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P-1848-1

Supp. Info. p1 of 25
(print-out of cif file)

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data_compound_(1)

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_chemical_formula_moiety             'C12 H12 Cd N6 Ni, (C7 H9 N)'
_chemical_formula_structural         'Cd (C4 N4 Ni) (C8 H12 N2) (C7 H9 N)'
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_symmetry_space_group_name_H-M       'P -1'
loop_
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   +x,+y,+z
   -x,-y,-z

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_cell_angle_beta                     91.72(2)
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_cell_volume                         520.4(2)
_cell_formula_units_Z                1
_exptl_crystal_density_diffrn        1.62
_exptl_crystal_density_meas          1.64(1)
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_exptl_absorpt_coefficient_mu        1.946
_cell_measurement_temperature        293
_exptl_crystal_description           block-like
_exptl_crystal_colour                yellow
_exptl_crystal_size_max              0.42
_exptl_crystal_size_mid              0.24
_exptl_crystal_size_min              0.18

_diffrn_measurement_device           'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method           '2¥q-¥w scans'
_exptl_absorpt_correction_type       none
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_reflns_number_total                 2971
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_reflns_observed_criterion           >4sigma(F)
_diffrn_reflns_av_R_equivalents      0.006
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_diffrn_reflns_limit_l_min           -13
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_diffrn_standards_number             3
_diffrn_standards_interval_count     200
_diffrn_standards_decay_%            0.0

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_refine_ls_number_parameters         148
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P-1848-2

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_refine_ls_shift/esd_max           0.165
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_refine_ls_extinction_method       none

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Cd      .0          .0          1.0          .02523(9) Uani  1.0  d  .
Ni      .5          .5          1.0          .0268(1)  Uani  1.0  d  .
N(1)    .1983(4)    .2366(3)    1.0630(3)    .0406(8)  Uani  1.0  d  .
N(2)    .7631(4)    .2020(4)    .9487(4)     .0465(9)  Uani  1.0  d  .
N(3)    .1184(4)    .0042(4)    .7747(3)     .0457(9)  Uani  1.0  d  .
C(1)    .3104(4)    .3397(4)    1.0418(3)    .0320(7)  Uani  1.0  d  .
C(2)    .6644(4)    .3173(4)    .9674(3)     .0347(8)  Uani  1.0  d  .
C(3)    .3229(6)    .0523(7)    .7667(4)     .060(1)   Uani  1.0  d  .
C(4)    .4112(5)    .0235(5)    .6266(3)     .043(1)   Uani  1.0  d  .
C(5)    .3245(6)    .0857(6)    .5065(4)     .051(1)   Uani  1.0  d  .
C(6)    .4142(6)    .0624(6)    .3804(4)     .049(1)   Uani  1.0  d  .
C(11)   -.078(4)    .478(2)     .427(4)      .16(2)    Uani  0.5  d  .
C(12)   -.087(3)    .445(1)     .573(2)      .145(7)   Uani  1.0  d  .
C(13)   .012(5)     .453(4)     .697(2)      .15(1)    Uani  0.5  d  .
C(14)   .207(3)     .554(2)     .663(2)      .193(9)   Uani  1.0  d  .
C(15)   .237(4)     .601(2)     .504(6)      .25(2)    Uani  0.5  d  .
C(16)   -.145(10)   .378(5)     .645(4)      .34(3)    Uani  0.5  d  .
H(1)    .04100      .08945      .71974       .076      Uiso  1.0  calc  N(3)
H(2)    .10102      -.11419     .73319       .076      Uiso  1.0  calc  N(3)
H(3)    .33699      .19076      .79338       .076      Uiso  1.0  calc  C(3)
H(4)    .40481      -.02472     .84287       .076      Uiso  1.0  calc  C(3)
H(5)    .18828      .15192      .51020       .076      Uiso  1.0  calc  C(5)
H(6)    .34669      .11192      .28713       .076      Uiso  1.0  calc  C(6)

loop_
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_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Cd      .0209(2)    .0210(2)    .0344(2)    .00045(9)   .0104(1)    .00043(9)
Ni      .0202(2)    .0191(2)    .0414(3)    .0003(2)    .0046(2)    -.0000(2)
N(1)    .040(1)     .032(1)     .050(2)     -.008(1)    .008(1)     -.003(1)
N(2)    .035(1)     .036(1)     .068(2)     .011(1)     .004(1)     -.001(1)
N(3)    .039(1)     .062(2)     .037(1)     -.004(1)    .017(1)     -.003(1)
C(1)    .030(1)     .025(1)     .041(1)     .000(1)     .004(1)     -.004(1)
C(2)    .028(1)     .029(1)     .048(2)     -.001(1)    .005(1)     .001(1)
C(3)    .046(2)     .094(3)     .042(2)     -.022(2)    .024(2)     -.017(2)
C(4)    .037(2)     .056(2)     .036(2)     -.009(1)    .015(1)     -.001(1)
C(5)    .042(2)     .067(2)     .043(2)     .007(2)     .013(1)     .002(2)
C(6)    .045(2)     .067(2)     .037(2)     .003(2)     .009(1)     .002(2)
C(11)   .14(2)      .042(7)     .30(5)      .03(1)      -.11(3)     -.03(1)
C(12)   .20(1)      .094(7)     .14(1)      .013(9)     -.00(1)     -.000(7)
C(13)   .20(3)      .19(2)      .065(8)     .13(2)      .01(1)      -.02(1)
C(14)   .29(2)      .113(9)     .18(1)      .05(1)      -.04(2)     .006(8)
C(15)   .14(2)      .041(7)     .56(4)      -.02(1)     -.14(3)     -.02(2)
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P-1848-3

C(16) .62(9) .25(4) .17(3) -.24(4) .23(4) -.08(2)

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 Ni    C(1)   1.863(3)  .    .
 Ni    C(2)   1.849(3)  .    .
 Cd    N(1)   2.350(3)  .    .
 Cd    N(2)   2.319(3)  .    1_455
 Cd    N(3)   2.357(3)  .    .
 C(1)  N(1)   1.137(4)  .    .
 C(2)  N(2)   1.142(4)  .    .
 N(3)  C(3)   1.475(5)  .    .
 C(3)  C(4)   1.521(4)  .    .
 C(4)  C(5)   1.386(6)  .    .
 C(5)  C(6)   1.399(5)  .    .
 C(6)  C(4)   1.389(6)  .    2_656
 C(11) C(12)  1.44(4)   .    .
 C(12) C(13)  1.37(3)   .    .
 C(13) C(14)  1.61(4)   .    .
 C(14) C(15)  1.61(6)   .    .
 C(15) C(12)  1.30(4)   .    2_566
 C(11) C(14)  1.25(4)   .    2_566
 C(12) C(16)  0.97(3)   .    .

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_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
 C(1)  Ni    C(2)   88.6(1)   .      .      .
 N(1)  Cd    N(2)   86.6(1)   .      .      1_455
 N(1)  Cd    N(3)   90.2(1)   .      .      .
 N(2)  Cd    N(3)   93.0(1)   1_455  .      .
 Ni    C(1)  N(1)   176.8(3)  .      .      .
 Ni    C(2)  N(2)   178.4(3)  .      .      .
 Cd    N(1)  C(1)   153.4(3)  .      .      .
 Cd    N(2)  C(2)   157.0(3)  .      1_455  1_455
 Cd    N(3)  C(3)   114.8(2)  .      .      .
 N(3)  C(3)  C(4)   115.4(3)  .      .      .
 C(3)  C(4)  C(5)   121.6(4)  .      .      .
 C(4)  C(5)  C(6)   119.8(4)  .      .      .
 C(5)  C(6)  C(4)   120.9(4)  .      .      2_656
 C(6)  C(4)  C(5)   119.3(3)  2_656  .      .
 C(3)  C(4)  C(6)   119.1(3)  .      .      2_656
 C(11) C(12) C(13)  145(3)    .      .      .
 C(12) C(13) C(14)  104(2)    .      .      .
 C(13) C(14) C(15)  116(2)    .      .      .
 C(14) C(15) C(12)  111(3)    .      .      2_566
 C(15) C(12) C(11)  145(3)    .      2_566  .
 C(12) C(11) C(12)  99(3)     2_566  .      .
 C(15) C(12) C(16)  86(4)     .      2_566  2_566
 C(11) C(12) C(16)  129(4)    .      2_566  2_566
 C(12) C(11) C(14)  135(4)    2_566  .      2_566
 C(12) C(11) C(14)  126(3)    .      .      2_566
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data_compound_(2)
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P-1848-4

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_chemical_formula_weight             654.72
_symmetry_cell_setting               triclinic
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   -x,-y,-z

_cell_length_a                       8.149(2)
_cell_length_b                       9.577(1)
_cell_length_c                       9.865(2)
_cell_angle_alpha                    81.03(1)
_cell_angle_beta                     94.08(2)
_cell_angle_gamma                    106.08(2)
_cell_volume                         730.4(2)
_cell_formula_units_Z                1
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_exptl_crystal_density_meas          1.47(1)
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        'flotation in mesitylene-bromoform'
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_diffrn_radiation_wavelength         0.70926
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_cell_measurement_theta_min          17.06
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_exptl_absorpt_coefficient_mu        1.404
_cell_measurement_temperature        293
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_exptl_crystal_colour                yellow
_exptl_crystal_size_max              0.32
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_exptl_crystal_size_min              0.12

_diffrn_measurement_device           'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method           '2¥q-¥w scans'
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_reflns_observed_criterion           >4sigma(F)
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_diffrn_reflns_limit_h_min           -11
_diffrn_reflns_limit_h_max           11
_diffrn_reflns_limit_k_min           0
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_diffrn_reflns_limit_l_min           -13
_diffrn_reflns_limit_l_max           13
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_refine_ls_wR_factor_obs             0.0567
_refine_ls_goodness_of_fit_obs       1.178
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_refine_ls_number_parameters         193
_refine_ls_hydrogen_treatment        noref
_refine_ls_weighting_scheme          unit
_refine_ls_shift/esd_max             0.016
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P-1848-5

