Synthesis and characterization of heterobimetallic complexes with pyridyl selenolato ligands. Crystal structure of [{Pt(C_5H_4N)(SeC_5H_4N)(dppp)}$ZnCl_2$]

Rohit Singh Chauhan, Neelam Shivran, Alexandra M. Z. Slawin and J. Derek Woollins

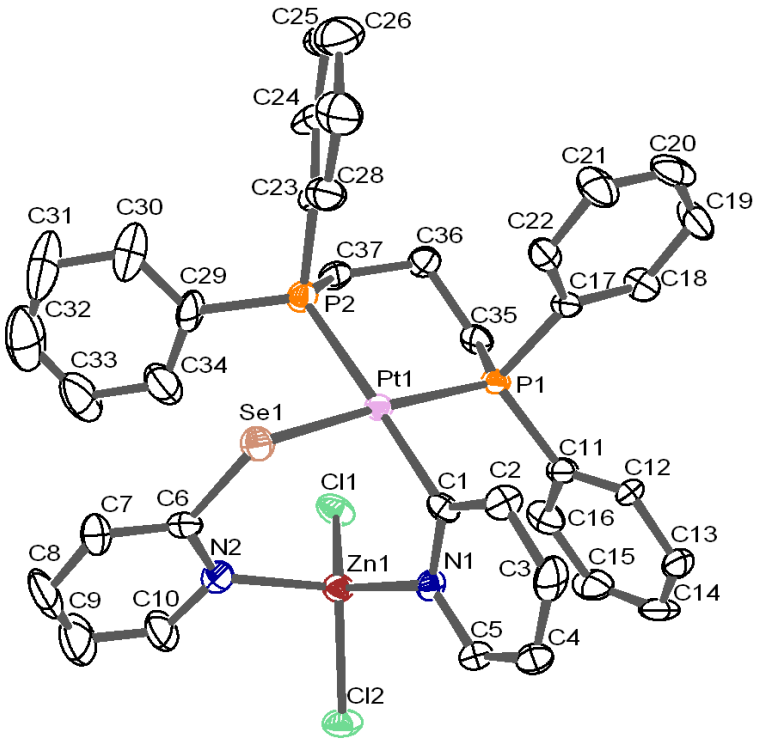

Figure S1- Crystal Structure of [{Pt(C_5H_4N)(SeC_5H_4N)(dppp)}$ZnCl_2$]

Crystal Information File of [{Pt(C_5H_4N)(SeC_5H_4N)(dppp)}$ZnCl_2$]

