 0.0312(16) -0.0009(12) 0.0047(13) -0.0061(14)
C11 0.050(2) 0.0406(18) 0.047(2) -0.0091(15) 0.0127(16) -0.0003(15)
C12 0.046(2) 0.057(2) 0.0406(19) -0.0132(16) 0.0195(15) -0.0096(16)
C13 0.056(2) 0.054(2) 0.0291(16) -0.0030(14) 0.0160(15) -0.0203(17)
C14 0.0443(19) 0.0357(15) 0.0280(15) -0.0016(12) 0.0086(13) -0.0126(13)
N5 0.0339(14) 0.0321(12) 0.0214(11) -0.0027(9) -0.0009(10) -0.0093(10)
C15 0.0436(19) 0.0463(17) 0.0233(14) -0.0050(12) -0.0005(13) -0.0128(14)
C16 0.051(2) 0.0530(19) 0.0333(17) -0.0054(14) -0.0144(15) -0.0130(16)
C17 0.0381(19) 0.062(2) 0.048(2) -0.0059(16) -0.0170(16) -0.0150(16)
C18 0.0302(17) 0.0477(18) 0.0408(18) -0.0018(14) -0.0035(14) -0.0092(14)
C19 0.0292(15) 0.0266(13) 0.0267(14) -0.0002(10) -0.0021(11) -0.0042(11)
C20 0.0295(16) 0.0295(14) 0.0257(14) -0.0011(11) 0.0023(11) -0.0039(12)
N6 0.0303(13) 0.0296(11) 0.0186(11) -0.0021(9) 0.0004(9) -0.0052(10)
N7 0.0329(14) 0.0364(12) 0.0185(11) -0.0062(9) 0.0006(10) -0.0064(10)
C21 0.0375(17) 0.0250(13) 0.0208(13) -0.0032(10) 0.0018(11) -0.0050(12)
S2 0.0501(5) 0.0462(4) 0.0191(3) -0.0057(3) 0.0051(3) -0.0270(4)
C22 0.0383(19) 0.071(2) 0.0370(18) -0.0051(16) 0.0094(15) -0.0158(17)
N8 0.0350(14) 0.0432(14) 0.0191(11) -0.0063(10) 0.0024(10) -0.0151(11)
C23 0.0404(17) 0.0315(14) 0.0171(13) -0.0029(10) 0.0037(11) -0.0062(12)
C24 0.060(2) 0.098(3) 0.0287(17) -0.0198(18) 0.0091(16) -0.043(2)
C25 0.066(3) 0.117(3) 0.039(2) -0.018(2) 0.0205(19) -0.053(3)
C26 0.064(2) 0.062(2) 0.0226(16) -0.0045(14) 0.0131(15) -0.0136(18)
C27 0.053(2) 0.058(2) 0.0185(14) -0.0047(13) -0.0040(14) -0.0058(16)
C28 0.0377(18) 0.0512(18) 0.0211(14) -0.0036(12) -0.0008(12) -0.0079(14)

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;
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.
;

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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2

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Cd1 N2 2.376(2) . ?
Cd1 N5 2.377(2) . ?
Cd1 N1 2.408(2) . ?
Cd1 S1 2.5477(7) . ?
Cd1 S2 2.5732(7) . ?
N1 C1 1.336(3) . ?
N1 C5 1.347(3) . ?
C1 C2 1.382(4) . ?
C1 H1 0.9400 . ?
C2 C3 1.362(4) . ?
C2 H2 0.9400 . ?
C3 C4 1.378(4) . ?
C3 H3 0.9400 . ?
C4 C5 1.387(4) . ?
C4 H4 0.9400 . ?
C5 C6 1.488(4) . ?
C6 N2 1.293(3) . ?
C6 C8 1.497(4) . ?
N2 N3 1.379(3) . ?
N3 C7 1.310(3) . ?
C7 N4 1.365(3) . ?
C7 S1 1.741(3) . ?
C8 H8A 0.9700 . ?
C8 H8B 0.9700 . ?
C8 H8C 0.9700 . ?
N4 C9 1.406(3) . ?
N4 H4N 0.8700 . ?
C9 C10 1.377(4) . ?
C9 C14 1.397(4) . ?
C10 C11 1.386(4) . ?
C10 H10 0.9400 . ?
C11 C12 1.368(5) . ?
C11 H11 0.9400 . ?
C12 C13 1.373(5) . ?
C12 H12 0.9400 . ?
C13 C14 1.372(4) . ?
C13 H13 0.9400 . ?
C14 H14 0.9400 . ?
N5 C15 1.330(3) . ?
N5 C19 1.341(3) . ?
C15 C16 1.377(4) . ?
C15 H15 0.9400 . ?
C16 C17 1.372(5) . ?
C16 H16 0.9400 . ?
C17 C18 1.382(4) . ?
C17 H17 0.9400 . ?
C18 C19 1.387(4) . ?
C18 H18 0.9400 . ?
C19 C20 1.486(4) . ?
C20 N6 1.286(3) . ?
C20 C22 1.493(4) . ?
N6 N7 1.382(3) . ?
N7 C21 1.313(4) . ?
C21 N8 1.366(3) . ?
C21 S2 1.751(3) . ?
C22 H22A 0.9700 . ?
C22 H22B 0.9700 . ?
C22 H22C 0.9700 . ?
N8 C23 1.412(3) . ?
N8 H8N 0.8700 . ?
C23 C24 1.368(4) . ?
C23 C28 1.384(4) . ?
C24 C25 1.392(4) . ?