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_atom_site_occupancy
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Ni    .5           .5           .0           .0367(3) Uani  1.0  d  .
N(1)  .7693(7)     .7838(5)     .0147(6)     .053(2)  Uani  1.0  d  .
N(2)  .7518(8)     .3296(7)     .1129(7)     .064(3)  Uani  1.0  d  .
N(3)  .9446(6)     1.0612(5)    .2158(5)     .044(2)  Uani  1.0  d  .
N(4)  .8297(7)     1.1530(6)    .8999(5)     .050(2)  Uani  1.0  d  .
C(1)  .6690(7)     .6759(6)     .0097(6)     .042(2)  Uani  1.0  d  .
C(2)  .6563(8)     .3937(6)     .0712(6)     .045(2)  Uani  1.0  d  .
C(3)  .7943(10)    .9677(8)     .2878(7)     .065(3)  Uani  1.0  d  .
C(4)  .7676(8)     1.0023(7)    .4284(6)     .045(2)  Uani  1.0  d  .
C(5)  .8302(10)    1.1423(7)    .4652(7)     .061(3)  Uani  1.0  d  .
C(6)  .7961(10)    1.1704(7)    .5934(7)     .058(3)  Uani  1.0  d  .
C(7)  .7013(7)     1.0603(7)    .6864(6)     .042(2)  Uani  1.0  d  .
C(8)  .6391(8)     .9196(7)     .6504(7)     .049(2)  Uani  1.0  d  .
C(9)  .6735(8)     .8925(7)     .5219(7)     .048(2)  Uani  1.0  d  .
C(10) .6651(8)     1.0930(8)    .8251(7)     .055(3)  Uani  1.0  d  .
N(11) .1093(14)    .4905(12)    .2333(11)    .056(4)  Uani  0.5  d  .
C(11) .2415(22)    .4820(14)    .3560(19)    .073(6)  Uani  0.5  d  .
C(12) .4204(17)    .5088(13)    .3404(14)    .048(4)  Uani  0.5  d  .
C(13) .5284(12)    .5121(8)     .4320(9)     .073(3)  Uani  1.0  d  .
C(14) .1901(21)    .4563(16)    .4933(16)    .061(6)  Uani  0.5  d  .
C(15) .7125(14)    .5400(10)    .4090(11)    .088(4)  Uani  1.0  d  .
H(1)  .93160       1.16337      .19872       .076     Uiso  1.0  calc  N(3)
H(2)  1.04647      1.05860      .27805       .076     Uiso  1.0  calc  N(3)
H(3)  .68129       .97638       .22262       .076     Uiso  1.0  calc  C(3)
H(4)  .80417       .85410       .30076       .076     Uiso  1.0  calc  C(3)
H(5)  .90578       1.22983      .39404       .076     Uiso  1.0  calc  C(5)
H(6)  .84469       1.27986      .62010       .076     Uiso  1.0  calc  C(6)
H(7)  .56439       .83182       .72178       .076     Uiso  1.0  calc  C(8)
H(8)  .62534       .78298       .49514       .076     Uiso  1.0  calc  C(9)
H(9)  .59184       .99125       .88571       .076     Uiso  1.0  calc  C(10)
H(10) .59042       1.17416      .81023       .076     Uiso  1.0  calc  C(10)
H(11) .90275       1.23035      .83278       .076     Uiso  1.0  calc  N(4)
H(12) .80078       1.19951      .97572       .076     Uiso  1.0  calc  N(4)

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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Cd    .0310(3)  .0250(3)  .0420(3) -.0012(2)  .0024(2) -.0084(2)
Ni    .0335(5)  .0235(4)  .0479(6) -.0035(4)  .0049(4) -.0082(4)
N(1)  .048(3)   .036(3)   .063(3)  -.008(2)   .004(3)  -.008(2)
N(2)  .066(4)   .059(4)   .075(4)   .026(3)  -.001(3)  -.018(3)
N(3)  .041(3)   .047(3)   .044(3)   .009(2)   .002(2)  -.012(2)
N(4)  .062(3)   .047(3)   .047(3)   .025(3)  -.005(2)  -.013(2)
C(1)  .040(3)   .033(3)   .048(3)   .001(2)   .004(2)  -.009(2)
```

P-1848-6

C(2)	.045(3)	.038(3)	.050(3)	.003(2)	.004(3)	-.015(3)
C(3)	.066(4)	.065(4)	.054(4)	-.013(3)	.023(3)	-.023(3)
C(4)	.042(3)	.046(3)	.045(3)	.007(2)	.005(2)	-.007(2)
C(5)	.082(5)	.043(3)	.052(4)	.001(3)	.014(3)	-.008(3)
C(6)	.080(5)	.046(3)	.049(4)	.014(3)	.011(3)	-.006(3)
C(7)	.037(3)	.054(3)	.039(3)	.020(2)	-.004(2)	-.004(2)
C(8)	.045(3)	.048(3)	.052(3)	.009(3)	.006(3)	-.001(3)
C(9)	.043(3)	.046(3)	.054(4)	.007(3)	.005(3)	-.006(3)
C(10)	.048(3)	.078(5)	.046(3)	.026(3)	.000(3)	-.016(3)
N(11)	.057(6)	.055(6)	.050(6)	.005(5)	.019(5)	-.006(5)
C(11)	.090(11)	.032(6)	.097(12)	.010(7)	.051(0)	-.003(7)
C(12)	.056(7)	.038(6)	.052(7)	.013(5)	.013(6)	-.005(5)
C(13)	.081(6)	.037(3)	.100(6)	.010(4)	.007(5)	-.014(4)
C(14)	.074(10)	.051(8)	.055(8)	.010(7)	.010(7)	-.007(6)
C(15)	.100(7)	.058(5)	.108(8)	.015(5)	.024(6)	-.015(5)

loop_
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Ni	C(1)	1.868(5)	.	.
Ni	C(2)	1.876(7)	.	.
Cd	N(1)	2.373(5)	.	.
Cd	N(3)	2.399(5)	.	.
Cd	N(4)	2.352(5)	.	1_554
C(1)	N(1)	1.132(7)	.	.
C(2)	N(2)	1.137(8)	.	.
N(3)	C(3)	1.457(8)	.	.
C(3)	C(4)	1.519(8)	.	.
C(4)	C(5)	1.392(8)	.	.
C(5)	C(6)	1.395(9)	.	.
C(6)	C(7)	1.378(9)	.	.
C(7)	C(8)	1.394(9)	.	.
C(8)	C(9)	1.395(9)	.	.
C(9)	C(4)	1.377(8)	.	.
C(7)	C(10)	1.516(8)	.	.
N(4)	C(10)	1.496(8)	.	.
N(11)	C(11)	1.57(2)	.	.
C(11)	C(12)	1.42(2)	.	.
C(12)	C(13)	1.21(2)	.	.
C(13)	C(13)	1.42(2)	.	2_666
C(13)	C(15)	1.48(1)	.	.
C(11)	C(14)	1.41(2)	.	.
C(14)	C(15)	1.20(2)	.	2_666

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2

N(2)	N(3)	3.362(9)	.	1_545
N(2)	N(4)	3.093(10)	.	1_544
N(2)	N(11)	3.141(12)	.	1_655

loop_
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2

P-1848-7

```
_geom_angle_site_symmetry_3
 C(1)   Ni     C(2)      90.1(2)    .       .       .
 N(1)   Cd     N(3)      94.0(2)    .       .       .
 N(1)   Cd     N(4)      93.8(2)    .       .       .
 N(3)   Cd     N(4)      86.3(2)    .       .       .
 Ni     C(1)   N(1)     178.8(6)    .       .       .
 Ni     C(2)   N(2)     179.2(6)    .       .       .
 Cd     N(1)   C(1)     171.6(5)    .       .       .
 Cd     N(3)   C(3)     117.3(4)    .       .       .
 Cd     N(4)   C(10)    121.2(4)    .     1_554   1_554
 N(3)   C(3)   C(4)     116.5(5)    .       .       .
 C(3)   C(4)   C(5)     122.4(6)    .       .       .
 C(3)   C(4)   C(9)     119.0(6)    .       .       .
 C(5)   C(4)   C(9)     118.5(6)    .       .       .
 C(4)   C(5)   C(6)     120.4(6)    .       .       .
 C(5)   C(6)   C(7)     120.9(6)    .       .       .
 C(6)   C(7)   C(8)     118.9(6)    .       .       .
 C(6)   C(7)   C(10)    120.1(6)    .       .       .
 C(8)   C(7)   C(10)    121.0(6)    .       .       .
 C(7)   C(8)   C(9)     119.9(6)    .       .       .
 C(4)   C(9)   C(8)     121.4(6)    .       .       .
 C(7)   C(10)  N(4)     109.8(5)    .       .       .
 N(11)  C(11)  C(12)    124.2(13)   .       .       .
 N(11)  C(11)  C(14)    121.0(14)   .       .       .
 C(12)  C(11)  C(14)    114.7(17)   .       .       .
 C(11)  C(12)  C(13)    126.5(13)   .       .       .
 C(12)  C(13)  C(15)    123.9(10)   .       .       .
 C(12)  C(13)  C(13)    117.0(11)   .       .     2_666
 C(13)  C(13)  C(15)    119.1(8)  2_666     .       .
 C(11)  C(14)  C(15)    123.9(16)   .       .     2_666
 C(13)  C(15)  C(14)    118.8(12) 2_666   2_666     .
#===END
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_chemical_formula_structural
          'Cd (C4 N4 Ni) (C8 H12 N2)2 ((C6 H6 O) (H2 O))'
_chemical_formula_weight             659.70
_symmetry_cell_setting               monoclinic
_symmetry_space_group_name_H-M       'P 1 21/m 1'
loop_
_symmetry_equiv_pos_as_xyz
   +x,+y,+z
   -x,+y+1/2,-z
   -x,-y,-z
   +x,-y+1/2,+z