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H37B H 0.2530 0.3281 0.6518 0.062 Uiso 1 1 calc R . .
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C15 C 0.0031(6) 0.4571(18) 0.3293(6) 0.077(4) Uani 1 1 d . . .
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C28 C 0.3448(6) 0.7564(15) 0.6274(6) 0.065(3) Uani 1 1 d . . .
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C3 C 0.1809(6) 0.8963(14) 0.3169(6) 0.068 Uani 1 1 d . . .
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C25 C 0.3347(8) 0.708(2) 0.7545(7) 0.102(6) Uani 1 1 d . . .
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C6 C 0.3844(6) 0.4448(13) 0.4122(5) 0.058(3) Uani 1 1 d . . .
C19 C 0.0474(7) 0.9141(15) 0.5779(7) 0.083(4) Uani 1 1 d . . .
H19 H 0.0038 0.9339 0.5827 0.100 Uiso 1 1 calc R . .
C36 C 0.1657(5) 0.4326(12) 0.6077(5) 0.052(3) Uani 1 1 d . . .
H36A H 0.1739 0.5315 0.6264 0.063 Uiso 1 1 calc R . .
H36B H 0.1435 0.3749 0.6359 0.063 Uiso 1 1 calc R . .
C21 C 0.1617(7) 0.9761(14) 0.5987(6) 0.077(4) Uani 1 1 d . . .
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C9 C 0.4199(9) 0.202(2) 0.3483(9) 0.116(6) Uani 1 1 d . . .
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C12 C 0.0517(5) 0.7242(13) 0.3845(4) 0.046(3) Uani 1 1 d . . .
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C10 C 0.3535(7) 0.2348(16) 0.3456(6) 0.085(4) Uani 1 1 d . . .
H10 H 0.3203 0.1711 0.3227 0.102 Uiso 1 1 calc R . .
C5 C 0.1754(5) 0.6512(13) 0.2781(5) 0.049(3) Uani 1 1 d . . .
H5 H 0.1637 0.5844 0.2435 0.058 Uiso 1 1 calc R . .
C35 C 0.1170(5) 0.4461(11) 0.5393(5) 0.049(3) Uani 1 1 d . . .
H35A H 0.0716 0.4650 0.5448 0.059 Uiso 1 1 calc R . .
H35B H 0.1165 0.3524 0.5161 0.059 Uiso 1 1 calc R . .
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C2 C 0.2074(5) 0.8424(10) 0.3793(5) 0.048(3) Uani 1 1 d . . .
H2 H 0.2188 0.9082 0.4143 0.057 Uiso 1 1 calc R . .
C27 C 0.3633(6) 0.8672(17) 0.6740(7) 0.088(5) Uani 1 1 d . . .
H27 H 0.3792 0.9584 0.6627 0.105 Uiso 1 1 calc R . .
C34 C 0.3622(8) 0.2445(18) 0.5393(7) 0.105(6) Uani 1 1 d . . .
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H34 H 0.3247 0.2391 0.5045 0.126 Uiso 1 1 calc R . .
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C16 C 0.0516(6) 0.4596(14) 0.3880(6) 0.062(3) Uani 1 1 d . . .
H16 H 0.0672 0.3706 0.4087 0.074 Uiso 1 1 calc R . .
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C13 C 0.0028(6) 0.7178(17) 0.3253(5) 0.072(4) Uani 1 1 d . . .
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C28 0.064(9) 0.080(10) 0.053(7) -0.013(7) 0.019(6) -0.009(8)
C3 0.069 0.059 0.078 0.041 0.024 0.017
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C34 0.135(15) 0.114(13) 0.081(10) 0.022(10) 0.053(10) 0.068(12)
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C8 0.083(13) 0.17(2) 0.142(16) -0.067(14) 0.037(12) 0.052(13)
C30 0.058(10) 0.107(13) 0.157(16) 0.031(11) -0.001(11) 0.018(10)
C33 0.20(2) 0.132(16) 0.109(14) 0.058(13) 0.081(15) 0.117(17)
C31 0.063(12) 0.106(16) 0.25(3) 0.028(17) -0.018(15) 0.025(13)
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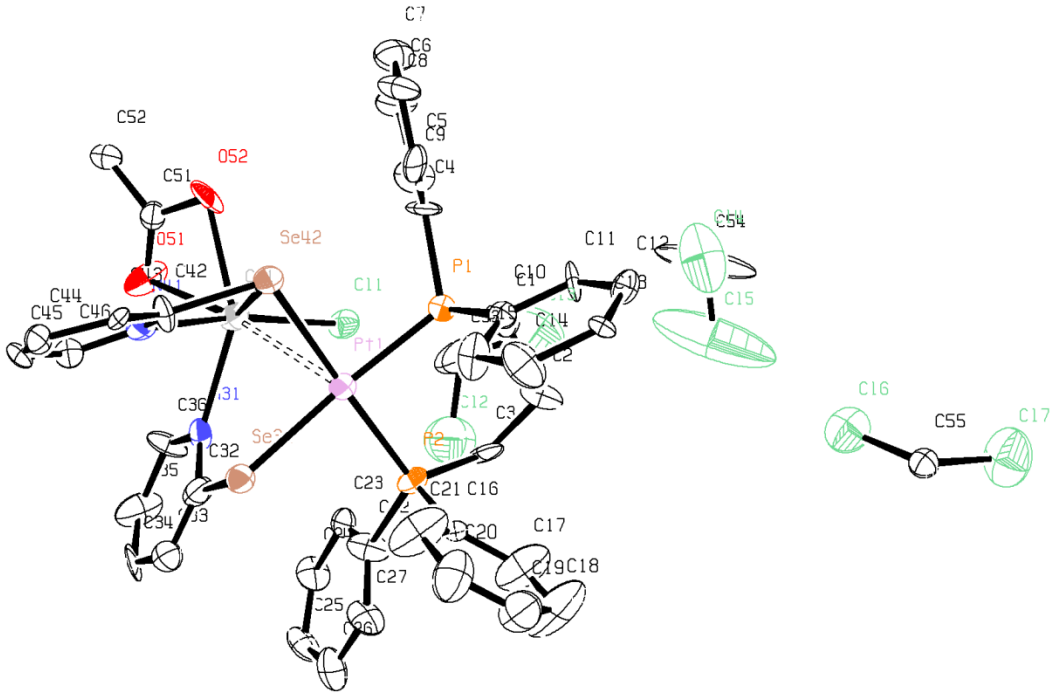

Figure S2- Crystal Structure of [{Pt(SeC$_5$H$_4$N)$_2$(dppp)}CdCl(OAc)]. 3CH$_2$Cl$_2$

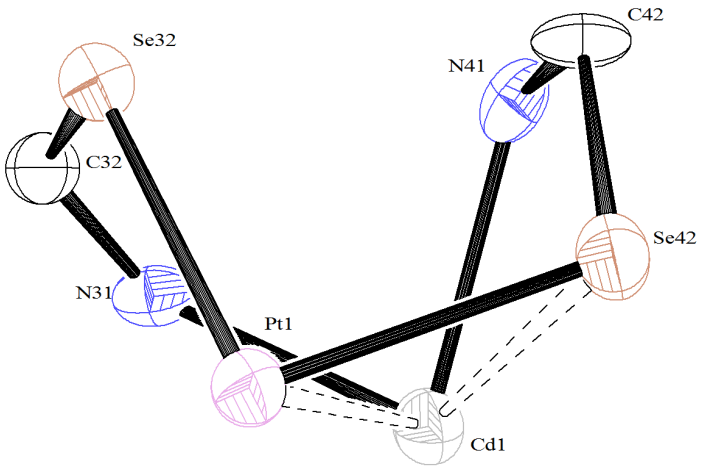

Figure S3- Depiction of twisted boat form of eight-member ring in compound [{Pt(SeC$_5$H$_4$N)$_2$(dppp)}CdCl(OAc)].3CH$_2$Cl$_2$ (2b).3CH$_2$Cl$_2$

Crystal Information File of [{Pt(SeC$_5$H$_4$N)$_2$(dppp)}CdCl(OAc)].3CH$_2$Cl$_2$

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    L. Palatinus, G. Chapuis (2007)
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    SuperFlip

    Sheldrick, G.M. (2008), Acta Cryst. A64, 112-122.

