Electronic Supplementary Information for Dalton Transactions

Supplementary material

Bis(2-pyridyl)ditelluride, bis(3-methyl-2-pyridyl)ditelluride and their tellurolate complexes of zinc, cadmium, mercury: Synthesis, characterization and their conversion to metal telluride nanoparticles

G. Kedarnath, Vimal K. Jain,* Amey Wadawale and Gautam K. Dey

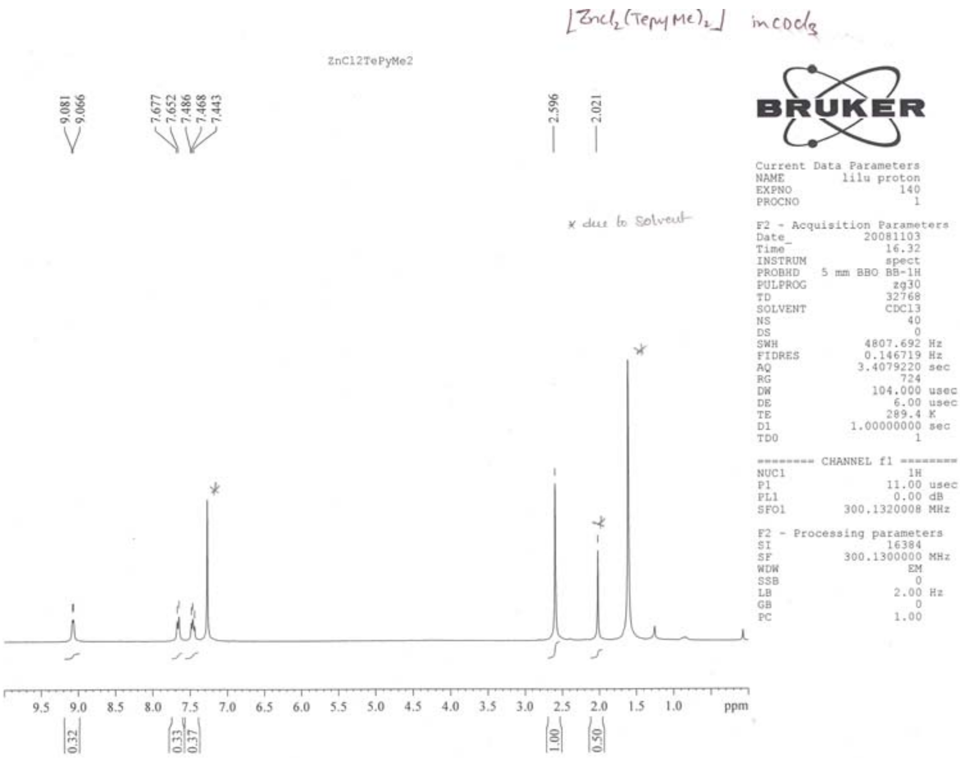

Fig. 1 ^{1}H NMR spectrum of $[ZnCl_2\{Te_2(pyMe)_2\}]$.

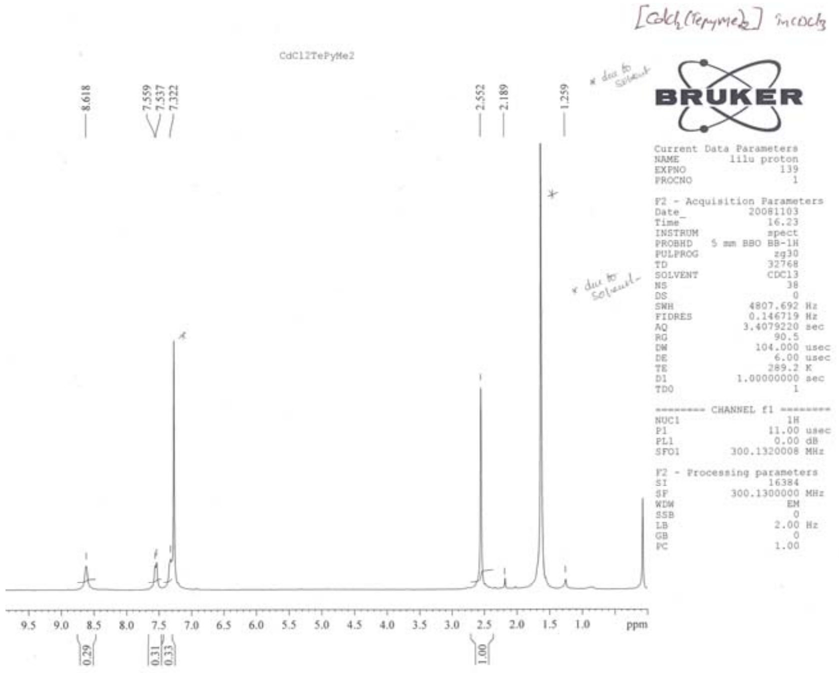

Fig. 2 ^{1}H NMR spectrum of $[CdCl_2\{Te_2(pyMe)_2\}]$.