_cell_length_a                       8.615(3)
_cell_length_b                       17.568(2)
_cell_length_c                       9.950(2)
_cell_angle_alpha                    90.00
_cell_angle_beta                     105.30(2)
_cell_angle_gamma                    90.00
_cell_volume                         1452.6(5)
_cell_formula_units_Z                2
_exptl_crystal_density_diffrn        1.51
_exptl_crystal_density_meas          1.50(1)
_exptl_crystal_density_method
         'flotation in mesitylene-bromoform'
_diffrn_radiation_type               'Mo K¥a'
_diffrn_radiation_wavelength         0.70926
_cell_measurement_reflns_used        25
_cell_measurement_theta_min          12.64
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P-1848-8

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_exptl_absorpt_coefficient_mu      1.416
_cell_measurement_temperature      293
_exptl_crystal_description         plate-like
_exptl_crystal_colour              yellow
_exptl_crystal_size_max            0.28
_exptl_crystal_size_mid            0.24
_exptl_crystal_size_min            0.18

_diffrn_measurement_device         'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method         '2¥q-¥w scans'
_exptl_absorpt_correction_type     none
_diffrn_reflns_number              4761
_reflns_number_total               3832
_reflns_number_observed            2792
_reflns_observed_criterion         >4sigma(F)
_diffrn_reflns_av_R_equivalents    0.007
_diffrn_reflns_theta_max           30.00
_diffrn_reflns_limit_h_min         0
_diffrn_reflns_limit_h_max         12
_diffrn_reflns_limit_k_min         0
_diffrn_reflns_limit_k_max         24
_diffrn_reflns_limit_l_min         -14
_diffrn_reflns_limit_l_max         13
_diffrn_standards_number           3
_diffrn_standards_interval_count   200
_diffrn_standards_decay_%          0.0

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_refine_ls_R_factor_obs            0.0519
_refine_ls_wR_factor_obs           0.0520
_refine_ls_goodness_of_fit_obs     1.304
_refine_ls_number_reflns           2792
_refine_ls_number_parameters       187
_refine_ls_hydrogen_treatment      noref
_refine_ls_weighting_scheme        'calc w=1/(¥s^2^(Fo)+0.0003Fo^2^)'
_refine_ls_shift/esd_max           0.039
_refine_diff_density_max           0.75
_refine_diff_density_min           -0.59
_refine_ls_extinction_method       none