    Rigaku (1998). REQAB.
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_diffrn_measurement_method              \w
_diffrn_detector_area_resol_mean        14.629
_diffrn_reflns_number                   14846
_diffrn_reflns_av_R_equivalents         0.1415
_diffrn_reflns_theta_min          1.539
_diffrn_reflns_theta_max          25.348
_diffrn_reflns_theta_full         25.242
_diffrn_measured_fraction_theta_max   0.943
_diffrn_measured_fraction_theta_full  0.947
_diffrn_reflns_limit_h_min             -8
_diffrn_reflns_limit_h_max              14
_diffrn_reflns_limit_k_min             -16
_diffrn_reflns_limit_k_max              16
_diffrn_reflns_limit_l_min             -18
_diffrn_reflns_limit_l_max              18
_diffrn_standards_number                0
_diffrn_standards_interval_count        .
_diffrn_standards_decay_%               ?

#========================================================================
=====
# REFINEMENT DATA

_refine_special_details
;
    Refinement was performed using all reflections. The weighted
```

```
    R-factor (wR) and goodness of fit (S) are based on F^2^.
    R-factor (gt) are based on F. The threshold expression of
    F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt).
;
_reflns_number_total                    8363
_reflns_number_gt                       4756
_reflns_threshold_expression            F^2^>2.0\s(F^2^)
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_R_factor_gt                  0.1453
_refine_ls_wR_factor_ref                0.4447
_refine_ls_number_restraints            12
_refine_ls_hydrogen_treatment           constr
_refine_ls_number_reflns                8363
_refine_ls_number_parameters            532
_refine_ls_goodness_of_fit_ref          1.087
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
         'w = 1/[\s^2^(Fo^2^)+(0.1900P)^2^+219.1236P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_primary            direct
_atom_sites_solution_secondary          difmap
_refine_ls_shift/su_max                 0.004
_refine_diff_density_max                2.610
_refine_diff_density_min               -2.610
_refine_ls_extinction_method            none
_refine_ls_extinction_coef              ?

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International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'H' 'H'  0.0000 0.0000
;
International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.4)
;
  'Cd' 'Cd'  -0.8075 1.2024
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'Cl' 'Cl'  0.1484 0.1585
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International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
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  'N' 'N'  0.0061 0.0033
;
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'O' 'O'  0.0106 0.0060
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'P' 'P'  0.1023 0.0942
;
International Tables for Crystallography
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;
  'Pt' 'Pt'  -1.7033 8.3905
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'Se' 'Se'  -0.0929 2.2259
;
International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;