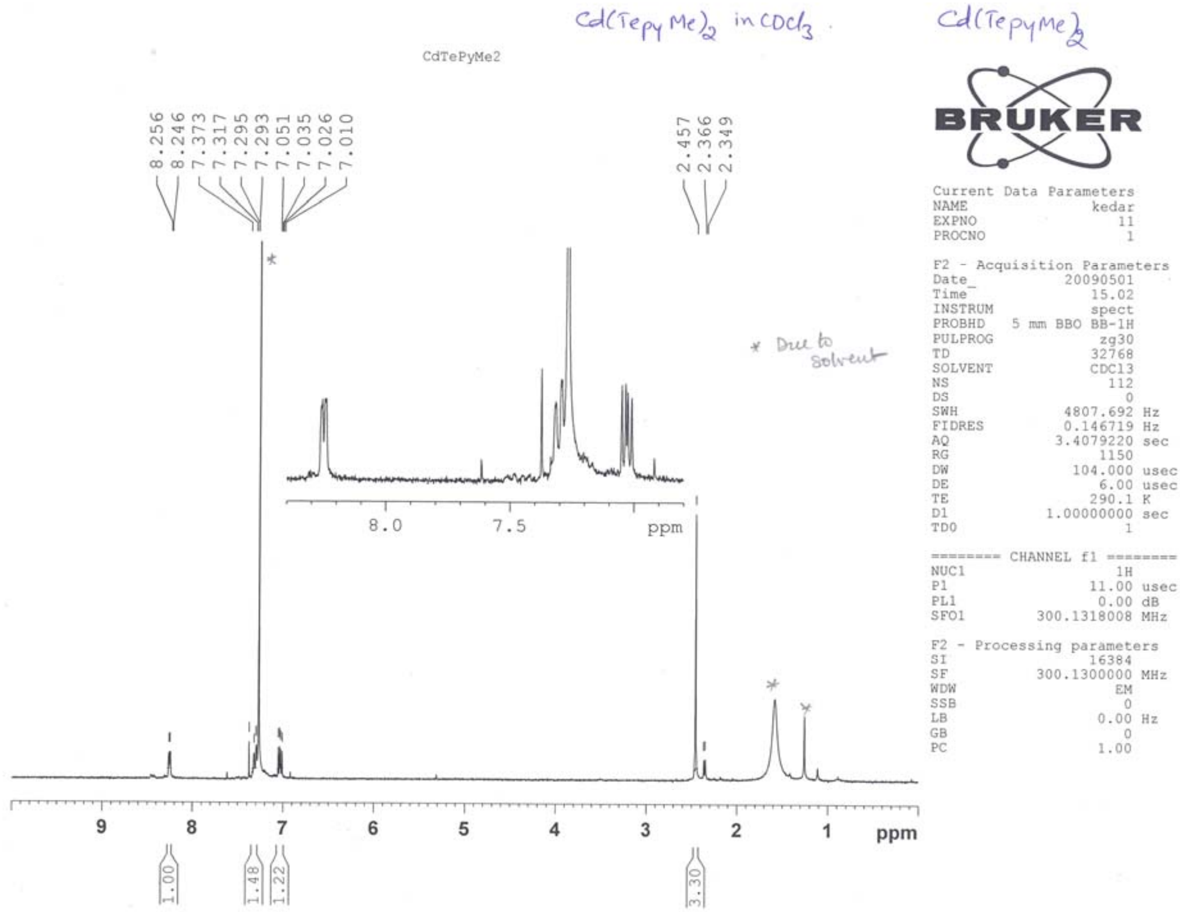

Fig. 3 ^{1}H NMR spectrum of [Cd(TepyMe)$_2$].