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
Cd    .0          .0          .0          .0298(2) Uani  d    .
Ni    .3493(1)    .25         .0542(1)    .0304(3) Uani  d    .
N(1)  .1032(7)    .1277(3)    .0320(6)    .048(2)  Uani  d    .
N(2)  .6077(8)    .1320(4)    .0810(7)    .072(3)  Uani  d    .
N(3)  .2404(6)    -.0541(3)   .1307(5)    .038(2)  Uani  d    .
N(4)  .0973(6)    -.0179(3)   .8002(5)    .039(2)  Uani  d    .
C(1)  .1952(7)    .1740(3)    .0406(6)    .034(2)  Uani  d    .
C(2)  .5070(8)    .1754(4)    .0699(7)    .046(2)  Uani  d    .
C(3)  .3638(7)    -.0086(4)   .2325(6)    .045(2)  Uani  d    .
C(4)  .3085(6)    .0062(4)    .3630(6)    .037(2)  Uani  d    .
C(5)  .2752(8)    .0811(4)    .4004(7)    .047(2)  Uani  d    .
C(6)  .2249(8)    .0933(4)    .5220(7)    .045(2)  Uani  d    .
C(7)  .2060(7)    .0312(4)    .6051(6)    .036(2)  Uani  d    .
C(8)  .2388(8)    -.0414(4)   .5671(7)    .046(3)  Uani  d    .
```

P-1848-9

C(9)	.2900(8)	-.0542(4)	.4466(7)	.044(2)	Uani	d	.
C(10)	.1582(9)	.0474(4)	.7392(7)	.049(3)	Uani	d	.
O(11)	.9717(10)	.25	.5106(11)	.090(4)	Uani	d	.
C(11)	.8427(17)	.25	.5615(14)	.064(5)	Uani	d	.
C(12)	.8662(21)	.25	.7089(14)	.081(6)	Uani	d	.
C(13)	.7368(28)	.25	.7634(18)	.100(9)	Uani	d	.
C(14)	.5821(23)	.25	.6802(21)	.096(8)	Uani	d	.
C(15)	.5564(17)	.25	.5315(18)	.084(7)	Uani	d	.
C(16)	.6866(15)	.25	.4723(12)	.062(5)	Uani	d	.
O(12)	.9111(13)	.25	.2276(12)	.151(7)	Uani	d	.
H(1)	.29541	-.07518	.06202	.076	Uiso	calc	N(3)
H(2)	.20925	-.09680	.18481	.076	Uiso	calc	N(3)
H(3)	.47803	-.04020	.26052	.076	Uiso	calc	C(3)
H(4)	.38158	.04611	.18481	.076	Uiso	calc	C(3)
H(5)	.28832	.12865	.33549	.076	Uiso	calc	C(5)
H(6)	.20085	.15038	.55156	.076	Uiso	calc	C(6)
H(7)	.22474	-.08913	.63134	.076	Uiso	calc	C(8)
H(8)	.31515	-.11148	.41877	.076	Uiso	calc	C(9)
H(9)	.06384	.09127	.71670	.076	Uiso	calc	C(10)
H(10)	.26479	.06919	.81651	.076	Uiso	calc	C(10)
H(11)	.00675	-.03989	.72586	.076	Uiso	calc	N(4)
H(12)	.18700	-.05574	.82613	.076	Uiso	calc	N(4)
H(13)	.93743	.25	.41060	.076	Uiso	calc	O(11)
H(14)	.98658	.25	.77726	.076	Uiso	calc	C(12)
H(15)	.75664	.25	.87520	.076	Uiso	calc	C(13)
H(16)	.48131	.25	.72563	.076	Uiso	calc	C(14)
H(17)	.43513	.25	.46476	.076	Uiso	calc	C(15)
H(18)	.66743	.25	.36056	.076	Uiso	calc	C(16)

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23

Cd	.0272(3)	.0262(3)	.0366(3)	-.0026(3)	.0094(2)	-.0025(3)
Ni	.0302(5)	.0221(5)	.0408(6)	.0	.0127(5)	.0
N(1)	.045(3)	.032(3)	.063(4)	-.012(3)	.008(3)	-.003(3)
N(2)	.067(4)	.069(5)	.086(5)	.036(4)	.034(4)	.008(4)
N(3)	.032(3)	.044(3)	.033(3)	.005(2)	.002(2)	-.003(2)
N(4)	.042(3)	.040(3)	.039(3)	.001(2)	.018(2)	-.001(2)
C(1)	.036(3)	.023(3)	.040(3)	.004(2)	.008(3)	-.002(2)
C(2)	.046(4)	.044(4)	.055(4)	.004(3)	.024(3)	.005(3)
C(3)	.037(3)	.059(4)	.040(3)	-.004(3)	.013(3)	.000(3)
C(4)	.024(2)	.046(3)	.037(3)	-.005(3)	.004(2)	-.006(3)
C(5)	.046(4)	.049(4)	.042(4)	-.005(3)	.006(3)	.004(3)
C(6)	.045(4)	.048(4)	.040(4)	-.001(3)	.008(3)	.003(3)
C(7)	.032(3)	.039(3)	.035(3)	-.001(3)	.006(3)	-.001(3)
C(8)	.054(4)	.041(4)	.045(4)	.006(3)	.016(3)	-.002(3)
C(9)	.048(4)	.043(4)	.038(3)	-.003(3)	.007(3)	.001(3)
C(10)	.064(5)	.041(4)	.052(4)	-.011(3)	.032(4)	-.009(3)
O(11)	.064(6)	.077(6)	.127(8)	.0	.021(6)	.0
C(11)	.081(9)	.029(5)	.082(9)	.0	.019(7)	.0
C(12)	.127(13)	.038(6)	.063(8)	.0	-.001(9)	.0
C(13)	.160(18)	.039(7)	.104(13)	.0	.040(13)	.0
C(14)	.138(16)	.041(7)	.128(15)	.0	.069(13)	.0
C(15)	.087(10)	.034(6)	.130(14)	.0	.027(10)	.0
C(16)	.065(8)	.035(5)	.074(8)	.0	.001(7)	.0
O(12)	.089(8)	.274(17)	.099(8)	.0	.043(7)	.0

loop_
_geom_bond_atom_site_label_1

P-1848-10

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_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
 Ni      C(1)      1.862(6)   .   .
 Ni      C(2)      1.864(7)   .   .
 Cd      N(1)      2.403(5)   .   .
 Cd      N(3)      2.337(5)   .   .
 Cd      N(4)      2.374(5)   .   1_554
 C(1)    N(1)      1.124(7)   .   .
 C(2)    N(2)      1.138(8)   .   .
 N(3)    C(3)      1.493(8)   .   .
 C(3)    C(4)      1.519(8)   .   .
 C(4)    C(5)      1.418(9)   .   .
 C(5)    C(6)      1.406(9)   .   .
 C(6)    C(7)      1.404(9)   .   .
 C(7)    C(8)      1.381(9)   .   .
 C(8)    C(9)      1.401(9)   .   .
 C(9)    C(4)      1.383(9)   .   .
 C(7)    C(10)     1.523(9)   .   .
 N(4)    C(10)     1.458(8)   .   .
 O(11)   C(11)     1.338(14)  .   .
 C(11)   C(12)     1.426(17)  .   .
 C(12)   C(13)     1.362(22)  .   .
 C(13)   C(14)     1.370(23)  .   .
 C(14)   C(15)     1.437(21)  .   .
 C(15)   C(16)     1.398(18)  .   .
 C(16)   C(11)     1.403(16)  .   .

loop_
_geom_contact_atom_site_label_1
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_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
 N(2)    N(3)      3.079(9)   .   3_655
 N(2)    N(4)      3.207(8)   .   3_656
 N(2)    O(12)     3.354(10)  .   .
 O(11)   O(12)     2.725(15)  .   .

loop_
_geom_angle_atom_site_label_1
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_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
 C(1)    Ni      C(2)       89.6(3)    .    .    .
 N(1)    Cd      N(3)       93.6(2)    .    .    .
 N(1)    Cd      N(4)       92.0(2)    .    .    1_554
 N(3)    Cd      N(4)       87.4(2)    .    .    1_554
 Ni      C(1)    N(1)      179.3(5)    .    .    .
 Ni      C(2)    N(2)      177.4(7)    .    .    .
 Cd      N(1)    C(1)      156.3(5)    .    .    .
 Cd      N(3)    C(3)      121.8(4)    .    .    .
 Cd      N(4)    C(10)     119.3(4)    .    1_554  1_554
 N(3)    C(3)    C(4)      110.1(5)    .    .    .
 C(3)    C(4)    C(5)      120.9(6)    .    .    .
 C(3)    C(4)    C(9)      119.7(6)    .    .    .
 C(4)    C(5)    C(6)      119.8(6)    .    .    .
 C(5)    C(6)    C(7)      119.9(6)    .    .    .
 C(6)    C(7)    C(8)      119.6(6)    .    .    .
 C(7)    C(8)    C(9)      121.1(6)    .    .    .
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P-1848-11

C(8)	C(9)	C(4)	120.2(6)	.	.	.
C(9)	C(4)	C(12)	119.4(6)	.	.	.
C(6)	C(7)	C(10)	118.1(6)	.	.	.
C(10)	C(7)	C(8)	122.3(6)	.	.	.
N(4)	C(10)	C(7)	115.4(5)	.	.	.
O(11)	C(11)	C(12)	118.9(13)	.	.	.
O(11)	C(11)	C(16)	120.9(12)	.	.	.
C(11)	C(12)	C(13)	120.0(15)	.	.	.
C(12)	C(13)	C(14)	121.8(16)	.	.	.
C(13)	C(14)	C(15)	118.9(16)	.	.	.
C(14)	C(15)	C(16)	120.7(14)	.	.	.
C(15)	C(16)	C(11)	118.4(12)	.	.	.
C(16)	C(11)	C(12)	120.2(13)	.	.	.

#===END

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_chemical_formula_structural 'Cd (C4 N4 Ni) (C8 H12 N2)2 (C9 H7 N)'
_chemical_formula_weight 676.73
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 1 21/m 1'
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z
-x,+y+1/2,-z
-x,-y,-z
+x,-y+1/2,+z

_cell_length_a 8.505(1)
_cell_length_b 17.737(1)
_cell_length_c 10.106(1)
_cell_angle_alpha 90.00
_cell_angle_beta 102.64(1)
_cell_angle_gamma 90.00
_cell_volume 1487.5(3)
_cell_formula_units_Z 2
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_exptl_crystal_density_meas 1.50(1)
_exptl_crystal_density_method
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_diffrn_radiation_type 'Mo K¥a'
_diffrn_radiation_wavelength 0.70926
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_cell_measurement_theta_max 17.41
_exptl_absorpt_coefficient_mu 1.381
_cell_measurement_temperature 293
_exptl_crystal_description plate-like
_exptl_crystal_colour yellow
_exptl_crystal_size_max 0.30
_exptl_crystal_size_mid 0.30
_exptl_crystal_size_min 0.25

_diffrn_measurement_device 'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method '2¥q-¥w scans'
_exptl_absorpt_correction_type none
_diffrn_reflns_number 4842
_reflns_number_total 4150
_reflns_number_observed 3430
_reflns_observed_criterion >4sigma(F)
_diffrn_reflns_av_R_equivalents 0.005
_diffrn_reflns_theta_max 30.00
_diffrn_reflns_limit_h_min 0

P-1848-12

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_diffrn_reflns_limit_l_min          -14
_diffrn_reflns_limit_l_max          13
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_refine_ls_wR_factor_obs            0.0474
_refine_ls_goodness_of_fit_obs      1.379
_refine_ls_number_reflns            3430
_refine_ls_number_parameters        199
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_refine_ls_weighting_scheme         'calc w=1/(¥s^2^(Fo)+0.0003Fo^2^)'
_refine_ls_shift/esd_max            0.009
_refine_diff_density_max            0.93
_refine_diff_density_min            -0.39
_refine_ls_extinction_method        none

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_atom_site_fract_y
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_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
Cd      .0          .0          .0          .0279(1) Uani  d      .
Ni      .33512(9)   .25         .04288(8)   .0288(2) Uani  d      .
N(1)    .0936(5)    .1258(2)    .0328(4)    .047(1)  Uani  d      .
N(2)    .5862(5)    .1283(3)    .0593(5)    .058(2)  Uani  d      .
N(3)    .2330(4)    -.0532(2)   .1317(3)    .038(1)  Uani  d      .
N(4)    .1093(5)    -.0202(2)   .8049(4)    .041(1)  Uani  d      .
C(1)    .1825(5)    .1744(2)    .0373(4)    .033(1)  Uani  d      .
C(2)    .4910(5)    .1748(3)    .0512(5)    .039(2)  Uani  d      .
C(3)    .3574(5)    -.0072(3)   .2279(4)    .046(2)  Uani  d      .
C(4)    .3040(5)    .0074(3)    .3584(4)    .036(1)  Uani  d      .
C(5)    .2756(7)    .0795(3)    .4005(5)    .046(2)  Uani  d      .
C(6)    .2300(7)    .0911(3)    .5239(5)    .046(2)  Uani  d      .
C(7)    .2134(5)    .0307(3)    .6062(4)    .036(1)  Uani  d      .
C(8)    .2432(7)    -.0426(3)   .5647(5)    .049(2)  Uani  d      .
C(9)    .2905(7)    -.0534(3)   .4420(5)    .049(2)  Uani  d      .
C(10)   .1662(7)    .0468(3)    .7408(5)    .049(2)  Uani  d      .
N(11)   .9927(11)   .25         .5295(10)   .082(4)  Uani  d      .
C(12)   .9680(15)   .25         .3952(13)   .086(5)  Uani  d      .
C(13)   .8112(16)   .25         .3096(11)   .083(5)  Uani  d      .
C(14)   .6798(15)   .25         .3678(10)   .076(4)  Uani  d      .
C(15)   .5727(15)   .25         .5773(12)   .081(5)  Uani  d      .
C(16)   .5969(18)   .25         .7172(12)   .092(5)  Uani  d      .
C(17)   .7597(22)   .25         .7922(11)   .099(6)  Uani  d      .
C(18)   .8916(17)   .25         .7311(10)   .086(5)  Uani  d      .
C(19)   .8619(13)   .25         .5887(9)    .066(4)  Uani  d      .
C(20)   .7026(12)   .25         .5087(9)    .062(3)  Uani  d      .
H(1)    .29099      -.07731     .06668      .076     Uiso  calc   N(3)
H(2)    .19613      -.09300     .18809      .076     Uiso  calc   N(3)
H(3)    .47219      -.03819     .25041      .076     Uiso  calc   C(3)
H(4)    .37410      .04701      .17994      .076     Uiso  calc   C(3)
H(5)    .28872      .12724      .33738      .076     Uiso  calc   C(5)
H(6)    .20761      .14765      .55503      .076     Uiso  calc   C(6)
H(7)    .22952      -.09037     .62746      .076     Uiso  calc   C(8)
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P-1848-13

H(8)	.31691	-.10957	.41187	.076	Uiso	calc	C(9)
H(9)	.06894	.08900	.72252	.076	Uiso	calc	C(10)
H(10)	.27200	.07001	.81168	.076	Uiso	calc	C(10)
H(11)	.02393	-.04503	.73473	.076	Uiso	calc	N(4)
H(12)	.20319	-.05506	.83204	.076	Uiso	calc	N(4)
H(13)	1.07115	.25	.34906	.076	Uiso	calc	C(12)
H(14)	.79585	.25	.20064	.076	Uiso	calc	C(13)
H(15)	.55950	.25	.30493	.076	Uiso	calc	C(14)
H(16)	.45067	.25	.51760	.076	Uiso	calc	C(15)
H(17)	.49700	.25	.76734	.076	Uiso	calc	C(16)
H(18)	.78188	.25	.90163	.076	Uiso	calc	C(17)
H(19)	1.01327	.25	.79156	.076	Uiso	calc	C(18)

loop_
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Cd	.0275(2)	.0259(2)	.0315(2)	-.0027(2)	.0091(2)	-.0018(2)
Ni	.0301(4)	.0207(3)	.0369(4)	.0	.0100(3)	.0
N(1)	.045(2)	.031(2)	.061(3)	-.009(2)	.004(2)	.000(2)
N(2)	.053(3)	.048(3)	.077(3)	.014(2)	.025(2)	-.007(2)
N(3)	.037(2)	.041(2)	.035(2)	.009(2)	.003(2)	-.005(2)
N(4)	.050(2)	.045(2)	.035(2)	.003(2)	.022(2)	.001(2)
C(1)	.032(2)	.027(2)	.039(2)	.003(2)	.004(2)	-.002(2)
C(2)	.038(2)	.034(2)	.048(2)	.001(2)	.017(2)	-.003(2)
C(3)	.034(2)	.075(4)	.031(2)	-.008(2)	.010(2)	-.007(2)
C(4)	.029(2)	.047(3)	.031(2)	-.004(2)	.003(2)	-.001(2)
C(5)	.061(3)	.038(3)	.041(3)	-.001(2)	.012(2)	.005(2)
C(6)	.061(3)	.034(2)	.046(3)	.001(2)	.018(2)	.001(2)
C(7)	.037(2)	.038(2)	.037(2)	-.002(2)	.013(2)	-.000(2)
C(8)	.073(4)	.038(3)	.044(3)	-.000(3)	.029(3)	-.001(2)
C(9)	.071(4)	.037(3)	.043(3)	.000(3)	.021(3)	-.002(2)
C(10)	.068(3)	.043(3)	.046(3)	-.006(2)	.034(3)	-.006(2)
N(11)	.087(6)	.053(5)	.097(7)	.0	-.003(6)	.0
C(12)	.106(9)	.049(5)	.098(8)	.0	.017(7)	.0
C(13)	.115(9)	.047(5)	.075(7)	.0	-.005(7)	.0
C(14)	.106(8)	.045(5)	.068(6)	.0	.001(6)	.0
C(15)	.107(9)	.043(5)	.094(8)	.0	.021(7)	.0
C(16)	.149(12)	.048(5)	.077(7)	.0	.019(8)	.0
C(17)	.184(15)	.036(5)	.070(7)	.0	.016(9)	.0
C(18)	.148(11)	.036(4)	.058(6)	.0	-.014(7)	.0
C(19)	.088(7)	.033(4)	.067(6)	.0	-.007(5)	.0
C(20)	.084(6)	.027(3)	.064(5)	.0	-.005(5)	.0

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Ni	C(1)	1.859(4)	.	.
Ni	C(2)	1.869(5)	.	.
Cd	N(1)	2.368(4)	.	.
Cd	N(3)	2.331(3)	.	.
Cd	N(4)	2.383(3)	.	1_554
C(1)	N(1)	1.141(5)	.	.
C(2)	N(2)	1.146(6)	.	.
N(3)	C(3)	1.510(6)	.	.
C(3)	C(4)	1.508(6)	.	.
C(4)	C(5)	1.386(6)	.	.

P-1848-14

C(5)	C(6)	1.400(7)	.	.
C(6)	C(7)	1.382(6)	.	.
C(7)	C(8)	1.406(7)	.	.
C(8)	C(9)	1.398(7)	.	.
C(9)	C(4)	1.389(6)	.	.
C(7)	C(10)	1.527(6)	.	.
N(4)	C(10)	1.484(6)	.	.
N(11)	C(12)	1.327(14)	.	.
C(12)	C(13)	1.421(16)	.	.
C(13)	C(14)	1.372(16)	.	.
C(15)	C(16)	1.384(15)	.	.
C(16)	C(17)	1.426(18)	.	.
C(17)	C(18)	1.394(18)	.	.
C(18)	C(19)	1.406(13)	.	.
C(19)	C(20)	1.418(13)	.	.
N(11)	C(19)	1.373(13)	.	.
C(20)	C(14)	1.394(13)	.	.
C(20)	C(15)	1.427(14)	.	.

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_geom_contact_site_symmetry_1
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N(2)	N(3)	3.027(7)	.	3_655
N(2)	N(4)	3.273(6)	.	3_656

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C(1)	Ni	C(2)	88.3(2)	.	.	.
N(1)	Cd	N(3)	94.8(1)	.	.	.
N(1)	Cd	N(4)	94.4(1)	.	.	1_554
N(3)	Cd	N(4)	88.6(1)	.	.	1_554
Ni	C(1)	N(1)	177.1(4)	.	.	.
Ni	C(2)	N(2)	178.5(5)	.	.	.
Cd	N(1)	C(1)	156.4(4)	.	.	.
Cd	N(3)	C(3)	122.5(3)	.	.	.
Cd	N(4)	C(10)	117.7(3)	.	1_554	1_554
N(3)	C(3)	C(4)	110.7(4)	.	.	.
C(3)	C(4)	C(5)	122.2(4)	.	.	.
C(3)	C(4)	C(9)	118.6(4)	.	.	.
C(4)	C(5)	C(6)	120.6(4)	.	.	.
C(5)	C(6)	C(7)	120.4(4)	.	.	.
C(6)	C(7)	C(8)	119.3(4)	.	.	.
C(7)	C(8)	C(9)	119.8(4)	.	.	.
C(8)	C(9)	C(4)	120.7(5)	.	.	.
C(9)	C(4)	C(12)	119.1(4)	.	.	.
C(6)	C(7)	C(10)	118.2(4)	.	.	.
C(10)	C(7)	C(8)	122.6(4)	.	.	.
N(4)	C(10)	C(7)	114.4(4)	.	.	.
N(11)	C(12)	C(13)	122.7(12)	.	.	.
N(11)	C(19)	C(18)	117.7(10)	.	.	.
N(11)	C(19)	C(20)	121.0(9)	.	.	.
C(12)	N(11)	C(19)	118.9(10)	.	.	.
C(12)	C(13)	C(14)	118.8(10)	.	.	.
C(13)	C(14)	C(20)	119.6(10)	.	.	.
C(14)	C(20)	C(15)	123.1(10)	.	.	.