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# ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_fract_y
_atom_site_fract_z
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_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
 Pt1 Pt 0.07255(10) 0.30401(9) 0.19329(8) 0.0263(4) Uani 1.0 2 d . . .
 Cd1 Cd 0.1095(2) 0.07686(18) 0.23814(16) 0.0310(6) Uani 1.0 2 d . . .
 Se32 Se -0.1331(3) 0.2710(3) 0.2311(2) 0.0292(8) Uani 1.0 2 d . . .
 Se42 Se 0.1169(3) 0.1945(3) 0.0675(2) 0.0311(8) Uani 1.0 2 d . . .
 Cl1 Cl 0.2335(7) 0.1416(6) 0.3317(5) 0.0324(18) Uani 1.0 2 d . . .
 Cl2 Cl 0.2424(16) 0.2472(15) 0.5673(13) 0.109(6) Uani 1.0 2 d . . .
 Cl3 Cl 0.4418(15) 0.2985(16) 0.4451(13) 0.110(6) Uani 1.0 2 d . . .
 Cl4 Cl 0.5705(16) 0.5517(14) 0.1923(10) 0.101(6) Uani 1.0 2 d . . .
 Cl5 Cl 0.5502(19) 0.547(4) 0.3749(13) 0.27(3) Uani 1.0 2 d . . .
 Cl6 Cl 0.4783(12) 0.8195(10) 0.3148(8) 0.070(4) Uani 1.0 2 d . . .
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Cl7 Cl 0.5599(14) 1.0206(12) 0.3049(12) 0.093(5) Uani 1.0 2 d . . .
P1 P 0.2521(7) 0.3545(7) 0.1466(6) 0.0285(18) Uani 1.0 2 d . . .
P2 P 0.0344(8) 0.4106(7) 0.3042(6) 0.0297(19) Uani 1.0 2 d . . .
O51 O 0.113(3) -0.0993(17) 0.2802(15) 0.044(7) Uani 1.0 2 d . . .
O52 O 0.246(2) -0.0467(19) 0.1715(17) 0.044(7) Uani 1.0 2 d . . .
N31 N -0.060(3) 0.1051(18) 0.3385(18) 0.027(6) Uani 1.0 2 d . . .
N41 N -0.024(3) 0.0565(18) 0.1458(18) 0.029(6) Uani 1.0 2 d . . .
C1 C 0.328(3) 0.382(3) 0.233(3) 0.030(7) Uani 1.0 2 d . . .
C2 C 0.266(3) 0.468(3) 0.2894(18) 0.031(8) Uani 1.0 2 d . . .
C3 C 0.158(3) 0.430(3) 0.354(3) 0.035(8) Uani 1.0 2 d . . .
C4 C 0.361(3) 0.268(3) 0.083(2) 0.030(8) Uani 1.0 2 d . . .
C5 C 0.373(3) 0.275(3) -0.011(3) 0.035(8) Uani 1.0 2 d . . .
C6 C 0.451(3) 0.210(3) -0.060(3) 0.042(9) Uani 1.0 2 d . . .
C7 C 0.524(4) 0.136(3) -0.019(3) 0.048(10) Uani 1.0 2 d . . .
C8 C 0.504(4) 0.126(3) 0.069(3) 0.045(10) Uani 1.0 2 d . . .
C9 C 0.427(4) 0.194(3) 0.121(3) 0.048(11) Uani 1.0 2 d . . .
C10 C 0.253(3) 0.473(3) 0.073(2) 0.025(7) Uani 1.0 2 d . . .
C11 C 0.352(3) 0.521(3) 0.057(2) 0.029(8) Uani 1.0 2 d . . .
C12 C 0.353(3) 0.614(3) 0.001(3) 0.033(8) Uani 1.0 2 d . . .
C13 C 0.258(3) 0.650(3) -0.031(3) 0.032(8) Uani 1.0 2 d . . .
C14 C 0.151(4) 0.600(4) -0.015(3) 0.054(11) Uani 1.0 2 d . . .
C15 C 0.154(3) 0.505(3) 0.044(3) 0.035(9) Uani 1.0 2 d . . .
C16 C -0.022(3) 0.534(3) 0.263(3) 0.030(8) Uani 1.0 2 d . . .
C17 C -0.008(5) 0.622(4) 0.297(4) 0.076(16) Uani 1.0 2 d . . .
C18 C -0.053(6) 0.712(4) 0.269(4) 0.09(3) Uani 1.0 2 d . . .
C19 C -0.111(4) 0.715(4) 0.200(4) 0.070(15) Uani 1.0 2 d . . .
C20 C -0.127(5) 0.632(4) 0.165(4) 0.069(14) Uani 1.0 2 d . . .
C21 C -0.081(5) 0.537(4) 0.193(3) 0.072(16) Uani 1.0 2 d . . .
C22 C -0.066(3) 0.376(3) 0.402(2) 0.039(9) Uani 1.0 2 d . . .
C23 C -0.029(3) 0.287(3) 0.458(3) 0.041(9) Uani 1.0 2 d . . .
C24 C -0.107(4) 0.264(4) 0.534(2) 0.043(10) Uani 1.0 2 d . . .
C25 C -0.216(3) 0.318(3) 0.557(3) 0.040(9) Uani 1.0 2 d . . .
C26 C -0.243(4) 0.405(3) 0.509(3) 0.046(10) Uani 1.0 2 d . . .
C27 C -0.165(4) 0.434(4) 0.427(2) 0.044(10) Uani 1.0 2 d . . .
C32 C -0.151(3) 0.172(3) 0.333(3) 0.037(8) Uani 1.0 2 d . . .
C33 C -0.256(3) 0.177(3) 0.384(3) 0.034(8) Uani 1.0 2 d . . .
C34 C -0.273(3) 0.101(3) 0.453(3) 0.038(9) Uani 1.0 2 d . . .
C35 C -0.183(5) 0.035(3) 0.468(3) 0.059(13) Uani 1.0 2 d . . .
C36 C -0.079(3) 0.033(3) 0.406(3) 0.040(9) Uani 1.0 2 d . . .
C42 C -0.012(3) 0.114(3) 0.079(3) 0.031(8) Uani 1.0 2 d . . .
C43 C -0.081(3) 0.119(3) 0.017(3) 0.038(9) Uani 1.0 2 d . . .
C44 C -0.172(3) 0.055(2) 0.023(2) 0.025(7) Uani 1.0 2 d . . .
C45 C -0.183(3) -0.003(3) 0.096(3) 0.036(9) Uani 1.0 2 d . . .
C46 C -0.115(3) -0.004(3) 0.162(3) 0.029(7) Uani 1.0 2 d . . .
C51 C 0.192(3) -0.121(3) 0.218(2) 0.031(8) Uani 1.0 2 d . . .
C52 C 0.238(3) -0.231(3) 0.198(3) 0.045(10) Uani 1.0 2 d . . .
C53 C 0.362(7) 0.206(5) 0.494(5) 0.13(3) Uani 1.0 2 d . . .
C54 C 0.619(5) 0.507(8) 0.281(4) 0.15(5) Uani 1.0 2 d . . .
C55 C 0.468(8) 0.949(4) 0.279(5) 0.14(4) Uani 1.0 2 d . . .
H1A H 0.3371 0.3196 0.2714 0.0359 Uiso 1.0 2 calc R . .
H1B H 0.4057 0.3996 0.2054 0.0359 Uiso 1.0 2 calc R . .
H2A H 0.2412 0.5259 0.2511 0.0371 Uiso 1.0 2 calc R . .
H2B H 0.3187 0.4911 0.3234 0.0371 Uiso 1.0 2 calc R . .
H3A H 0.1313 0.4799 0.3988 0.0422 Uiso 1.0 2 calc R . .
```