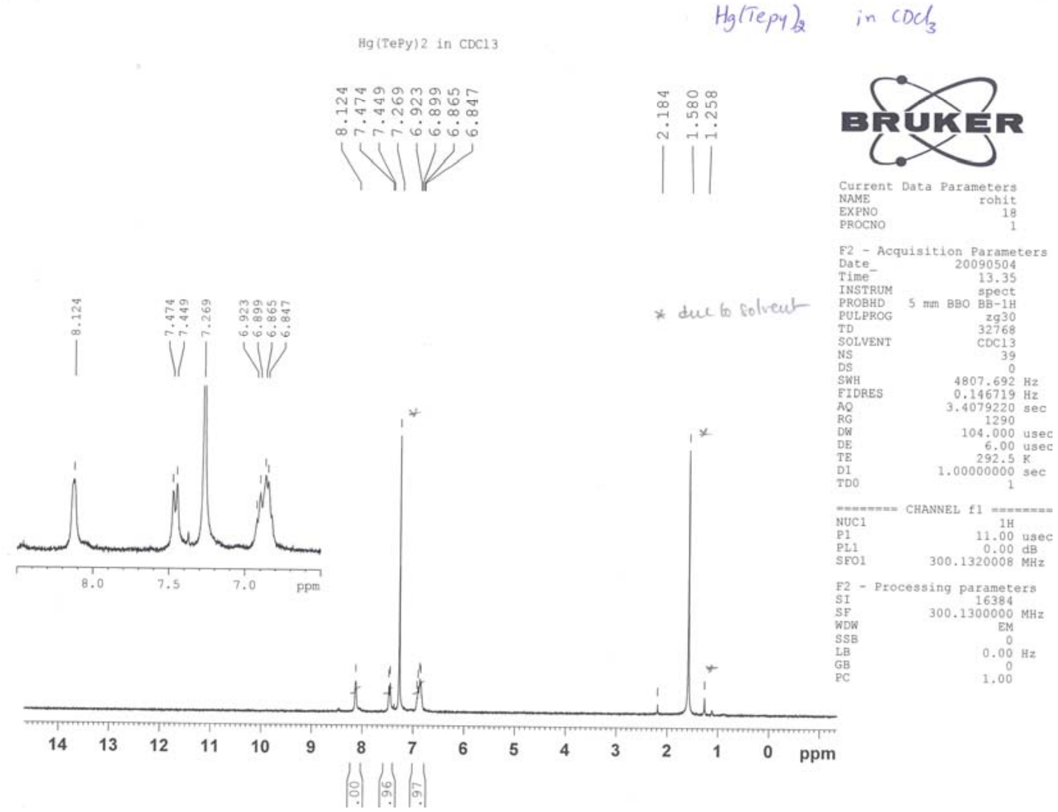

Fig. 4 ^{1}H NMR spectrum of $[Hg(Tepy)_2]$.

Electronic Supplementary Information for Dalton Transactions

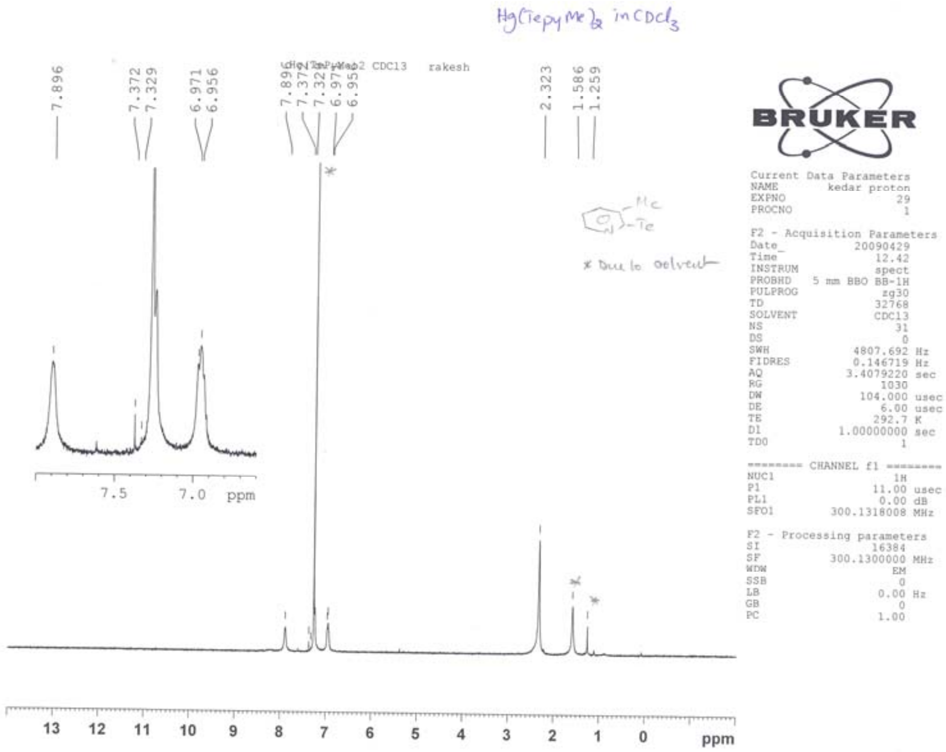

Fig. 5 ^{1}H NMR spectrum of $[Hg(TepyMe)_2]$.