C24 H24 0.9400 . ?
C25 C26 1.367(5) . ?
C25 H25 0.9400 . ?
C26 C27 1.359(5) . ?
C26 H26 0.9400 . ?
C27 C28 1.375(4) . ?
C27 H27 0.9400 . ?
C28 H28 0.9400 . ?

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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
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N6 Cd1 N5 68.15(7) . . ?
N2 Cd1 N5 98.57(7) . . ?
N6 Cd1 N1 84.60(7) . . ?
N2 Cd1 N1 68.19(7) . . ?
N5 Cd1 N1 93.65(8) . . ?
N6 Cd1 S1 131.75(5) . . ?
N2 Cd1 S1 74.35(5) . . ?
N5 Cd1 S1 93.03(6) . . ?
N1 Cd1 S1 142.53(6) . . ?
N6 Cd1 S2 73.50(6) . . ?
N2 Cd1 S2 124.08(6) . . ?
N5 Cd1 S2 137.33(6) . . ?
N1 Cd1 S2 100.80(6) . . ?
S1 Cd1 S2 98.91(2) . . ?
C1 N1 C5 118.5(2) . . ?
```

C1 N1 Cd1 124.22(19) . . ?
C5 N1 Cd1 117.26(16) . . ?
N1 C1 C2 122.9(3) . . ?
N1 C1 H1 118.5 . . ?
C2 C1 H1 118.5 . . ?
C3 C2 C1 118.6(3) . . ?
C3 C2 H2 120.7 . . ?
C1 C2 H2 120.7 . . ?
C2 C3 C4 119.4(3) . . ?
C2 C3 H3 120.3 . . ?
C4 C3 H3 120.3 . . ?
C3 C4 C5 119.5(3) . . ?
C3 C4 H4 120.2 . . ?
C5 C4 H4 120.2 . . ?
N1 C5 C4 121.0(3) . . ?
N1 C5 C6 117.1(2) . . ?
C4 C5 C6 121.8(3) . . ?
N2 C6 C5 116.6(2) . . ?
N2 C6 C8 123.0(2) . . ?
C5 C6 C8 120.4(2) . . ?
C6 N2 N3 116.2(2) . . ?
C6 N2 Cd1 120.77(17) . . ?
N3 N2 Cd1 122.99(15) . . ?
C7 N3 N2 114.2(2) . . ?
N3 C7 N4 118.3(2) . . ?
N3 C7 S1 129.25(19) . . ?
N4 C7 S1 112.42(18) . . ?
C7 S1 Cd1 99.19(8) . . ?
C6 C8 H8A 109.5 . . ?
C6 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
C6 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
C7 N4 C9 132.7(2) . . ?
C7 N4 H4N 113.7 . . ?
C9 N4 H4N 113.7 . . ?
C10 C9 C14 118.9(3) . . ?
C10 C9 N4 125.9(2) . . ?
C14 C9 N4 115.2(2) . . ?
C9 C10 C11 119.3(3) . . ?
C9 C10 H10 120.3 . . ?
C11 C10 H10 120.4 . . ?
C12 C11 C10 121.6(3) . . ?
C12 C11 H11 119.2 . . ?
C10 C11 H11 119.2 . . ?
C11 C12 C13 119.1(3) . . ?
C11 C12 H12 120.5 . . ?
C13 C12 H12 120.5 . . ?
C14 C13 C12 120.3(3) . . ?
C14 C13 H13 119.8 . . ?
C12 C13 H13 119.8 . . ?
C13 C14 C9 120.7(3) . . ?
C13 C14 H14 119.6 . . ?
C9 C14 H14 119.6 . . ?
C15 N5 C19 119.4(2) . . ?
C15 N5 Cd1 123.2(2) . . ?
C19 N5 Cd1 117.31(17) . . ?
N5 C15 C16 123.0(3) . . ?
N5 C15 H15 118.5 . . ?
C16 C15 H15 118.5 . . ?
C17 C16 C15 118.0(3) . . ?
C17 C16 H16 121.0 . . ?
C15 C16 H16 121.0 . . ?
C16 C17 C18 119.6(3) . . ?
C16 C17 H17 120.2 . . ?
C18 C17 H17 120.2 . . ?
C17 C18 C19 119.3(3) . . ?
C17 C18 H18 120.3 . . ?
C19 C18 H18 120.3 . . ?
N5 C19 C18 120.6(3) . . ?
N5 C19 C20 116.9(2) . . ?
C18 C19 C20 122.5(3) . . ?
N6 C20 C19 116.1(2) . . ?
N6 C20 C22 122.6(3) . . ?
C19 C20 C22 121.3(3) . . ?
C20 N6 N7 117.0(2) . . ?
C20 N6 Cd1 119.65(17) . . ?
N7 N6 Cd1 121.64(16) . . ?
C21 N7 N6 113.6(2) . . ?
N7 C21 N8 118.4(2) . . ?
N7 C21 S2 128.7(2) . . ?
N8 C21 S2 112.9(2) . . ?
C21 S2 Cd1 97.46(9) . . ?
C20 C22 H22A 109.5 . . ?
C20 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
C20 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
C21 N8 C23 131.9(2) . . ?
C21 N8 H8N 114.0 . . ?
C23 N8 H8N 114.0 . . ?
C24 C23 C28 118.6(3) . . ?
C24 C23 N8 125.7(3) . . ?
C28 C23 N8 115.7(3) . . ?
C23 C24 C25 119.6(3) . . ?
C23 C24 H24 120.2 . . ?