```
 H3B H 0.1821 0.3656 0.3839 0.0422 Uiso 1.0 2 calc R . .
 H5 H 0.3267 0.3258 -0.0388 0.0424 Uiso 1.0 2 calc R . .
 H6 H 0.4563 0.2125 -0.1220 0.0509 Uiso 1.0 2 calc R . .
 H7 H 0.5845 0.0963 -0.0530 0.0578 Uiso 1.0 2 calc R . .
 H8 H 0.5444 0.0712 0.0973 0.0543 Uiso 1.0 2 calc R . .
 H9 H 0.4209 0.1876 0.1824 0.0578 Uiso 1.0 2 calc R . .
 H11 H 0.4171 0.4945 0.0808 0.0345 Uiso 1.0 2 calc R . .
 H12 H 0.4189 0.6502 -0.0120 0.0399 Uiso 1.0 2 calc R . .
 H13 H 0.2601 0.7107 -0.0671 0.0387 Uiso 1.0 2 calc R . .
 H14 H 0.0863 0.6260 -0.0398 0.0646 Uiso 1.0 2 calc R . .
 H15 H 0.0885 0.4680 0.0606 0.0425 Uiso 1.0 2 calc R . .
 H17 H 0.0356 0.6187 0.3427 0.0906 Uiso 1.0 2 calc R . .
 H18 H -0.0449 0.7722 0.2950 0.1133 Uiso 1.0 2 calc R . .
 H19 H -0.1411 0.7783 0.1775 0.0846 Uiso 1.0 2 calc R . .
 H20 H -0.1704 0.6380 0.1196 0.0833 Uiso 1.0 2 calc R . .
 H21 H -0.0897 0.4777 0.1657 0.0868 Uiso 1.0 2 calc R . .
 H23 H 0.0433 0.2478 0.4421 0.0495 Uiso 1.0 2 calc R . .
 H24 H -0.0860 0.2094 0.5731 0.0518 Uiso 1.0 2 calc R . .
 H25 H -0.2708 0.2945 0.6046 0.0486 Uiso 1.0 2 calc R . .
 H26 H -0.3120 0.4472 0.5281 0.0552 Uiso 1.0 2 calc R . .
 H27 H -0.1840 0.4927 0.3921 0.0525 Uiso 1.0 2 calc R . .
 H33 H -0.3147 0.2279 0.3741 0.0408 Uiso 1.0 2 calc R . .
 H34 H -0.3465 0.0970 0.4882 0.0462 Uiso 1.0 2 calc R . .
 H35 H -0.1892 -0.0097 0.5187 0.0706 Uiso 1.0 2 calc R . .
 H36 H -0.0204 -0.0197 0.4120 0.0483 Uiso 1.0 2 calc R . .
 H43 H -0.0669 0.1661 -0.0325 0.0460 Uiso 1.0 2 calc R . .
 H44 H -0.2194 0.0557 -0.0194 0.0299 Uiso 1.0 2 calc R . .
 H45 H -0.2406 -0.0480 0.1048 0.0436 Uiso 1.0 2 calc R . .
 H46 H -0.1315 -0.0442 0.2157 0.0353 Uiso 1.0 2 calc R . .
 H52A H 0.3173 -0.2445 0.2059 0.0542 Uiso 1.0 2 calc R . .
 H52B H 0.2337 -0.2418 0.1369 0.0542 Uiso 1.0 2 calc R . .
 H52C H 0.1902 -0.2777 0.2371 0.0542 Uiso 1.0 2 calc R . .
 H53A H 0.4102 0.1563 0.5253 0.1529 Uiso 1.0 2 calc R . .
 H53B H 0.3373 0.1709 0.4487 0.1529 Uiso 1.0 2 calc R . .
 H54A H 0.6201 0.4321 0.2846 0.1844 Uiso 1.0 2 calc R . .
 H54B H 0.6999 0.5222 0.2739 0.1844 Uiso 1.0 2 calc R . .
 H55A H 0.4768 0.9529 0.2141 0.1695 Uiso 1.0 2 calc R . .
 H55B H 0.3890 0.9785 0.3021 0.1695 Uiso 1.0 2 calc R . .