```
C(14)  C(20)  C(19)     119.0(11)   .     .     .
C(15)  C(16)  C(17)     117.0(12)   .     .     .
C(15)  C(20)  C(19)     117.9(9)    .     .     .
C(16)  C(17)  C(18)     123.1(10)   .     .     .
C(16)  C(15)  C(20)     122.6(11)   .     .     .
C(17)  C(18)  C(19)     118.2(11)   .     .     .
C(18)  C(19)  C(20)     121.3(12)   .     .     .

#===END
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_chemical_formula_moiety             'C32 H36 Cd2 N14 Ni2, 2(C4 H5 N)'
_chemical_formula_structural         'Cd2 (C4 N4 Ni)2 (C8 H12 N2)3 2(C4 H5 N)'
_chemical_formula_weight             1093.12
_symmetry_cell_setting               monoclinic
_symmetry_space_group_name_H-M       'C 1 2/c 1'
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   -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+1/2,-y+1/2,-z
   +x+1/2,-y+1/2,+z+1/2

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_cell_length_b                       7.738(2)
_cell_length_c                       31.213(1)
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_cell_angle_beta                     109.138(5)
_cell_angle_gamma                    90.00
_cell_volume                         4522(1)
_cell_formula_units_Z                4
_exptl_crystal_density_diffrn        1.63
_exptl_crystal_density_meas          1.60(1)
_exptl_crystal_density_method
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_diffrn_radiation_type               'Mo K¥a'
_diffrn_radiation_wavelength         0.70926
_cell_measurement_reflns_used        25
_cell_measurement_theta_min          16.40
_cell_measurement_theta_max          17.26
_exptl_absorpt_coefficient_mu        1.796
_cell_measurement_temperature        293
_exptl_crystal_description           flaky
_exptl_crystal_colour                yellow
_exptl_crystal_size_max              0.28
_exptl_crystal_size_mid              0.23
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_diffrn_measurement_device           'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method           '¥w scans'
_exptl_absorpt_correction_type       none
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_reflns_number_total                 5757
_reflns_number_observed              4092
_reflns_observed_criterion           >4sigma(F)
_diffrn_reflns_av_R_equivalents      0.004
_diffrn_reflns_theta_max             30.00
_diffrn_reflns_limit_h_min           0
_diffrn_reflns_limit_h_max           27
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P-1848-16

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_diffrn_reflns_limit_k_min          0
_diffrn_reflns_limit_k_max          10
_diffrn_reflns_limit_l_min          -44
_diffrn_reflns_limit_l_max          41
_diffrn_standards_number            3
_diffrn_standards_interval_count    200
_diffrn_standards_decay_%           0.0

_refine_ls_structure_factor_coef    F
_refine_ls_R_factor_obs             0.0480
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_refine_ls_number_reflns            4092
_refine_ls_number_parameters        273
_refine_ls_hydrogen_treatment       noref
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_refine_ls_shift/esd_max            0.029
_refine_diff_density_max            0.83
_refine_diff_density_min            -0.67
_refine_ls_extinction_method        none

loop_
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_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
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_atom_site_calc_attached_atom
Cd      .36285(2)   .39190(5)   .14136(1)   .0317(1) Uani  d      .
Ni(1)   .5          .8904(1)    .25         .0310(3) Uani  d      .
Ni(2)   .25         .75         .0          .0356(4) Uani  d      .
N(1)    .4397(3)    .6098(7)    .1821(2)    .049(2)  Uani  d      .
N(2)    .4293(3)   1.1667(7)    .1831(2)    .054(2)  Uani  d      .
N(3)    .2962(3)    .6262(8)    .0960(2)    .055(2)  Uani  d      .
N(4)    .3313(5)   1.0829(11)   .0211(3)    .106(4)  Uani  d      .
N(5)    .4215(3)    .3584(7)    .0883(2)    .050(2)  Uani  d      .
N(6)    .3061(3)    .4356(8)    .1971(2)    .050(2)  Uani  d      .
N(7)    .2386(3)    .7370(7)    .4037(2)    .051(2)  Uani  d      .
C(1)    .4625(3)    .7188(8)    .2072(2)    .037(2)  Uani  d      .
C(2)    .4577(3)   1.0609(8)    .2080(2)    .039(2)  Uani  d      .
C(3)    .2796(3)    .6798(8)    .0601(2)    .041(2)  Uani  d      .
C(4)    .3021(4)    .9542(10)   .0146(2)    .055(3)  Uani  d      .
C(5)    .4591(4)    .5159(10)   .0815(2)    .059(3)  Uani  d      .
C(6)    .4798(3)    .5066(8)    .0390(2)    .043(2)  Uani  d      .
C(7)    .5436(4)    .4275(10)   .0402(2)    .056(3)  Uani  d      .
C(8)    .5630(4)    .4208(11)   .0011(2)    .060(3)  Uani  d      .
C(9)    .3494(4)    .3882(11)   .2429(2)    .071(3)  Uani  d      .
C(10)   .3186(4)    .4480(9)    .2796(2)    .046(2)  Uani  d      .
C(11)   .2529(4)    .3850(10)   .2804(2)    .053(3)  Uani  d      .
C(12)   .2298(4)    .4293(9)    .3166(2)    .048(3)  Uani  d      .
C(13)   .2706(3)    .5313(8)    .3522(2)    .041(2)  Uani  d      .
C(14)   .3349(4)    .6000(9)    .3501(2)    .049(3)  Uani  d      .
C(15)   .3583(4)    .5552(10)   .3136(2)    .052(3)  Uani  d      .
C(16)   .2478(4)    .5538(9)    .3936(2)    .054(3)  Uani  d      .
N(21)   .1059(6)    .5059(11)   .0723(3)    .101(5)  Uani  d      .
C(22)   .1351(5)    .5817(12)   .1141(4)    .084(5)  Uani  d      .
C(23)   .0885(7)    .5585(12)   .1366(3)    .092(5)  Uani  d      .
C(24)   .0289(6)    .4721(14)   .1088(5)    .096(6)  Uani  d      .
C(25)   .0390(7)    .4401(12)   .0697(4)    .092(5)  Uani  d      .
H(1)    .38540      .32582      .05859      .076     Uiso  calc   N(5)
H(2)    .45733      .26339      .09878      .076     Uiso  calc   N(5)
H(3)    .42379      .62789      .07887      .076     Uiso  calc   C(5)
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P-1848-17