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C25 C24 H24 120.2 . . ?
C26 C25 C24 121.3(3) . . ?
C26 C25 H25 119.4 . . ?
C24 C25 H25 119.4 . . ?
C27 C26 C25 119.1(3) . . ?
C27 C26 H26 120.5 . . ?
C25 C26 H26 120.5 . . ?
C26 C27 C28 120.4(3) . . ?
C26 C27 H27 119.8 . . ?
C28 C27 H27 119.8 . . ?
C27 C28 C23 121.1(3) . . ?
C27 C28 H28 119.4 . . ?
C23 C28 H28 119.4 . . ?

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 _geom_torsion_site_symmetry_2
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N1 C1 C2 C3 -0.4(5) . . . . ?
C1 C2 C3 C4 -0.1(5) . . . . ?
C2 C3 C4 C5 0.5(5) . . . . ?
C1 N1 C5 C4 -0.4(4) . . . . ?
Cd1 N1 C5 C4 179.2(2) . . . . ?
C1 N1 C5 C6 179.8(2) . . . . ?
Cd1 N1 C5 C6 -0.7(3) . . . . ?
C3 C4 C5 N1 -0.2(5) . . . . ?
C3 C4 C5 C6 179.7(3) . . . . ?
N1 C5 C6 N2 1.4(4) . . . . ?
C4 C5 C6 N2 -178.4(3) . . . . ?
N1 C5 C6 C8 -179.4(3) . . . . ?
C4 C5 C6 C8 0.8(4) . . . . ?
C5 C6 N2 N3 179.8(2) . . . . ?
C8 C6 N2 N3 0.7(4) . . . . ?
C5 C6 N2 Cd1 -1.4(3) . . . . ?
C8 C6 N2 Cd1 179.4(2) . . . . ?
C6 N2 N3 C7 178.0(2) . . . . ?
Cd1 N2 N3 C7 -0.7(3) . . . . ?
N2 N3 C7 N4 -179.4(2) . . . . ?
N2 N3 C7 S1 0.1(4) . . . . ?
N3 C7 S1 Cd1 0.4(3) . . . . ?
N4 C7 S1 Cd1 179.89(18) . . . . ?
N3 C7 N4 C9 0.3(5) . . . . ?
S1 C7 N4 C9 -179.3(2) . . . . ?
C7 N4 C9 C10 6.1(5) . . . . ?
C7 N4 C9 C14 -174.4(3) . . . . ?
C14 C9 C10 C11 -1.5(5) . . . . ?
N4 C9 C10 C11 178.0(3) . . . . ?
C9 C10 C11 C12 0.7(5) . . . . ?
C10 C11 C12 C13 0.4(6) . . . . ?
C11 C12 C13 C14 -0.7(5) . . . . ?
C12 C13 C14 C9 -0.1(5) . . . . ?
C10 C9 C14 C13 1.2(5) . . . . ?
N4 C9 C14 C13 -178.3(3) . . . . ?
C19 N5 C15 C16 1.0(4) . . . . ?
Cd1 N5 C15 C16 -175.4(2) . . . . ?
N5 C15 C16 C17 0.5(5) . . . . ?
C15 C16 C17 C18 -0.7(5) . . . . ?
C16 C17 C18 C19 -0.4(5) . . . . ?
C15 N5 C19 C18 -2.1(4) . . . . ?
Cd1 N5 C19 C18 174.5(2) . . . . ?
C15 N5 C19 C20 177.1(2) . . . . ?
Cd1 N5 C19 C20 -6.3(3) . . . . ?
C17 C18 C19 N5 1.8(4) . . . . ?
C17 C18 C19 C20 -177.4(3) . . . . ?
N5 C19 C20 N6 -5.2(3) . . . . ?
C18 C19 C20 N6 174.0(3) . . . . ?
N5 C19 C20 C22 174.8(3) . . . . ?
C18 C19 C20 C22 -5.9(4) . . . . ?
C19 C20 N6 N7 179.7(2) . . . . ?
C22 C20 N6 N7 -0.4(4) . . . . ?
C19 C20 N6 Cd1 14.5(3) . . . . ?
C22 C20 N6 Cd1 -165.6(2) . . . . ?
C20 N6 N7 C21 176.0(2) . . . . ?
Cd1 N6 N7 C21 -19.2(3) . . . . ?
N6 N7 C21 N8 179.4(2) . . . . ?
N6 N7 C21 S2 -0.3(4) . . . . ?
N7 C21 S2 Cd1 15.5(3) . . . . ?
N8 C21 S2 Cd1 -164.27(18) . . . . ?
N7 C21 N8 C23 -2.4(4) . . . . ?
S2 C21 N8 C23 177.3(2) . . . . ?
C21 N8 C23 C24 3.4(5) . . . . ?
C21 N8 C23 C28 -177.2(3) . . . . ?
C28 C23 C24 C25 0.5(6) . . . . ?
N8 C23 C24 C25 179.9(3) . . . . ?
C23 C24 C25 C26 0.0(7) . . . . ?
C24 C25 C26 C27 -0.6(6) . . . . ?
C25 C26 C27 C28 0.7(5) . . . . ?
C26 C27 C28 C23 -0.1(5) . . . . ?
C24 C23 C28 C27 -0.5(5) . . . . ?
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N8 C23 C28 C27 -179.9(3) . . . . ?