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 Cd1 0.0323(14) 0.0302(13) 0.0308(13) 0.0006(10) -0.0071(10) -0.0063(10)
 Se32 0.0287(17) 0.0306(17) 0.0287(17) -0.0021(13) -0.0056(13) -0.0051(14)
 Se42 0.0308(18) 0.0350(18) 0.0275(17) -0.0047(14) -0.0015(14) -0.0090(14)
 Cl1 0.037(5) 0.038(5) 0.023(4) -0.002(4) -0.008(4) -0.007(4)
 Cl2 0.093(12) 0.120(14) 0.115(14) -0.003(10) -0.018(10) -0.029(11)
```

Cl3 0.075(11) 0.138(15) 0.117(14) -0.005(10) -0.027(10) 0.002(12)
Cl4 0.121(13) 0.128(13) 0.073(9) -0.065(11) -0.045(9) 0.032(10)
Cl5 0.081(14) 0.62(8) 0.066(12) 0.08(3) -0.010(10) 0.00(3)
Cl6 0.081(9) 0.066(8) 0.062(7) -0.006(7) -0.015(7) -0.004(6)
Cl7 0.090(11) 0.089(10) 0.116(13) -0.016(8) -0.057(10) -0.009(9)
P1 0.024(5) 0.027(5) 0.034(5) -0.003(4) -0.002(4) -0.006(4)
P2 0.036(5) 0.029(5) 0.025(4) -0.000(4) -0.004(4) -0.011(4)
O51 0.08(2) 0.023(12) 0.023(12) 0.014(12) -0.012(13) 0.006(10)
O52 0.021(12) 0.051(15) 0.052(16) -0.016(11) 0.010(11) 0.011(13)
N31 0.025(14) 0.021(13) 0.038(16) -0.007(11) -0.012(12) 0.004(12)
N41 0.028(15) 0.015(13) 0.041(16) 0.007(11) -0.002(12) -0.004(12)
C1 0.032(18) 0.030(17) 0.031(17) -0.006(14) -0.012(14) 0.000(14)
C2 0.023(16) 0.06(3) 0.010(14) 0.008(15) -0.004(12) 0.009(14)
C3 0.030(19) 0.032(18) 0.04(2) 0.021(14) -0.011(15) -0.020(16)
C4 0.015(15) 0.05(2) 0.027(17) 0.008(14) 0.004(13) -0.020(15)
C5 0.05(2) 0.014(15) 0.05(2) -0.015(14) -0.002(17) 0.002(15)
C6 0.020(17) 0.07(3) 0.033(19) 0.007(17) 0.000(14) -0.013(18)
C7 0.05(3) 0.04(2) 0.04(3) 0.000(18) 0.009(19) 0.005(18)
C8 0.05(3) 0.021(17) 0.05(3) 0.014(16) 0.008(18) 0.012(17)
C9 0.06(3) 0.021(17) 0.05(3) 0.002(17) 0.013(19) 0.024(17)
C10 0.024(7) 0.025(7) 0.025(7) -0.0023(12) -0.0045(16) -0.0016(11)
C11 0.034(18) 0.032(17) 0.027(16) -0.028(15) -0.010(14) 0.008(14)
C12 0.04(2) 0.031(18) 0.032(18) -0.008(15) -0.012(15) -0.011(15)
C13 0.011(15) 0.030(17) 0.05(2) -0.003(13) 0.007(14) -0.013(16)
C14 0.05(3) 0.07(3) 0.04(2) -0.02(3) 0.001(18) 0.02(2)
C15 0.05(2) 0.033(18) 0.037(19) -0.008(16) -0.039(17) 0.013(16)
C16 0.021(16) 0.025(16) 0.043(19) -0.006(13) 0.010(14) -0.018(15)
C17 0.11(5) 0.06(3) 0.06(3) 0.02(3) -0.03(3) -0.02(3)
C18 0.13(5) 0.05(3) 0.12(5) 0.05(4) -0.10(5) -0.03(3)
C19 0.04(3) 0.07(3) 0.11(5) 0.01(3) -0.04(3) -0.04(3)
C20 0.09(4) 0.06(3) 0.06(3) -0.02(3) -0.02(3) -0.01(3)
C21 0.12(5) 0.05(3) 0.04(3) 0.03(3) -0.04(3) -0.00(2)
C22 0.03(2) 0.07(3) 0.012(15) 0.008(18) -0.008(14) -0.003(16)
C23 0.030(19) 0.05(2) 0.05(3) -0.013(16) -0.005(17) -0.030(19)
C24 0.05(3) 0.06(3) 0.012(15) -0.02(2) 0.008(15) -0.003(16)
C25 0.03(2) 0.07(3) 0.021(16) -0.020(18) 0.003(15) -0.000(17)
C26 0.04(3) 0.05(3) 0.05(3) -0.015(18) -0.029(19) 0.01(2)
C27 0.04(3) 0.07(3) 0.017(16) -0.016(19) 0.006(15) -0.004(17)
C32 0.034(19) 0.029(18) 0.05(3) 0.006(15) -0.017(17) -0.016(16)
C33 0.034(8) 0.034(8) 0.034(8) -0.0034(13) -0.0063(17) -0.0021(12)
C34 0.024(17) 0.028(18) 0.07(3) -0.023(14) -0.009(17) 0.007(17)
C35 0.09(4) 0.03(2) 0.04(3) 0.01(2) 0.01(3) 0.010(18)
C36 0.024(18) 0.06(3) 0.026(17) -0.000(16) 0.012(14) 0.011(17)
C42 0.022(16) 0.031(17) 0.04(2) -0.013(14) -0.016(15) 0.005(16)
C43 0.029(18) 0.035(19) 0.05(3) -0.014(15) 0.014(16) -0.034(17)
C44 0.027(17) 0.017(15) 0.030(17) -0.003(12) -0.005(13) 0.003(13)
C45 0.009(15) 0.038(19) 0.06(3) -0.003(13) -0.002(15) -0.017(18)
C46 0.029(7) 0.029(7) 0.029(7) -0.0030(12) -0.0055(16) -0.0018(11)
C51 0.033(18) 0.031(17) 0.028(17) -0.011(14) -0.001(15) -0.006(15)
C52 0.03(2) 0.04(2) 0.06(3) -0.003(16) 0.009(18) -0.016(19)
C53 0.16(8) 0.07(4) 0.11(6) -0.01(5) 0.06(5) -0.04(4)
C54 0.05(3) 0.34(12) 0.04(3) 0.10(5) -0.00(3) 0.01(5)
C55 0.31(11) 0.04(3) 0.11(5) -0.11(5) -0.11(6) 0.05(4)

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2009)'
_computing_cell_refinement             'CrystalClear-SM Expert 2.0 rc13'
_computing_data_reduction              'CrystalClear-SM Expert 2.0 rc13'
_computing_structure_solution          'Superflip (Palatinus, et al.,
2007)'