H(4)	.50780	.53237	.11089	.076	Uiso	calc	C(5)
H(5)	.57806	.37148	.07139	.076	Uiso	calc	C(7)
H(6)	.61215	.35780	.00221	.076	Uiso	calc	C(8)
H(7)	.26142	.36476	.18843	.076	Uiso	calc	N(6)
H(8)	.29353	.56083	.19702	.076	Uiso	calc	N(6)
H(9)	.35438	.24663	.24464	.076	Uiso	calc	C(9)
H(10)	.40260	.44645	.25006	.076	Uiso	calc	C(9)
H(11)	.22061	.30330	.25341	.076	Uiso	calc	C(11)
H(12)	.17864	.38264	.31687	.076	Uiso	calc	C(12)
H(13)	.36613	.68653	.37620	.076	Uiso	calc	C(14)
H(14)	.40843	.60585	.31240	.076	Uiso	calc	C(15)
H(15)	.28872	.49615	.42295	.076	Uiso	calc	C(16)
H(16)	.19668	.48628	.38773	.076	Uiso	calc	C(16)
H(17)	.23797	.74150	.43559	.076	Uiso	calc	N(7)
H(18)	.28146	.80018	.40169	.076	Uiso	calc	N(7)
H(19)	.12856	.49895	.04805	.076	Uiso	calc	N(21)
H(20)	.18641	.64509	.12367	.076	Uiso	calc	C(22)
H(21)	.09771	.60190	.17093	.076	Uiso	calc	C(23)
H(22)	-.01813	.43573	.11687	.076	Uiso	calc	C(24)
H(23)	.00515	.37635	.03955	.076	Uiso	calc	C(25)

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_atom_site_aniso_U_33
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_atom_site_aniso_U_23

Cd	.0453(2)	.0281(2)	.0238(2)	-.0023(2)	.0144(2)	.0012(2)
Ni(1)	.0387(5)	.0222(4)	.0300(5)	.0	.0083(4)	.0
Ni(2)	.0442(6)	.0338(6)	.0286(5)	.0026(5)	.0117(4)	.0023(4)
N(1)	.060(4)	.037(3)	.046(3)	-.007(3)	.013(3)	-.007(3)
N(2)	.080(4)	.041(3)	.045(3)	.017(3)	.025(3)	.015(3)
N(3)	.063(4)	.054(4)	.039(3)	.003(3)	.007(3)	.013(3)
N(4)	.152(8)	.094(6)	.082(5)	-.075(6)	.053(5)	-.033(5)
N(5)	.074(4)	.040(3)	.050(3)	-.015(3)	.042(3)	-.004(2)
N(6)	.063(4)	.064(4)	.026(2)	.004(3)	.017(2)	-.004(2)
N(7)	.067(4)	.053(3)	.034(3)	.022(3)	.016(3)	.003(2)
C(1)	.043(4)	.029(3)	.034(3)	.004(3)	.007(3)	.005(2)
C(2)	.049(4)	.036(3)	.034(3)	.003(3)	.016(3)	-.001(2)
C(3)	.042(4)	.039(3)	.038(3)	.001(3)	.006(3)	.001(3)
C(4)	.075(5)	.055(4)	.041(4)	-.015(4)	.026(4)	-.012(3)
C(5)	.076(5)	.063(5)	.055(4)	-.030(4)	.044(4)	-.014(4)
C(6)	.053(4)	.038(3)	.048(3)	-.006(3)	.031(3)	.000(3)
C(7)	.064(5)	.064(5)	.044(4)	.011(4)	.022(3)	.007(3)
C(8)	.047(4)	.084(6)	.054(4)	.014(4)	.025(3)	.001(4)
C(9)	.090(6)	.100(6)	.032(3)	.036(5)	.034(4)	.006(4)
C(10)	.057(4)	.052(4)	.032(3)	.014(3)	.019(3)	.007(3)
C(11)	.063(4)	.057(4)	.047(4)	-.007(4)	.027(3)	-.008(3)
C(12)	.056(4)	.048(4)	.044(3)	.002(3)	.024(3)	.000(3)
C(13)	.056(4)	.033(3)	.041(3)	.014(3)	.024(3)	.008(3)
C(14)	.056(4)	.051(4)	.043(3)	.003(4)	.020(3)	-.003(3)
C(15)	.046(4)	.067(5)	.046(4)	-.002(4)	.019(3)	.003(3)
C(16)	.085(5)	.043(4)	.045(4)	.023(4)	.036(4)	.006(3)
N(21)	.144(9)	.071(6)	.104(7)	.052(6)	.064(7)	.038(5)
C(22)	.063(6)	.070(7)	.109(8)	.009(5)	.016(6)	.026(6)
C(23)	.128(9)	.056(6)	.094(7)	.024(6)	.040(7)	.002(5)
C(24)	.084(7)	.067(6)	.145(11)	-.002(6)	.049(8)	.008(7)
C(25)	.100(8)	.051(6)	.100(8)	-.004(5)	-.001(7)	.011(5)

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2

P-1848-18

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_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
 Ni(1)  C(1)      1.856(6)   .   .
 Ni(1)  C(2)      1.855(6)   .   .
 Ni(2)  C(3)      1.854(6)   .   .
 Ni(2)  C(4)      1.860(7)   .   .
 Cd     N(1)      2.347(5)   .   .
 Cd     N(2)      2.311(5)   .   1_545
 Cd     N(3)      2.410(6)   .   .
 Cd     N(5)      2.329(5)   .   .
 Cd     N(6)      2.385(5)   .   .
 Cd     N(7)      2.367(5)   .   6_545
 C(1)   N(1)      1.140(7)   .   .
 C(2)   N(2)      1.143(7)   .   .
 C(3)   N(3)      1.137(7)   .   .
 C(4)   N(4)      1.136(9)   .   .
 N(5)   C(5)      1.479(8)   .   .
 C(5)   C(6)      1.513(8)   .   .
 C(6)   C(7)      1.395(9)   .   .
 C(7)   C(8)      1.395(9)   .   .
 C(8)   C(6)      1.380(9)   .   3_665
 N(6)   C(9)      1.453(8)   .   .
 C(9)   C(10)     1.534(8)   .   .
 C(10)  C(11)     1.398(9)   .   .
 C(11)  C(12)     1.393(8)   .   .
 C(12)  C(13)     1.386(9)   .   .
 C(13)  C(14)     1.402(9)   .   .
 C(14)  C(15)     1.405(9)   .   .
 C(15)  C(10)     1.375(9)   .   .
 C(13)  C(16)     1.512(8)   .   .
 N(7)   C(16)     1.477(8)   .   .
 N(21)  C(22)     1.371(12)  .   .
 C(22)  C(23)     1.343(13)  .   .
 C(23)  C(24)     1.386(14)  .   .
 C(24)  C(25)     1.322(14)  .   .
 C(25)  N(21)     1.399(13)  .   .

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
 N(4)   N(5)      3.111(9)  1_545   .
 N(4)   N(7)      3.313(12) 6_545   .
 N(4)   N(21)     3.592(15) 7_565   .
 N(7)   N(21)     3.588(12) 6_545   .