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Table S3. CIF file for [Cd(acpy-mdtc)(NCS)]2(3)

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_shelx_SHELXL_version_number '2014/7'
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'C20 H20 Cd2 N8 S6'
_chemical_formula_weight 789.60

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'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'
'N' 'N' 0.0061 0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'S' 'S' 0.1246 0.1234
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Cd' 'Cd' -0.8075 1.2024
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_space_group_crystal_system monoclinic
_space_group_IT_number 15
_space_group_name_H-M_alt 'C 2/c'
_space_group_name_Hall '-C 2yc'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names.
They are only intended as comments.
;

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

_cell_length_a 18.3005(6)
_cell_length_b 10.9377(4)
_cell_length_c 15.0362(9)
_cell_angle_alpha 90
_cell_angle_beta 116.4921(10)
_cell_angle_gamma 90
_cell_volume 2693.7(2)
_cell_formula_units_Z 4
_cell_measurement_temperature 223(2)
_cell_measurement_reflns_used 9719
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_exptl_crystal_density_method ?
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_exptl_crystal_F_000 1552
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_exptl_transmission_factor_max ?
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_exptl_crystal_size_min 0.050
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_diffrn_radiation_type MoK\a
_diffrn_source ?
_diffrn_measurement_device_type 'PHOTON 100 CMOS'

_diffrn_measurement_method '\f and \w scans'
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_diffrn_reflns_theta_full 25.242
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_diffrn_measured_fraction_theta_full 1.000
_diffrn_reflns_Laue_measured_fraction_max 0.997
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_reflns_Friedel_fraction_max .
_reflns_Friedel_fraction_full .

_reflns_special_details
;
Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique
Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.
;

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_computing_cell_refinement 'Bruker SAINT'
_computing_data_reduction 'Bruker SAINT'
_computing_structure_solution 'Bruker SHELXTL'
_computing_structure_refinement 'SHELXL-2014/7 (Sheldrick, 2014)'
_computing_molecular_graphics 'Bruker SHELXTL'
_computing_publication_material 'Bruker SHELXTL'
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_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
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_atom_sites_solution_secondary ?
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_refine_ls_extinction_method none
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N1 N 0.25335(9) 0.49907(14) 0.14147(12) 0.0247(3) Uani 1 1 d . . . . .
C1 C 0.25237(12) 0.37764(18) 0.14474(15) 0.0308(4) Uani 1 1 d . . . . .
H1 H 0.2046 0.3367 0.1010 0.037 Uiso 1 1 calc R U . . .
C2 C 0.31774(12) 0.30865(19) 0.20893(15) 0.0308(4) Uani 1 1 d . . . . .
H2 H 0.3148 0.2228 0.2089 0.037 Uiso 1 1 calc R U . . .

C3 C 0.38740(13) 0.36908(19) 0.27313(15) 0.0323(4) Uani 1 1 d . . . . .
H3 H 0.4329 0.3250 0.3185 0.039 Uiso 1 1 calc R U . . .
C4 C 0.38963(12) 0.49562(18) 0.27010(15) 0.0292(4) Uani 1 1 d . . . . .
H4 H 0.4368 0.5383 0.3132 0.035 Uiso 1 1 calc R U . . .
C5 C 0.32164(10) 0.55877(17) 0.20289(13) 0.0215(4) Uani 1 1 d . . . . .
C6 C 0.32078(10) 0.69428(17) 0.19495(13) 0.0220(4) Uani 1 1 d . . . . .
N2 N 0.25622(9) 0.74092(14) 0.12440(11) 0.0227(3) Uani 1 1 d . . . . .
N3 N 0.25440(9) 0.86643(14) 0.11405(12) 0.0263(3) Uani 1 1 d . . . . .
C7 C 0.18393(10) 0.91001(16) 0.04968(13) 0.0215(4) Uani 1 1 d . . . . .
S1 S 0.09457(3) 0.83721(4) -0.02736(4) 0.02626(10) Uani 1 1 d . . . . .
C8 C 0.39178(11) 0.76749(18) 0.26621(15) 0.0317(4) Uani 1 1 d . . . . .
H8A H 0.4376 0.7570 0.2509 0.048 Uiso 1 1 calc R U . . .
H8B H 0.4070 0.7397 0.3335 0.048 Uiso 1 1 calc R U . . .
H8C H 0.3768 0.8532 0.2605 0.048 Uiso 1 1 calc R U . . .
S2 S 0.18995(3) 1.07093(5) 0.04943(4) 0.03039(11) Uani 1 1 d . . . . .
C9 C 0.09038(12) 1.11963(18) -0.03943(17) 0.0352(5) Uani 1 1 d . . . . .
H9A H 0.0769 1.0813 -0.1030 0.053 Uiso 1 1 calc R U . . .
H9B H 0.0900 1.2078 -0.0466 0.053 Uiso 1 1 calc R U . . .
H9C H 0.0504 1.0961 -0.0166 0.053 Uiso 1 1 calc R U . . .
S3 S 0.08460(3) 0.46952(5) -0.11432(4) 0.03060(11) Uani 1 1 d . . . . .
C10 C -0.00240(11) 0.44324(17) -0.10858(13) 0.0247(4) Uani 1 1 d . . . . .
N4 N -0.06310(10) 0.42354(17) -0.10628(13) 0.0333(4) Uani 1 1 d . . . . .