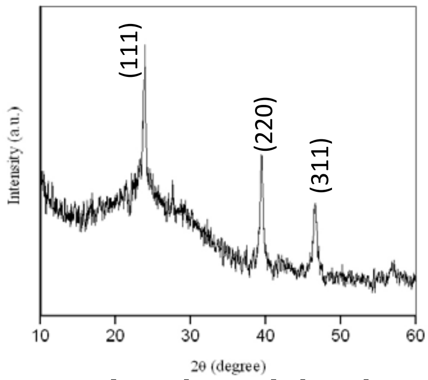

Fig. 6 CdTe nanoparticles obtained by the pyrolysis of $[Cd(Tepy)_2]$ at 350 ^{o}C in a furnace for 1h.

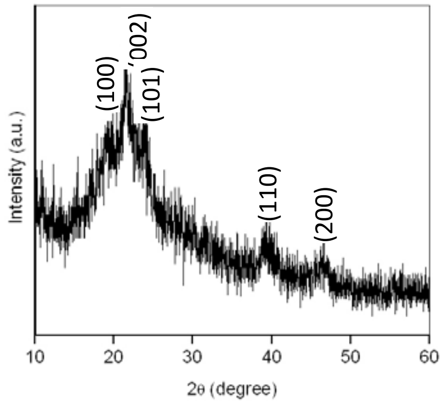

Fig. 7 CdTe nanoparticles obtained by the pyrolysis of [Cd(Tepy)$_2$] in HDA at 160 ^{o}C for 20 min.

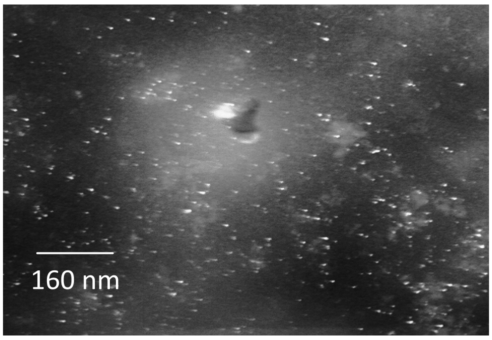

Fig. 8 TEM image of CdTe nanoparticles obtained by the pyrolysis of $[Cd(Tepy)_2]$ in HDA at 160 ^oC for 20 min.

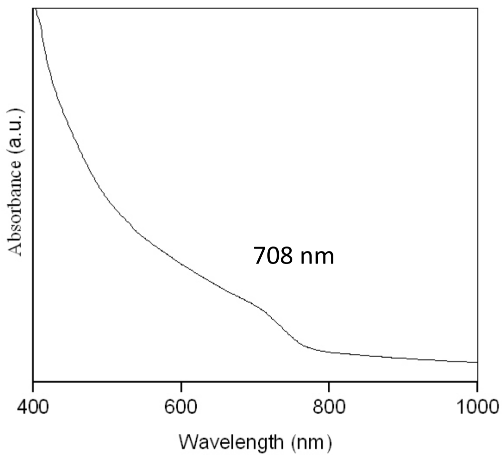

Fig. 9 Absoption spectrum of CdTe nanoparticles obtained by the pyrolysis of $[Cd(Tepy)_2]$ in HDA at 160 ^oC for 20 min.

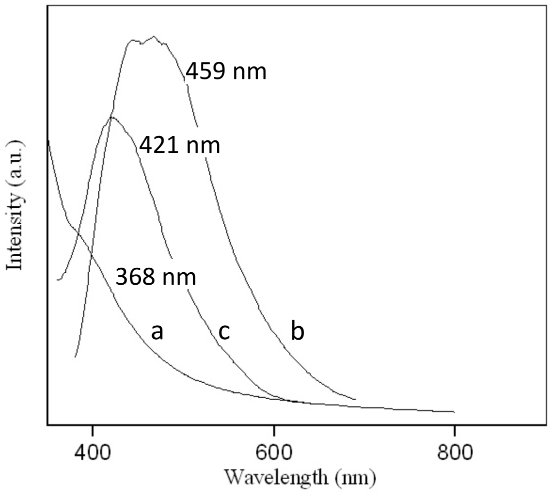

Fig. 10 a) Absoption, b) emission spectra of CdTe nanoparticles obtained by the pyrolysis of $[Cd(Tepy)_2]$ in TOPO (2 g) at 160 ^oC for 20 min (**experiment 2**) and c) emission spectrum of CdTe nanoparticles recapped with TGA.

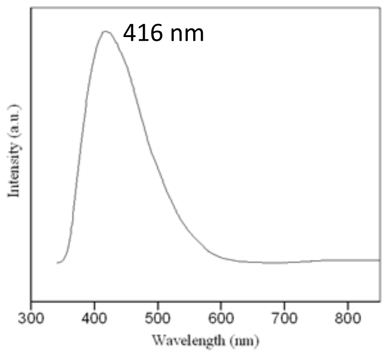

Fig. 11 Emission spectrum of CdTe nanoparticles obtained by the pyrolysis of $[Cd(Tepy)_2]$ in HDA/TOPO at 160 ^oC for 20 min (**experiment 4**).