_computing_structure_refinement        'SHELXL97 (Sheldrick, 2008)'
_computing_publication_material        'CrystalStructure 4.0 (Rigaku,
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Pt1 Se32 2.490(4) yes . .
Pt1 Se42 2.484(4) yes . .
Pt1 P1 2.282(9) yes . .
Pt1 P2 2.277(9) yes . .
Cd1 Se42 2.969(4) yes . .
Cd1 Cl1 2.533(10) yes . .
Cd1 O51 2.39(3) yes . .
Cd1 O52 2.34(3) yes . .
Cd1 N31 2.32(3) yes . .
Cd1 N41 2.40(3) yes . .
Se32 C32 1.98(4) yes . .
Se42 C42 1.94(4) yes . .
Cl2 C53 1.71(7) yes . .
Cl3 C53 1.69(7) yes . .
Cl4 C54 1.65(6) yes . .
Cl5 C54 1.63(6) yes . .
Cl6 C55 1.77(6) yes . .
Cl7 C55 1.67(9) yes . .
P1 C1 1.84(4) yes . .
P1 C4 1.83(3) yes . .
P1 C10 1.88(3) yes . .
P2 C3 1.84(4) yes . .
P2 C16 1.82(3) yes . .
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O52 C51 1.33(4) yes . .
N31 C32 1.33(4) yes . .
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N41 C42 1.24(5) yes . .
N41 C46 1.39(5) yes . .
C1 C2 1.54(5) yes . .
C2 C3 1.58(5) yes . .
C4 C5 1.45(5) yes . .
C4 C9 1.36(5) yes . .
C5 C6 1.37(5) yes . .
C6 C7 1.43(6) yes . .
C7 C8 1.35(6) yes . .
C8 C9 1.40(5) yes . .
C10 C11 1.37(5) yes . .
C10 C15 1.36(5) yes . .
C11 C12 1.46(5) yes . .
C12 C13 1.35(5) yes . .
C13 C14 1.46(6) yes . .
C14 C15 1.51(6) yes . .
C16 C17 1.37(7) yes . .
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C42 C43 1.39(6) yes . .
C43 C44 1.44(5) yes . .
C44 C45 1.31(5) yes . .
C45 C46 1.44(6) yes . .
C51 C52 1.55(5) yes . .
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C1 H1B 0.990 no . .
C2 H2A 0.990 no . .
C2 H2B 0.990 no . .
C3 H3A 0.990 no . .
C3 H3B 0.990 no . .
C5 H5 0.950 no . .
C6 H6 0.950 no . .
C7 H7 0.950 no . .
C8 H8 0.950 no . .
C9 H9 0.950 no . .
C11 H11 0.950 no . .
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C52 H52B 0.980 no . .
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C53 H53A 0.990 no . .
C53 H53B 0.990 no . .
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Cd1 Pt1 Se42 63.83(10) yes . . .
Cd1 Pt1 P1 105.4(2) yes . . .
Cd1 Pt1 P2 118.7(3) yes . . .
Se32 Pt1 Se42 94.06(12) yes . . .
Se32 Pt1 P1 171.6(3) yes . . .
Se32 Pt1 P2 87.3(3) yes . . .
Se42 Pt1 P1 86.4(3) yes . . .
Se42 Pt1 P2 177.3(3) yes . . .
P1 Pt1 P2 91.9(4) yes . . .
Pt1 Cd1 Se42 48.67(8) yes . . .
Pt1 Cd1 Cl1 79.6(2) yes . . .
Pt1 Cd1 O51 172.8(7) yes . . .
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Se42 Cd1 O52 90.3(7) yes . . .
Se42 Cd1 N31 115.0(7) yes . . .
Se42 Cd1 N41 59.0(6) yes . . .
Cl1 Cd1 O51 103.7(8) yes . . .
Cl1 Cd1 O52 97.3(7) yes . . .
Cl1 Cd1 N31 94.7(8) yes . . .
Cl1 Cd1 N41 166.6(6) yes . . .
O51 Cd1 O52 55.9(9) yes . . .
O51 Cd1 N31 89.3(9) yes . . .
O51 Cd1 N41 89.0(9) yes . . .
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O52 Cd1 N41 93.3(9) yes . . .
N31 Cd1 N41 81.1(10) yes . . .
Pt1 Se32 C32 107.9(11) yes . . .
Pt1 Se42 Cd1 67.50(10) yes . . .
Pt1 Se42 C42 106.2(10) yes . . .
Cd1 Se42 C42 74.7(11) yes . . .
Pt1 P1 C1 116.0(11) yes . . .
Pt1 P1 C4 118.0(12) yes . . .
Pt1 P1 C10 113.1(11) yes . . .
C1 P1 C4 100.7(15) yes . . .
C1 P1 C10 104.2(15) yes . . .
C4 P1 C10 102.9(14) yes . . .
Pt1 P2 C3 115.7(11) yes . . .
Pt1 P2 C16 108.7(12) yes . . .
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C3 P2 C16 107.2(16) yes . . .
C3 P2 C22 99.5(16) yes . . .
C16 P2 C22 106.6(16) yes . . .
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Cd1 N31 C36 115.9(19) yes . . .
C32 N31 C36 114(3) yes . . .
Cd1 N41 C42 112(3) yes . . .
Cd1 N41 C46 128(2) yes . . .
C42 N41 C46 119(4) yes . . .
P1 C1 C2 114(3) yes . . .
C1 C2 C3 110(3) yes . . .
P2 C3 C2 116(3) yes . . .
P1 C4 C5 118(3) yes . . .
P1 C4 C9 124(3) yes . . .
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C4 C5 C6 120(3) yes . . .
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C6 C7 C8 118(4) yes . . .
C7 C8 C9 122(4) yes . . .
C4 C9 C8 121(4) yes . . .
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C19 C20 C21 122(6) yes . . .
C16 C21 C20 116(5) yes . . .