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N1 0.0208(7) 0.0228(8) 0.0256(8) -0.0006(6) 0.0061(6) -0.0034(6)
C1 0.0272(10) 0.0252(10) 0.0327(10) -0.0017(8) 0.0067(8) -0.0069(8)
C2 0.0343(10) 0.0220(10) 0.0332(11) 0.0021(8) 0.0124(9) -0.0004(8)
C3 0.0294(10) 0.0298(11) 0.0294(10) 0.0048(8) 0.0058(8) 0.0044(8)
C4 0.0226(9) 0.0288(10) 0.0271(10) -0.0016(8) 0.0030(8) -0.0020(8)
C5 0.0198(8) 0.0235(9) 0.0214(9) -0.0006(7) 0.0092(7) -0.0007(7)
C6 0.0174(8) 0.0246(9) 0.0226(9) -0.0018(7) 0.0078(7) -0.0027(7)
N2 0.0173(7) 0.0204(8) 0.0272(8) 0.0002(6) 0.0071(6) -0.0025(6)
N3 0.0209(7) 0.0198(8) 0.0317(9) 0.0002(6) 0.0060(6) -0.0032(6)
C7 0.0198(8) 0.0206(9) 0.0249(9) -0.0018(7) 0.0107(7) -0.0027(6)
S1 0.0177(2) 0.0228(2) 0.0304(2) -0.00069(18) 0.00367(18) -0.00123(17)
C8 0.0232(9) 0.0280(10) 0.0314(11) -0.0013(8) 0.0009(8) -0.0051(8)
S2 0.0261(2) 0.0199(2) 0.0389(3) -0.0011(2) 0.0088(2) -0.00206(18)
C9 0.0316(10) 0.0234(10) 0.0442(13) 0.0026(9) 0.0113(9) 0.0053(8)
S3 0.0237(2) 0.0370(3) 0.0317(3) -0.0090(2) 0.0129(2) -0.0074(2)
C10 0.0270(9) 0.0205(9) 0.0222(9) -0.0020(7) 0.0069(7) -0.0046(7)
N4 0.0287(9) 0.0355(10) 0.0348(9) -0.0046(8) 0.0133(7) -0.0106(7)

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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.
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Cd1 N1 2.3489(16) . ?
Cd1 S1 2.5526(5) . ?
Cd1 S3 2.5713(5) . ?
N1 C1 1.330(2) . ?
N1 C5 1.346(2) . ?
C1 C2 1.379(3) . ?
C1 H1 0.9400 . ?
C2 C3 1.377(3) . ?
C2 H2 0.9400 . ?
C3 C4 1.386(3) . ?
C3 H3 0.9400 . ?
C4 C5 1.387(3) . ?
C4 H4 0.9400 . ?
C5 C6 1.486(3) . ?
C6 N2 1.290(2) . ?
C6 C8 1.495(2) . ?
N2 N3 1.380(2) . ?
N3 C7 1.309(2) . ?
C7 S1 1.7205(18) . ?
C7 S2 1.7636(19) . ?
C8 H8A 0.9700 . ?
C8 H8B 0.9700 . ?
C8 H8C 0.9700 . ?
S2 C9 1.794(2) . ?
C9 H9A 0.9700 . ?
C9 H9B 0.9700 . ?
C9 H9C 0.9700 . ?
S3 C10 1.6575(19) . ?
C10 N4 1.147(2) . ?
N4 Cd1 2.2816(17) 5_565 ?

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N2 Cd1 S1 76.35(4) . . ?
N1 Cd1 S1 146.08(4) . . ?
N4 Cd1 S3 99.18(4) 5_565 . ?
N2 Cd1 S3 144.06(4) . . ?
N1 Cd1 S3 98.13(4) . . ?
S1 Cd1 S3 110.403(17) . . ?
C1 N1 C5 118.89(16) . . ?
C1 N1 Cd1 124.76(13) . . ?
C5 N1 Cd1 116.33(12) . . ?
N1 C1 C2 123.41(18) . . ?
N1 C1 H1 118.3 . . ?
C2 C1 H1 118.3 . . ?
C3 C2 C1 118.08(19) . . ?
C3 C2 H2 121.0 . . ?
C1 C2 H2 121.0 . . ?
C2 C3 C4 119.21(19) . . ?
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C4 C3 H3 120.4 . . ?
C3 C4 C5 119.41(18) . . ?
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N1 C5 C4 120.99(17) . . ?
N1 C5 C6 117.09(15) . . ?
C4 C5 C6 121.93(16) . . ?
N2 C6 C5 115.69(15) . . ?
N2 C6 C8 124.19(17) . . ?
C5 C6 C8 120.12(16) . . ?
C6 N2 N3 116.96(15) . . ?
C6 N2 Cd1 120.74(12) . . ?
N3 N2 Cd1 121.99(11) . . ?
C7 N3 N2 114.32(15) . . ?
N3 C7 S1 131.01(14) . . ?
N3 C7 S2 108.85(13) . . ?
S1 C7 S2 120.13(11) . . ?
C7 S1 Cd1 96.28(6) . . ?
C6 C8 H8A 109.5 . . ?
C6 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
C6 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
C7 S2 C9 104.73(9) . . ?
S2 C9 H9A 109.5 . . ?
S2 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
S2 C9 H9C 109.5 . . ?
H9A C9 H9C 109.5 . . ?
H9B C9 H9C 109.5 . . ?
C10 S3 Cd1 96.97(7) . . ?
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C1 C2 C3 C4 -0.8(3) . . . . ?
C2 C3 C4 C5 0.3(3) . . . . ?
C1 N1 C5 C4 -1.2(3) . . . . ?
Cd1 N1 C5 C4 -179.53(14) . . . . ?
C1 N1 C5 C6 178.48(17) . . . . ?