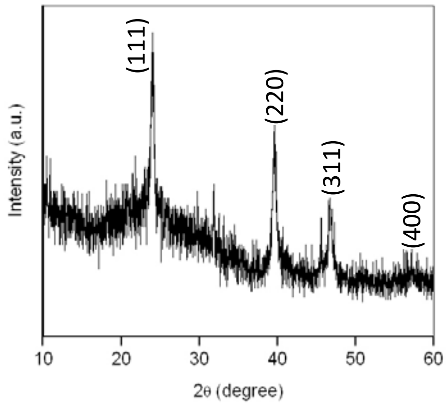

Fig. 12 XRD pattern of HgTe obtained by the pyrolysis of $[Hg(pyTe)_2]$ in a furnace at 175 ^oC for 1 h.

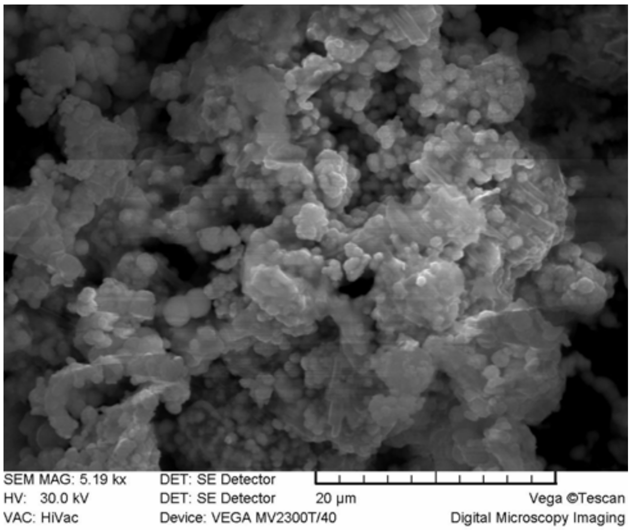

Fig. 13 SEM picture of HgTe obtained by the pyrolysis of $[Hg(pyTe)_2]$ in a furnace at 175 ^oC for 1 h.

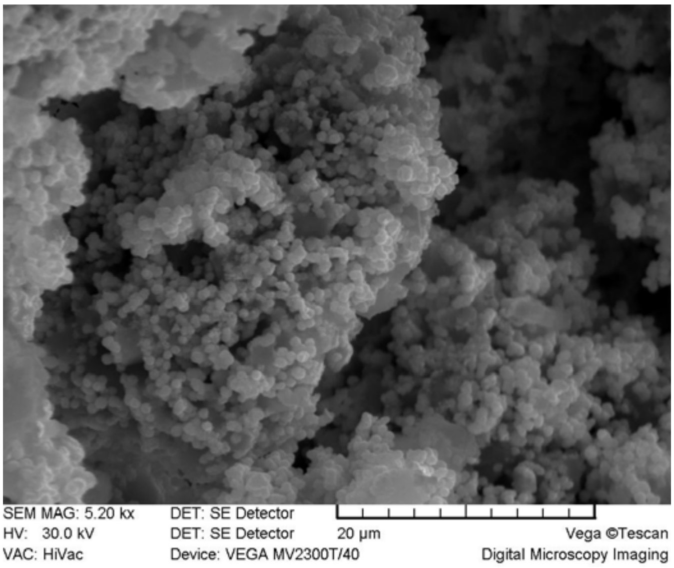

Fig. 14 SEM picture of HgTe obtained by the pyrolysis of $[Hg(TepyMe)_2]$ in a furnace at 250 ^{o}C for 1 h.

Crystal information (.cif) for $[ZnCl_2(TepyMe)_2].CH_3CN$ (1b)