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_2
_geom_angle_site_symmetry_3
 C(1)   Ni(1)  C(2)      91.1(2)    .    .    .
 C(3)   Ni(2)  C(4)      92.1(3)    .    .    .
 N(1)   Cd     N(2)      95.0(2)    .    .    1_545
 N(1)   Cd     N(3)      84.9(2)    .    .    .
 N(1)   Cd     N(5)      94.5(2)    .    .    .
 N(1)   Cd     N(6)      83.2(2)    .    .    .
 N(1)   Cd     N(7)      163.7(2)   .    .    6_545
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P-1848-19

```
 N(2)   Cd     N(3)      177.8(2)   1_545   .      .
 N(2)   Cd     N(5)       89.5(2)   1_545   .      .
 N(2)   Cd     N(6)       90.8(2)   1_545   .      .
 N(2)   Cd     N(7)       99.7(2)   1_545   .      6_545
 N(3)   Cd     N(5)       88.3(2)    .      .      .
 N(3)   Cd     N(6)       91.3(2)    .      .      .
 N(3)   Cd     N(7)       80.6(2)    .      .      6_545
 N(5)   Cd     N(6)      177.6(2)    .      .      .
 N(5)   Cd     N(7)       92.6(2)    .      .      6_545
 N(6)   Cd     N(7)       89.6(2)    .      .      6_545
 Ni(1)  C(1)   N(1)      177.9(5)    .      .      .
 Ni(1)  C(2)   N(2)      176.8(6)    .      .      .
 Ni(2)  C(3)   N(3)      175.5(6)    .      .      .
 Ni(2)  C(4)   N(4)      176.0(8)    .      .      .
 Cd     N(1)   C(1)      160.8(5)    .      .      .
 Cd     N(2)   C(2)      170.5(5)    .      1_545  1_545
 Cd     N(3)   C(3)      141.2(6)    .      .      .
 Cd     N(5)   C(5)      113.8(4)    .      .      .
 Cd     N(6)   C(9)      114.4(4)    .      .      .
 Cd     N(7)   C(16)     120.0(4)    .      6_545  6_545
 N(5)   C(5)   C(6)      112.4(5)    .      .      .
 C(5)   C(6)   C(7)      120.1(6)    .      .      .
 C(6)   C(7)   C(8)      120.0(6)    .      .      .
 C(7)   C(8)   C(6)      121.0(7)    .      .      3_665
 N(6)   C(9)   C(10)     114.0(6)    .      .      .
 C(9)   C(10)  C(11)     120.6(7)    .      .      .
 C(9)   C(10)  C(15)     119.4(7)    .      .      .
 C(11)  C(10)  C(15)     119.8(6)    .      .      .
 C(10)  C(11)  C(12)     119.0(6)    .      .      .
 C(11)  C(12)  C(13)     122.0(6)    .      .      .
 C(12)  C(13)  C(14)     118.5(6)    .      .      .
 C(12)  C(13)  C(16)     119.5(6)    .      .      .
 C(14)  C(13)  C(16)     121.8(6)    .      .      .
 C(13)  C(14)  C(15)     119.4(6)    .      .      .
 C(10)  C(15)  C(14)     121.1(6)    .      .      .
 N(7)   C(16)  C(13)     112.7(5)    .      .      .
 N(21)  C(22)  C(23)     107.1(9)    .      .      .
 C(22)  C(23)  C(24)     109.1(10)   .      .      .
 C(23)  C(24)  C(25)     108.2(10)   .      .      .
 C(24)  C(25)  N(21)     107.8(10)   .      .      .
 C(25)  N(21)  C(22)     107.8(9)    .      .      .
#===END
data_compound_(5)

_chemical_formula_sum                'C24 H26 Cd N8 Ni'
_chemical_formula_moiety             'C24 H26 Cd N8 Ni'
_chemical_formula_structural         'Cd (C4 N4 Ni) (C8 H12 N2) (C6 H7 N)'
_chemical_formula_weight             597.63
_symmetry_cell_setting               monoclinic
_symmetry_space_group_name_H-M       'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
   +x,+y,+z
   -x,+y,-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
   -x+1/2,-y+1/2,-z
   +x+1/2,-y+1/2,+z+1/2

_cell_length_a                       22.240(1)
_cell_length_b                       9.254(1)
_cell_length_c                       16.241(1)
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P-1848-20

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_cell_angle_alpha                    90.00
_cell_angle_beta                     130.668(3)
_cell_angle_gamma                     90.00
_cell_volume                          2545.5(4)
_cell_formula_units_Z                 4
_exptl_crystal_density_diffrn        1.56
_exptl_crystal_density_meas           1.54(1)
_exptl_crystal_density_method
          'flotation in mesitylene-bromoform'
_diffrn_radiation_type               'Mo K¥a'
_diffrn_radiation_wavelength          0.70926
_cell_measurement_reflns_used          25
_cell_measurement_theta_min            16.28
_cell_measurement_theta_max            17.48
_exptl_absorpt_coefficient_mu        1.434
_cell_measurement_temperature          293
_exptl_crystal_description           block-like
_exptl_crystal_colour                yellow
_exptl_crystal_size_max               0.30
_exptl_crystal_size_mid               0.25
_exptl_crystal_size_min               0.20

_diffrn_measurement_device             'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method              '2¥q-¥w scans'
_exptl_absorpt_correction_type       empirical
_exptl_absorpt_correction_T_min       0.854
_exptl_absorpt_correction_T_max       0.998
_diffrn_reflns_number                 4100
_reflns_number_total                  3407
_reflns_number_observed                2810
_reflns_observed_criterion           >4sigma(F)
_diffrn_reflns_av_R_equivalents       0.006
_diffrn_reflns_theta_max              30.00
_diffrn_reflns_limit_h_min            0
_diffrn_reflns_limit_h_max            31
_diffrn_reflns_limit_k_min            0
_diffrn_reflns_limit_k_max            13
_diffrn_reflns_limit_l_min           -22
_diffrn_reflns_limit_l_max           17
_diffrn_standards_number               3
_diffrn_standards_interval_count     200
_diffrn_standards_decay_%              0.0

_refine_ls_structure_factor_coef   F
_refine_ls_R_factor_obs               0.0389
_refine_ls_wR_factor_obs              0.0444
_refine_ls_goodness_of_fit_obs       1.174
_refine_ls_number_reflns              2810
_refine_ls_number_parameters           156
_refine_ls_hydrogen_treatment         noref
_refine_ls_weighting_scheme           'calc w=1/(¥s^2^(Fo)+0.0004Fo^2^)'
_refine_ls_shift/esd_max              0.002
_refine_diff_density_max              0.60
_refine_diff_density_min             -0.90
_refine_ls_extinction_method          none

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_calc_flag
```

P-1848-21

_atom_site_calc_attached_atom

Cd	.0	.0	.0	.0255(2)	Uani	d	.
Ni	.0	.36207(8)	.25	.0256(4)	Uani	d	.
N(1)	.0165(2)	.1385(4)	.1321(3)	.038(3)	Uani	d	.
N(2)	.0044(3)	.5968(5)	.1266(4)	.054(4)	Uani	d	.
N(3)	.0991(2)	.1359(4)	.0220(3)	.035(2)	Uani	d	.
C(1)	.0094(3)	.2222(5)	.1771(3)	.029(2)	Uani	d	.
C(2)	.0045(3)	.5066(5)	.1746(4)	.035(3)	Uani	d	.
C(3)	.1257(3)	.0782(5)	-.0351(5)	.044(4)	Uani	d	.
C(4)	.1904(3)	.1678(5)	-.0159(4)	.033(3)	Uani	d	.
C(5)	.1719(3)	.2707(6)	-.0914(4)	.040(3)	Uani	d	.
C(6)	.2305(3)	.3521(6)	-.0768(4)	.042(3)	Uani	d	.
N(11)	.1013(2)	-.1607(4)	.1487(3)	.039(2)	Uani	d	.
C(11)	.1619(3)	-.2156(5)	.1490(4)	.035(3)	Uani	d	.
C(12)	.1447(3)	-.3286(6)	.0811(4)	.048(3)	Uani	d	.
C(13)	.1998(4)	-.3749(8)	.0745(5)	.067(5)	Uani	d	.
C(14)	.2743(4)	-.3111(9)	.1389(6)	.074(5)	Uani	d	.
C(15)	.2920(3)	-.2004(8)	.2102(6)	.063(4)	Uani	d	.
C(16)	.2360(3)	-.1512(6)	.2152(4)	.049(3)	Uani	d	.
H(1)	.14627	.14030	.10136	.076	Uiso	calc	N(3)
H(2)	.07813	.23574	-.00575	.076	Uiso	calc	N(3)
H(3)	.14800	-.03240	-.00614	.076	Uiso	calc	C(3)
H(4)	.07461	.07591	-.12276	.076	Uiso	calc	C(3)
H(5)	.11068	.28773	-.16296	.076	Uiso	calc	C(5)
H(6)	.21497	.43066	-.13714	.076	Uiso	calc	C(6)
H(7)	.12857	-.10615	.21795	.076	Uiso	calc	N(11)
H(8)	.07310	-.24595	.14735	.076	Uiso	calc	N(11)
H(9)	.08744	-.38056	.03293	.076	Uiso	calc	C(12)
H(10)	.18539	-.46105	.01940	.076	Uiso	calc	C(13)
H(11)	.31811	-.34674	.13385	.076	Uiso	calc	C(14)
H(12)	.35042	-.15264	.26206	.076	Uiso	calc	C(15)
H(13)	.24961	-.06443	.26953	.076	Uiso	calc	C(16)

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23

Cd	.0288(2)	.0252(2)	.0350(2)	-.0057(2)	.0264(2)	-.0052(2)
Ni	.0342(4)	.0218(3)	.0291(4)	.0	.0243(3)	.0
N(1)	.040(2)	.040(2)	.045(2)	-.011(2)	.033(2)	-.013(2)
N(2)	.073(3)	.041(2)	.059(3)	-.009(2)	.048(3)	.007(2)
N(3)	.032(2)	.041(2)	.045(2)	-.013(2)	.031(2)	-.007(2)
C(1)	.031(2)	.031(2)	.033(2)	-.005(2)	.025(2)	-.002(2)
C(2)	.043(2)	.031(2)	.038(2)	-.004(2)	.029(2)	-.003(2)
C(3)	.051(3)	.044(3)	.067(3)	-.018(2)	.052(3)	-.013(3)
C(4)	.035(2)	.038(2)	.044(3)	-.008(2)	.033(2)	-.006(2)
C(5)	.033(2)	.050(3)	.042(3)	-.006(2)	.027(2)	.003(2)
C(6)	.040(3)	.047(3)	.047(3)	-.002(2)	.032(2)	.010(2)
N(11)	.040(2)	.040(2)	.040(2)	.003(2)	.027(2)	.007(2)
C(11)	.034(2)	.034(2)	.035(2)	.004(2)	.021(2)	.008(2)
C(12)	.048(3)	.046(3)	.042(3)	.008(2)	.025(3)	.005(2)
C(13)	.066(4)	.073(4)	.062(4)	.024(4)	.041(4)	.009(4)
C(14)	.063(4)	.093(5)	.077(5)	.031(4)	.051(4)	.031(4)
C(15)	.038(3)	.070(4)	.068(4)	.008(3)	.028(3)	.021(3)
C(16)	.035(3)	.049(3)	.048(3)	-.001(2)	.020(2)	.008(3)