Cd1 N1 C5 C6 0.2(2) . . . . ?
C3 C4 C5 N1 0.7(3) . . . . ?
C3 C4 C5 C6 -178.98(18) . . . . ?
N1 C5 C6 N2 -4.9(2) . . . . ?
C4 C5 C6 N2 174.81(17) . . . . ?
N1 C5 C6 C8 175.02(16) . . . . ?
C4 C5 C6 C8 -5.3(3) . . . . ?
C5 C6 N2 N3 -178.80(15) . . . . ?
C8 C6 N2 N3 1.3(3) . . . . ?
C5 C6 N2 Cd1 7.5(2) . . . . ?
C8 C6 N2 Cd1 -172.47(14) . . . . ?
C6 N2 N3 C7 -172.03(16) . . . . ?
Cd1 N2 N3 C7 1.6(2) . . . . ?
N2 N3 C7 S1 -2.8(3) . . . . ?
N2 N3 C7 S2 177.18(12) . . . . ?
N3 C7 S1 Cd1 2.19(19) . . . . ?
S2 C7 S1 Cd1 -177.74(10) . . . . ?
N3 C7 S2 C9 -179.22(14) . . . . ?
S1 C7 S2 C9 0.72(15) . . . . ?

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Table S4. CIF file for $[Cd(acpy\text{-}phTsc)(NCS)_2]_2$(4)

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 'H' 'H' 0.0000 0.0000
 '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'
 'S' 'S' 0.1246 0.1234
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_space_group_name_H-M_alt 'P 21/c'
_space_group_name_Hall '-P 2ybc'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is
uniquely defined by the following loop, which should
always be used as a source of symmetry information in
preference to the above space-group names.
They are only intended as comments.
;

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

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_reflns_special_details
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Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique
Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.
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N1 N 0.5895(2) 0.08970(8) 0.32668(11) 0.0285(3) Uani
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C1 C 0.5399(3) 0.11246(11) 0.40870(15) 0.0364(4) Uani
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Uani 1 1 d . . . . .
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1 1 d . . . . .
N4 N 0.8641(2) -0.08012(9) 0.00950(10) 0.0283(3) Uani
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C8 C 0.9242(2) -0.14873(10) -0.02076(12) 0.0277(4) Uani
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C10 C 0.9624(3) -0.22132(13) -0.15912(16) 0.0469(5) Uani
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C13 C 0.9972(3) -0.20530(11) 0.03884(14) 0.0387(4) Uani
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S1 S 0.85432(7) -0.10768(2) 0.19589(3) 0.03163(10) Uani
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C14 C 0.5828(3) 0.15012(11) 0.06864(15) 0.0391(4) Uani
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H14B H 0.4774 0.1806 0.0711 0.059 Uiso 1 1 calc R U . . .
H14C H 0.5582 0.1169 0.0143 0.059 Uiso 1 1 calc R U . . .
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1 1 d . . . . .
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C5 0.0228(8) 0.0238(8) 0.0379(10) -0.0008(7) 0.0010(7) -0.0015(6)
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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.
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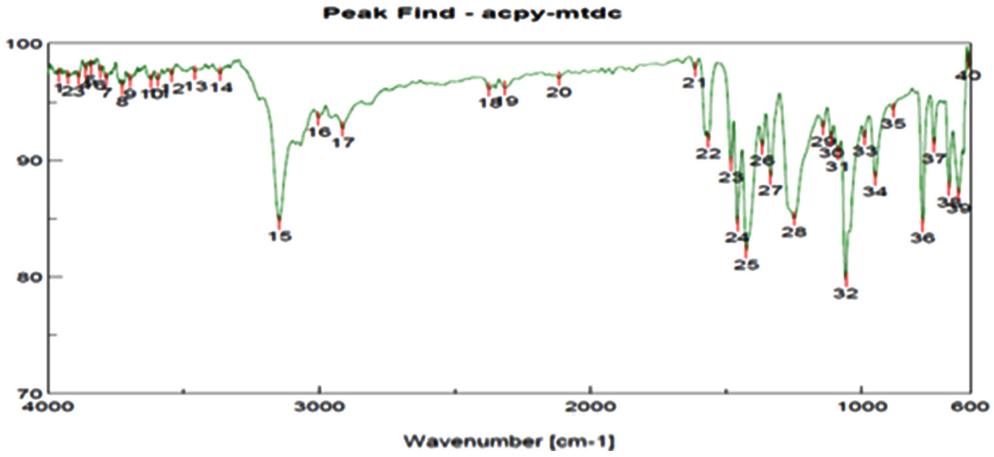