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H11A C11 H11B 109.5 . . ?
C2 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C1 C2 C11 114(2) . . ?
C1 C2 C3 119(2) . . ?
C11 C2 C3 127(2) . . ?
C6 Te2 Te1 93.9(7) . . ?
C1 Te1 Te2 96.3(5) . . ?
C2 C1 N1 122.5(19) . . ?
C2 C1 Te1 121.7(16) . . ?
N1 C1 Te1 115.7(14) . . ?
C10 N2 C6 115(2) . . ?
C10 N2 Zn1 116.1(15) . . ?
C6 N2 Zn1 128.8(16) . . ?
N2 C6 C7 124(2) . . ?
N2 C6 Te2 114.8(18) . . ?
C7 C6 Te2 121.0(15) . . ?
C8 C9 C10 118.2(19) . . ?
C8 C9 H10 120.9 . . ?
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C9 C8 C7 C12 178(2) . . . . ?
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Cl1 Zn1 N1 C1 149.0(15) . . . . ?
Cl2 Zn1 N1 C1 -88.4(16) . . . . ?
N2 Zn1 N1 C5 -156.3(14) . . . . ?
Cl1 Zn1 N1 C5 -37.2(15) . . . . ?
Cl2 Zn1 N1 C5 85.3(14) . . . . ?
C1 N1 C5 C4 4(3) . . . . ?
Zn1 N1 C5 C4 -170(2) . . . . ?
N1 C5 C4 C3 -5(4) . . . . ?
C2 C3 C4 C5 3(4) . . . . ?
C4 C3 C2 C1 0(4) . . . . ?
C4 C3 C2 C11 -173(3) . . . . ?
C6 Te2 Te1 C1 109.4(8) . . . . ?
C11 C2 C1 N1 172(2) . . . . ?
C3 C2 C1 N1 -1(3) . . . . ?
C11 C2 C1 Te1 -6(3) . . . . ?
C3 C2 C1 Te1 -179.0(18) . . . . ?
C5 N1 C1 C2 -1(3) . . . . ?
Zn1 N1 C1 C2 173.1(16) . . . . ?
C5 N1 C1 Te1 177.4(14) . . . . ?
Zn1 N1 C1 Te1 -9(2) . . . . ?
Te2 Te1 C1 C2 122.2(18) . . . . ?
Te2 Te1 C1 N1 -56.0(15) . . . . ?
N1 Zn1 N2 C10 -159.6(13) . . . . ?
Cl1 Zn1 N2 C10 81.2(14) . . . . ?
Cl2 Zn1 N2 C10 -42.8(14) . . . . ?
N1 Zn1 N2 C6 25(2) . . . . ?
Cl1 Zn1 N2 C6 -94.0(18) . . . . ?
Cl2 Zn1 N2 C6 142.0(18) . . . . ?
C10 N2 C6 C7 1(3) . . . . ?
Zn1 N2 C6 C7 175.9(19) . . . . ?
C10 N2 C6 Te2 -179.7(15) . . . . ?
Zn1 N2 C6 Te2 -4(3) . . . . ?
C8 C7 C6 N2 -1(4) . . . . ?
C12 C7 C6 N2 -180(2) . . . . ?
C8 C7 C6 Te2 179.5(17) . . . . ?
C12 C7 C6 Te2 1(3) . . . . ?
Te1 Te2 C6 N2 -58.0(17) . . . . ?
Te1 Te2 C6 C7 122(2) . . . . ?
C7 C8 C9 C10 2(3) . . . . ?
C6 N2 C10 C9 1(3) . . . . ?
Zn1 N2 C10 C9 -174.8(15) . . . . ?
C8 C9 C10 N2 -3(3) . . . . ?

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_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    2.265
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_refine_diff_density_min   -1.169
_refine_diff_density_rms    0.247
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Crystal information (.cif) for [Cd(Tepy)$_2$(tmeda)] (3)

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;
_chemical_name_common             ?
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 'C16 H24 Cd N4 Te2'
_chemical_formula_weight          639.99

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 _atom_type_scat_dispersion_imag
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 'C'  'C'   0.0033   0.0016
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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'
 'Te'  'Te'  -0.5308   1.6751
 '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'

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_symmetry_space_group_name_Hall       '-C 2yc'
_symmetry_Int_Tables_number            15

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-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                    20.900(5)
_cell_length_b                    7.3572(11)
_cell_length_c                    14.250(3)
_cell_angle_alpha                 90.00
_cell_angle_beta                  105.382(16)
_cell_angle_gamma                 90.00
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_cell_formula_units_Z             4
_cell_measurement_temperature     298(2)
_cell_measurement_reflns_used          25
_cell_measurement_theta_min            10.3
_cell_measurement_theta_max            16.1

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_exptl_crystal_density_diffrn     2.012
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_exptl_crystal_F_000              1200
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_exptl_absorpt_correction_type         psi-scan
_exptl_absorpt_process_details         '(North, Phillips & Mathews,
1968)'
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_exptl_special_details
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_diffrn_radiation_monochromator   graphite
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_diffrn_measurement_method             \w
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_diffrn_standards_interval_count       150
_diffrn_standards_decay_%              -5.93
_diffrn_reflns_number             3266
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_diffrn_reflns_theta_max          27.48
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_reflns_number_gt                 1920
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'WINAFC'
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_computing_molecular_graphics     'ORTEP-3 FOR WINDOWS'
_computing_publication_material   'WINGX 1.70.01'