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance

P-1848-22

```
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
 Ni    C(1)    1.855(4)   .   .
 Ni    C(2)    1.860(5)   .   .
 Cd    N(1)    2.315(4)   .   .
 Cd    N(3)    2.354(3)   .   .
 Cd    N(11)   2.455(4)   .   .
 C(1)  N(1)    1.144(5)   .   .
 C(2)  N(2)    1.141(6)   .   .
 N(3)  C(3)    1.486(6)   .   .
 C(3)  C(4)    1.506(6)   .   .
 C(4)  C(5)    1.387(6)   .   .
 C(5)  C(6)    1.386(6)   .   .
 C(6)  C(4)    1.394(6)   .   7_555
 N(11) C(11)   1.436(6)   .   .
 C(11) C(12)   1.381(7)   .   .
 C(12) C(13)   1.365(8)   .   .
 C(13) C(14)   1.390(10)  .   .
 C(14) C(15)   1.397(10)  .   .
 C(15) C(16)   1.377(8)   .   .
 C(16) C(11)   1.385(7)   .   .

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
 N(2)  N(3)    3.162(6)   .   3_565
 N(2)  N(11)   2.967(8)   .   1_565

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_2
_geom_angle_site_symmetry_3
 C(1)  Ni    C(2)    90.3(2)    .    .    .
 N(1)  Cd    N(3)    89.8(1)    .    .    .
 N(1)  Cd    N(11)   86.2(1)    .    .    .
 N(3)  Cd    N(11)   90.3(1)    .    .    .
 Ni    C(1)  N(1)   178.1(4)    .    .    .
 Ni    C(2)  N(2)   177.4(5)    .    .    .
 Cd    N(1)  C(1)   164.3(4)    .    .    .
 Cd    N(3)  C(3)   115.2(3)    .    .    .
 Cd    N(11) C(11)  118.4(3)    .    .    .
 N(3)  C(3)  C(4)   112.7(4)    .    .    .
 C(3)  C(4)  C(5)   120.2(4)    .    .    .
 C(4)  C(5)  C(6)   121.2(4)    .    .    .
 C(3)  C(4)  C(6)   120.9(5)    .    .    7_555
 C(5)  C(4)  C(6)   118.9(6)    .    .    7_555
 C(5)  C(6)  C(4)   119.9(6)    .    .    7_555
 N(11) C(11) C(12)  119.6(4)    .    .    .
 N(11) C(11) C(16)  119.3(5)    .    .    .
 C(11) C(12) C(13)  120.3(6)    .    .    .
 C(12) C(13) C(14)  120.0(6)    .    .    .
 C(13) C(14) C(15)  119.2(6)    .    .    .
 C(14) C(15) C(16)  121.0(6)    .    .    .
 C(15) C(16) C(11)  118.4(6)    .    .    .
 C(16) C(11) C(12)  121.1(5)    .    .    .
#===END
data_compound_(6)
```

P-1848-23

```
_chemical_formula_sum                'C12 H14 N6 Ni'
_chemical_formula_moiety             '(C4 N4 Ni), (C8 H14 N2)'
_chemical_formula_weight             300.98
_symmetry_cell_setting               triclinic
_symmetry_space_group_name_H-M       'P -1'
loop_
_symmetry_equiv_pos_as_xyz
   +x,+y,+z
   -x,-y,-z

_cell_length_a                       7.392(3)
_cell_length_b                       7.921(2)
_cell_length_c                       6.247(1)
_cell_angle_alpha                    90.89(2)
_cell_angle_beta                     101.49(2)
_cell_angle_gamma                    70.92(2)
_cell_volume                         338.2(2)
_cell_formula_units_Z                1
_exptl_crystal_density_diffrn        1.48
_exptl_crystal_density_meas          1.46(1)
_exptl_crystal_density_method
         'flotation in mesitylene-bromoform'
_diffrn_radiation_type               'Mo K¥a'
_diffrn_radiation_wavelength         0.70926
_cell_measurement_reflns_used        25
_cell_measurement_theta_min          16.70
_cell_measurement_theta_max          17.48
_exptl_absorpt_coefficient_mu        1.434
_cell_measurement_temperature        293
_exptl_crystal_description           plate-like
_exptl_crystal_colour                yellow
_exptl_crystal_size_max              0.26
_exptl_crystal_size_mid              0.20
_exptl_crystal_size_min              0.18

_diffrn_measurement_device           'RIGAKU AFC5R diffractometer'
_diffrn_measurement_method           '2¥q-¥w scans'
_exptl_absorpt_correction_type       none
_diffrn_reflns_number                2176
_reflns_number_total                 1890
_reflns_number_observed              1646
_reflns_observed_criterion           >4sigma(F)
_diffrn_reflns_av_R_equivalents      0.009
_diffrn_reflns_theta_max             30.00
_diffrn_reflns_limit_h_min           0
_diffrn_reflns_limit_h_max           10
_diffrn_reflns_limit_k_min           -10
_diffrn_reflns_limit_k_max           11
_diffrn_reflns_limit_l_min           -8
_diffrn_reflns_limit_l_max           8
_diffrn_standards_number             3
_diffrn_standards_interval_count     200
_diffrn_standards_decay_%            0.0

_refine_ls_structure_factor_coef     F
_refine_ls_R_factor_obs              0.0507
_refine_ls_wR_factor_obs             0.0456
_refine_ls_goodness_of_fit_obs       2.171
_refine_ls_number_reflns             1646
_refine_ls_number_parameters         116
_refine_ls_hydrogen_treatment        refall
_refine_ls_weighting_scheme          'calc w=1/(¥s^2^(Fo)+0.00005Fo^2^)'
_refine_ls_shift/esd_max             0.000
```

P-1848-24

```
_refine_diff_density_max          0.68
_refine_diff_density_min          -0.76
_refine_ls_extinction_method      none

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
Ni    .5          .5          .5          .0288(2) Uani
N(1)  .2182(4)    .8064(4)    .1959(5)    .047(1)  Uani
N(2)  .4417(4)    .2356(3)    .1681(4)    .046(1)  Uani
C(1)  .3267(4)    .6886(4)    .3079(5)    .033(1)  Uani
C(2)  .4638(4)    .3374(4)    .2929(5)    .034(1)  Uani
N(3)  .2101(4)    .0827(4)    .8555(4)    .035(1)  Uani
C(3)  .2448(6)    .1369(4)    .6441(6)    .041(1)  Uani
C(4)  .1174(4)    .3254(4)    .5709(5)    .034(1)  Uani
C(5)  .1314(5)    .4665(4)    .6960(5)    .038(1)  Uani
C(6)  .0147(5)    .6398(4)    .6260(5)    .039(1)  Uani
H(1)  .071(6)     .113(5)     .848(6)     .057(11) Uiso
H(2)  .256(5)     .138(5)     .969(6)     .054(11) Uiso
H(3)  .266(5)     -.038(5)    .886(5)     .052(10) Uiso
H(4)  .382(6)     .121(5)     .666(6)     .055(11) Uiso
H(5)  .218(5)     .048(5)     .539(5)     .050(10) Uiso
H(6)  .223(5)     .450(4)     .821(5)     .041(9)  Uiso
H(7)  .020(5)     .741(4)     .712(5)     .042(9)  Uiso

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Ni    .0298(3)  .0242(3)  .0257(3) -.0027(2)  .0010(2)  .0021(2)
N(1)  .037(2)   .045(2)   .047(2)  -.003(1)   .001(1)   .016(1)
N(2)  .052(2)   .035(1)   .037(1)  -.001(1)   -.000(1)  -.004(1)
C(1)  .029(2)   .035(2)   .031(2)  -.008(1)   .004(1)   .000(1)
C(2)  .031(2)   .029(2)   .031(2)   .002(1)   .002(1)   .004(1)
N(3)  .035(2)   .028(1)   .035(1)  -.005(1)   -.000(1)  .008(1)
C(3)  .044(2)   .031(2)   .037(2)   .001(2)   .009(2)   .010(1)
C(4)  .035(2)   .028(1)   .033(2)  -.002(1)   .010(1)   .008(1)
C(5)  .037(2)   .037(2)   .032(2)  -.008(1)   .000(1)   .009(1)
C(6)  .045(2)   .031(2)   .036(2)  -.006(2)   .007(2)   .004(1)

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
 Ni    C(1)    1.872(3)   .    .
 Ni    C(2)    1.855(3)   .    .
 C(1)  N(1)    1.145(4)   .    .
 C(2)  N(2)    1.141(4)   .    .
 N(3)  C(3)    1.489(4)   .    .
 C(3)  C(4)    1.502(4)   .    .
 C(4)  C(5)    1.373(4)   .    .
 C(5)  C(6)    1.383(4)   .    .
 C(6)  C(4)    1.378(4)   .    2_566
 N(3)  H(1)    0.97(4)    .    .
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P-1848-25

```
  N(3)   H(2)     0.89(4)    .   .
  N(3)   H(3)     0.92(4)    .   .
  C(3)   H(4)     0.96(4)    .   .
  C(3)   H(5)     1.00(3)    .   .
  C(5)   H(6)     0.91(3)    .   .
  C(6)   H(7)     0.97(3)    .   .

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
  N(3)   N(1)     2.947(4)   .   2_566
  N(3)   N(2)     2.857(4)   .   1_556
  N(3)   N(1)     3.053(4)   .   1_546
  N(3)   N(2)     2.983(4)   .   2_656
  H(1)   N(1)     1.99(4)    .   2_566
  H(2)   N(2)     2.01(4)    .   1_556
  H(3)   N(1)     2.45(4)    .   1_546
  H(3)   N(2)     2.30(3)    .   2_656

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_2
_geom_angle_site_symmetry_3
  C(1)   Ni      C(2)      90.2(1)    .      .      .
  Ni     C(1)    N(1)      177.9(3)   .      .      .
  Ni     C(2)    N(2)      179.0(3)   .      .      .
  N(3)   C(3)    C(4)      111.1(3)   .      .      .
  C(3)   C(4)    C(5)      121.1(3)   .      .      .
  C(4)   C(5)    C(6)      120.7(3)   .      .      .
  C(5)   C(6)    C(4)      120.7(3)   .      .      2_566
  C(3)   N(3)    H(1)      110(2)     .      .      .
  C(3)   N(3)    H(2)      113(2)     .      .      .
  C(3)   N(3)    H(3)      112(2)     .      .      .
  H(1)   N(3)    H(2)      107(3)     .      .      .
  H(1)   N(3)    H(3)      108(3)     .      .      .
  H(2)   N(3)    H(3)      108(3)     .      .      .
  N(3)   C(3)    H(4)      107(2)     .      .      .
  N(3)   C(3)    H(5)      106(2)     .      .      .
  C(4)   C(3)    H(4)      113(2)     .      .      .
  C(4)   C(3)    H(5)      113(2)     .      .      .
  H(4)   C(3)    H(5)      108(3)     .      .      .
  C(4)   C(5)    H(6)      121(2)     .      .      .
  C(6)   C(5)    H(6)      118(2)     .      .      .
  C(5)   C(6)    H(7)      122(2)     .      .      .
  C(4)   C(6)    H(7)      117(2)     2_566  .      .
#===END
# ----------------------end-of-file----------------------
```