***Figure* S1.** IR spectrum of acpy-mdtcH.

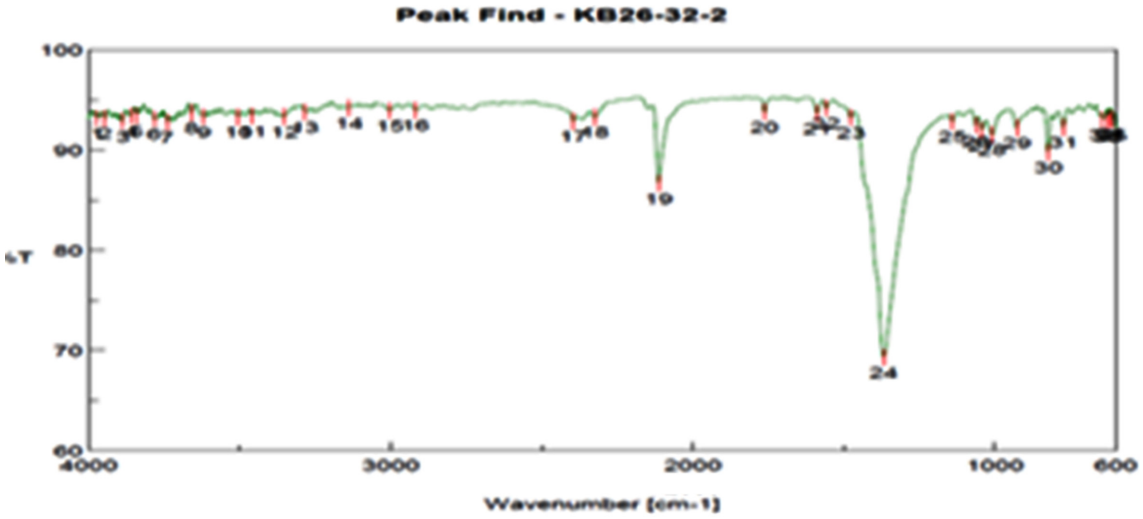

***Figure* S2.** IR spectrum of $[Cd(acpy\text{-}mdtc)(NCS)]_2$.

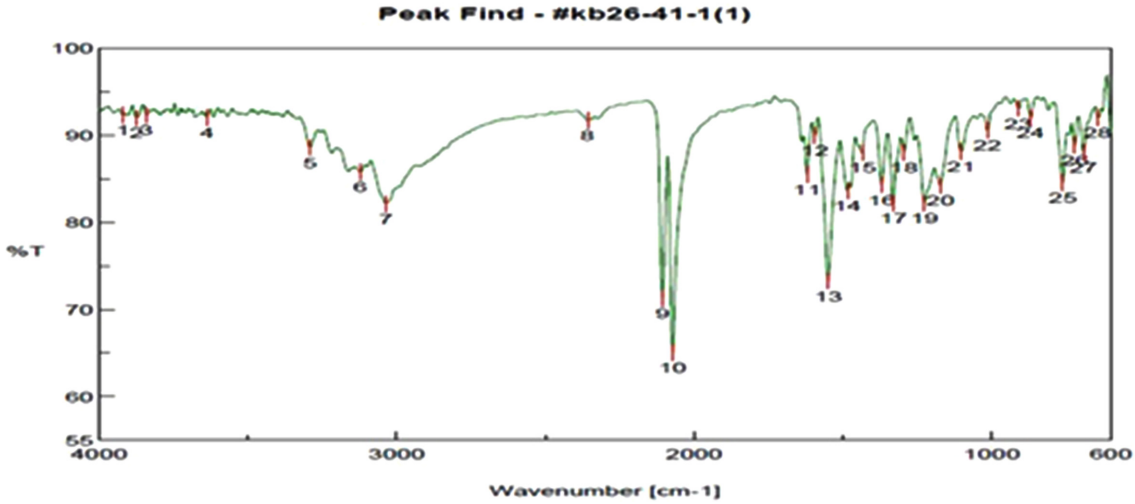

***Figure* S3.** IR spectrum of $[Cd(acpy\text{-}phTsc)(NCS)_2]_2$.

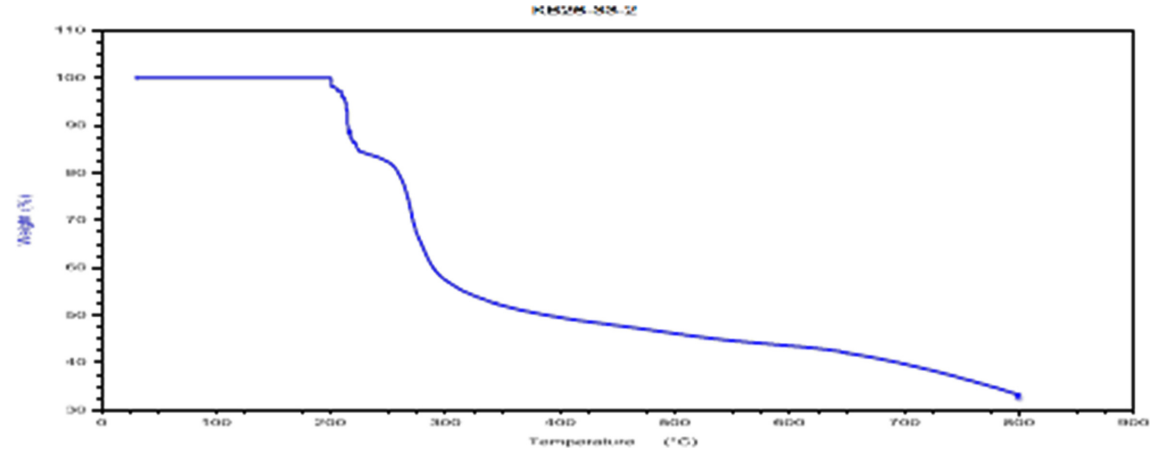