_refine_special_details
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 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.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0675P)^2^+5.1667P] 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     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0022(2)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          2433
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_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0399
_refine_ls_wR_factor_ref          0.1162
_refine_ls_wR_factor_gt           0.1070
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_refine_ls_restrained_S_all       1.027
_refine_ls_shift/su_max           0.000
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Cd1 Cd 0.0000 0.20270(7) 0.2500 0.0415(2) Uani 1 2 d S . .
N1 N 0.1290(3) 0.0419(7) 0.3348(4) 0.0539(12) Uani 1 1 d . . .
N2 N 0.0614(3) 0.4632(7) 0.3348(4) 0.0578(14) Uani 1 1 d . . .
C1 C 0.1435(3) 0.0097(8) 0.2512(4) 0.0445(12) Uani 1 1 d . . .
C2 C 0.2046(4) -0.0617(11) 0.2492(6) 0.067(2) Uani 1 1 d . . .
C5 C 0.1749(4) 0.0070(13) 0.4178(6) 0.074(2) Uani 1 1 d . . .
C4 C 0.2374(4) -0.0573(13) 0.4205(7) 0.082(3) Uani 1 1 d . . .
C7 C 0.1242(3) 0.4943(11) 0.3083(6) 0.0688(19) Uani 1 1 d . . .
H7A H 0.1150 0.5107 0.2391 0.103 Uiso 1 1 calc R . .
H7B H 0.1528 0.3913 0.3276 0.103 Uiso 1 1 calc R . .
H7C H 0.1455 0.6011 0.3408 0.103 Uiso 1 1 calc R . .
C3 C 0.2518(4) -0.0932(14) 0.3351(8) 0.085(3) Uani 1 1 d . . .
C8 C 0.0166(4) 0.6193(11) 0.3029(8) 0.094(3) Uani 1 1 d . . .
C6 C 0.0743(5) 0.4382(13) 0.4396(7) 0.089(3) Uani 1 1 d . . .
H6A H 0.1035 0.3363 0.4596 0.133 Uiso 1 1 calc R . .
H6B H 0.0333 0.4160 0.4558 0.133 Uiso 1 1 calc R . .
H6C H 0.0948 0.5457 0.4725 0.133 Uiso 1 1 calc R . .
H1 H 0.211(4) -0.079(11) 0.197(6) 0.07(3) Uiso 1 1 d . . .
H3 H 0.263(5) -0.067(12) 0.479(8) 0.11(4) Uiso 1 1 d . . .
H8B H -0.020(4) 0.597(9) 0.337(5) 0.06(2) Uiso 1 1 d . . .
H4 H 0.163(4) 0.045(10) 0.480(6) 0.08(2) Uiso 1 1 d . . .
H8A H 0.044(4) 0.745(12) 0.326(6) 0.09(2) Uiso 1 1 d . . .
H2 H 0.286(5) -0.143(14) 0.334(7) 0.10(3) Uiso 1 1 d . . .

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 _atom_site_aniso_U_33
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Te1 0.0441(3) 0.0541(3) 0.0495(3) -0.00150(15) 0.01645(17) 0.00397(16)
Cd1 0.0394(3) 0.0350(3) 0.0544(3) 0.000 0.0198(2) 0.000
N1 0.052(3) 0.060(3) 0.053(3) 0.003(2) 0.021(2) 0.003(3)
N2 0.045(3) 0.048(3) 0.084(4) -0.023(3) 0.023(3) -0.008(2)
C1 0.039(3) 0.039(3) 0.059(3) 0.005(2) 0.019(2) -0.003(2)
C2 0.047(4) 0.082(5) 0.077(5) 0.013(4) 0.025(3) 0.018(3)
C5 0.078(5) 0.083(5) 0.060(4) 0.009(4) 0.017(4) -0.001(5)
C4 0.061(5) 0.088(6) 0.083(6) 0.032(5) -0.006(4) -0.005(4)
C7 0.050(4) 0.051(4) 0.108(6) -0.012(4) 0.025(4) -0.015(3)
C3 0.038(4) 0.092(6) 0.124(8) 0.037(5) 0.019(4) 0.016(4)
C8 0.061(5) 0.041(4) 0.179(10) -0.034(5) 0.027(6) 0.003(3)
C6 0.078(6) 0.099(7) 0.094(6) -0.050(5) 0.030(5) -0.017(5)

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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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Te1 Cd1 2.7739(6) . ?
Cd1 N2 2.441(5) . ?
Cd1 N2 2.441(5) 2 ?
Cd1 Te1 2.7739(6) 2 ?
N1 C1 1.326(7) . ?
N1 C5 1.336(10) . ?
N2 C6 1.457(11) . ?
N2 C8 1.475(10) . ?
N2 C7 1.477(8) . ?
C1 C2 1.389(8) . ?
C2 C3 1.372(12) . ?
C2 H1 0.80(7) . ?
C5 C4 1.379(12) . ?
C5 H4 1.02(8) . ?
C4 C3 1.355(14) . ?
C4 H3 0.86(11) . ?
C7 H7A 0.9600 . ?
C7 H7B 0.9600 . ?
C7 H7C 0.9600 . ?
C3 H2 0.81(10) . ?
C8 C8 1.48(2) 2 ?
C8 H8B 1.02(6) . ?
C8 H8A 1.09(9) . ?
C6 H6A 0.9600 . ?
C6 H6B 0.9600 . ?
C6 H6C 0.9600 . ?

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N2 Cd1 N2 76.5(3) . 2 ?
N2 Cd1 Te1 104.67(13) . 2 ?
N2 Cd1 Te1 108.04(12) 2 2 ?
N2 Cd1 Te1 108.04(12) . . ?
N2 Cd1 Te1 104.67(13) 2 . ?
Te1 Cd1 Te1 138.00(3) 2 . ?
C1 N1 C5 118.7(6) . . ?
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```
C6 N2 C8 110.1(7) . . ?
C6 N2 C7 110.3(6) . . ?
C8 N2 C7 109.6(7) . . ?
C6 N2 Cd1 109.8(4) . . ?
C8 N2 Cd1 104.6(5) . . ?
C7 N2 Cd1 112.4(4) . . ?
N1 C1 C2 121.1(6) . . ?
N1 C1 Te1 116.6(4) . . ?
C2 C1 Te1 122.2(5) . . ?
C3 C2 C1 119.5(8) . . ?
C3 C2 H1 123(6) . . ?
C1 C2 H1 118(6) . . ?
N1 C5 C4 122.8(8) . . ?
N1 C5 H4 115(5) . . ?
C4 C5 H4 121(5) . . ?
C3 C4 C5 118.5(8) . . ?
C3 C4 H3 129(7) . . ?
C5 C4 H3 113(7) . . ?
N2 C7 H7A 109.5 . . ?
N2 C7 H7B 109.5 . . ?
H7A C7 H7B 109.5 . . ?
N2 C7 H7C 109.5 . . ?
H7A C7 H7C 109.5 . . ?
H7B C7 H7C 109.5 . . ?
C4 C3 C2 119.3(8) . . ?
C4 C3 H2 121(7) . . ?
C2 C3 H2 119(7) . . ?
N2 C8 C8 113.6(7) . 2 ?
N2 C8 H8B 103(4) . . ?
C8 C8 H8B 106(4) 2 . ?
N2 C8 H8A 109(4) . . ?
C8 C8 H8A 112(4) 2 . ?
H8B C8 H8A 113(6) . . ?
N2 C6 H6A 109.5 . . ?
N2 C6 H6B 109.5 . . ?
H6A C6 H6B 109.5 . . ?
N2 C6 H6C 109.5 . . ?
H6A C6 H6C 109.5 . . ?
H6B C6 H6C 109.5 . . ?

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C1 Te1 Cd1 N2 64.2(2) . . . . ?
C1 Te1 Cd1 N2 144.5(2) . . . 2 ?
C1 Te1 Cd1 Te1 -75.18(15) . . . 2 ?
N2 Cd1 N2 C6 132.3(6) 2 . . . ?
Te1 Cd1 N2 C6 26.9(5) 2 . . . ?
Te1 Cd1 N2 C6 -126.4(5) . . . . ?
N2 Cd1 N2 C8 14.2(5) 2 . . . ?
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Te1 Cd1 N2 C8 -91.2(6) 2 . . . ?
Te1 Cd1 N2 C8 115.5(5) . . . . ?
N2 Cd1 N2 C7 -104.6(6) 2 . . . ?
Te1 Cd1 N2 C7 149.9(5) 2 . . . ?
Te1 Cd1 N2 C7 -3.3(5) . . . . ?
C5 N1 C1 C2 1.0(10) . . . . ?
C5 N1 C1 Te1 179.9(6) . . . . ?
Cd1 Te1 C1 N1 4.9(4) . . . . ?
Cd1 Te1 C1 C2 -176.2(6) . . . . ?
N1 C1 C2 C3 -2.4(11) . . . . ?
Te1 C1 C2 C3 178.8(6) . . . . ?
C1 N1 C5 C4 1.5(12) . . . . ?
N1 C5 C4 C3 -2.6(14) . . . . ?
C5 C4 C3 C2 1.1(14) . . . . ?
C1 C2 C3 C4 1.3(13) . . . . ?
C6 N2 C8 C8 -161.1(9) . . . 2 ?
C7 N2 C8 C8 77.5(10) . . . 2 ?
Cd1 N2 C8 C8 -43.2(10) . . . 2 ?

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_diffrn_measured_fraction_theta_full   1.000
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_refine_diff_density_min   -0.834
_refine_diff_density_rms    0.146
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