***Figure* S4.** Thermogravimetric curve of [Cd(acpy-mdtc)$_2$].

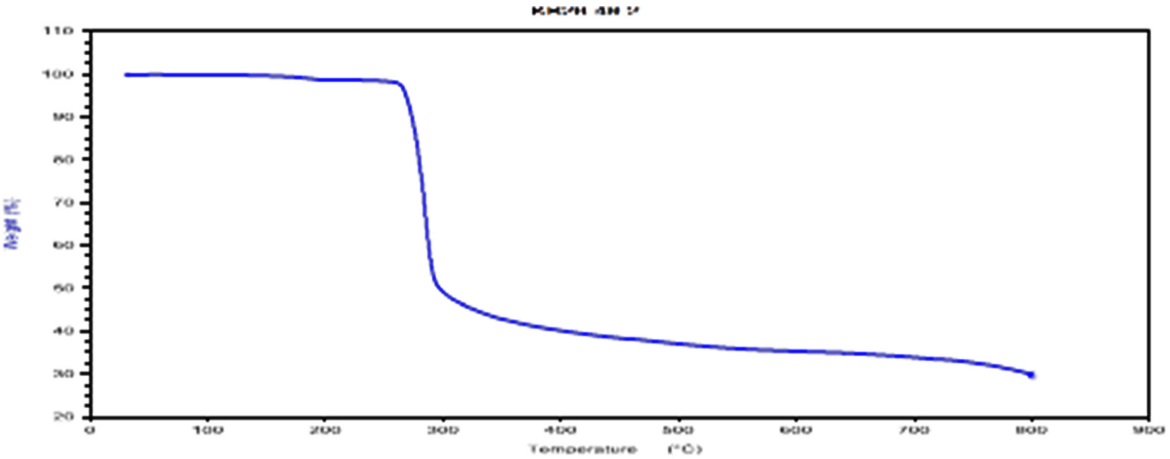

***Figure* S5.** Thermogravimetric curve of [Cd(acpy-phtsc)$_2$].

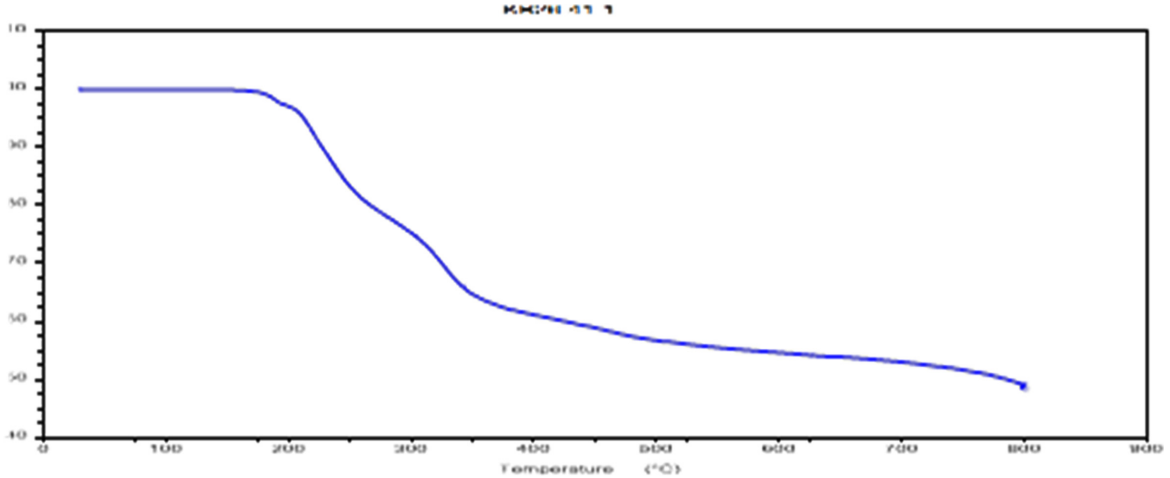

***Figure* S6.** Thermogravimetric curve of [Cd(acpy-mdtc)(NCS)]$_2$.

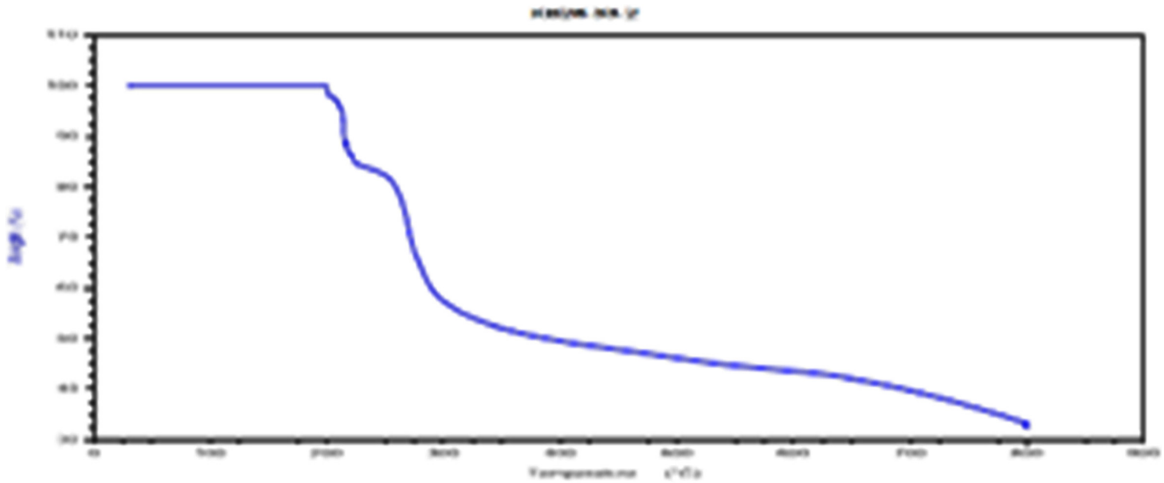

***Figure* S7.** Thermogravimetric curve of $[Cd(acpy\text{-}phtsc)(NCS)_2]_2$.