P2 C22 C23 117(3) yes . . .
P2 C22 C27 121(3) yes . . .
C23 C22 C27 122(3) yes . . .
C22 C23 C24 115(3) yes . . .
C23 C24 C25 123(4) yes . . .
C24 C25 C26 120(4) yes . . .
C25 C26 C27 119(4) yes . . .
C22 C27 C26 120(4) yes . . .
Se32 C32 N31 116(3) yes . . .
Se32 C32 C33 115(3) yes . . .
N31 C32 C33 129(4) yes . . .
C32 C33 C34 116(3) yes . . .
C33 C34 C35 119(4) yes . . .
C34 C35 C36 119(4) yes . . .
N31 C36 C35 123(4) yes . . .
Se42 C42 N41 114(3) yes . . .
Se42 C42 C43 123(3) yes . . .
N41 C42 C43 124(4) yes . . .
C42 C43 C44 122(3) yes . . .
C43 C44 C45 111(4) yes . . .
C44 C45 C46 126(4) yes . . .
N41 C46 C45 117(3) yes . . .
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O52 C51 C52 118(3) yes . . .
Cl2 C53 Cl3 114(4) yes . . .
Cl4 C54 Cl5 118(5) yes . . .
Cl6 C55 Cl7 118(5) yes . . .
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C2 C1 H1A 108.855 no . . .
C2 C1 H1B 108.849 no . . .
H1A C1 H1B 107.696 no . . .
C1 C2 H2A 109.685 no . . .
C1 C2 H2B 109.691 no . . .
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C3 C2 H2B 109.678 no . . .
H2A C2 H2B 108.176 no . . .
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H3A C3 H3B 107.342 no . . .
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C5 C6 H6 119.889 no . . .
C7 C6 H6 119.898 no . . .
C6 C7 H7 120.793 no . . .
C8 C7 H7 120.804 no . . .
C7 C8 H8 119.130 no . . .
C9 C8 H8 119.140 no . . .
C4 C9 H9 119.479 no . . .
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N31 C36 H36 118.729 no . . .
C35 C36 H36 118.726 no . . .
C42 C43 H43 118.810 no . . .
C44 C43 H43 118.826 no . . .
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C46 C45 H45 117.008 no . . .
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C45 C46 H46 121.461 no . . .
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C51 C52 H52B 109.474 no . . .
C51 C52 H52C 109.469 no . . .
H52A C52 H52B 109.474 no . . .
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H52B C52 H52C 109.469 no . . .
Cl2 C53 H53A 108.669 no . . .
Cl2 C53 H53B 108.674 no . . .
Cl3 C53 H53A 108.666 no . . .
Cl3 C53 H53B 108.664 no . . .
H53A C53 H53B 107.604 no . . .
Cl4 C54 H54A 107.908 no . . .
Cl4 C54 H54B 107.906 no . . .
Cl5 C54 H54A 107.912 no . . .
Cl5 C54 H54B 107.909 no . . .
H54A C54 H54B 107.198 no . . .
Cl6 C55 H55A 107.895 no . . .
Cl6 C55 H55B 107.899 no . . .
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Se32 Pt1 Cd1 Cl1 -128.74(10) no . . . .
Se32 Pt1 Cd1 O52 140.43(17) no . . . .
Se32 Pt1 Cd1 N31 -32.85(11) no . . . .
Se32 Pt1 Cd1 N41 48.48(10) no . . . .
Cd1 Pt1 Se42 Cd1 -0.00(6) no . . . .
Se42 Pt1 Cd1 Se42 -0.00(9) no . . . .
Se42 Pt1 Cd1 Cl1 132.85(11) no . . . .
Se42 Pt1 Cd1 O52 42.02(16) no . . . .
Se42 Pt1 Cd1 N31 -131.26(13) no . . . .
Se42 Pt1 Cd1 N41 -49.93(10) no . . . .
Cd1 Pt1 P1 C1 -83.7(4) no . . . .
Cd1 Pt1 P1 C4 35.9(5) no . . . .
Cd1 Pt1 P1 C10 156.0(4) no . . . .
P1 Pt1 Cd1 Se42 -78.0(3) no . . . .
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P1 Pt1 Cd1 N31 150.7(3) no . . . .
P1 Pt1 Cd1 N41 -128.0(3) no . . . .
Cd1 Pt1 P2 C3 74.8(5) no . . . .
Cd1 Pt1 P2 C16 -164.5(3) no . . . .
Cd1 Pt1 P2 C22 -42.9(6) no . . . .
P2 Pt1 Cd1 Se42 -179.0(3) no . . . .
P2 Pt1 Cd1 Cl1 -46.2(3) no . . . .
P2 Pt1 Cd1 O52 -137.0(3) no . . . .
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P2 Pt1 Cd1 N41 131.1(3) no . . . .
Se32 Pt1 Se42 Cd1 -79.34(9) no . . . .
Se32 Pt1 P2 C3 154.5(4) no . . . .
Se32 Pt1 P2 C16 -84.8(4) no . . . .
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Se42 Pt1 P1 C4 -25.8(5) no . . . .
Se42 Pt1 P1 C10 94.4(4) no . . . .
P1 Pt1 Se42 Cd1 109.1(3) no . . . .
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P1 Pt1 P2 C3 -33.9(5) no . . . .
P1 Pt1 P2 C16 86.8(5) no . . . .
P1 Pt1 P2 C22 -151.7(5) no . . . .
P2 Pt1 P1 C1 36.7(5) no . . . .
P2 Pt1 P1 C4 156.3(5) no . . . .
P2 Pt1 P1 C10 -83.5(5) no . . . .
Pt1 Cd1 Se42 Pt1 0.00(3) no . . . .
Pt1 Cd1 O52 C51 -170.1(7) no . . . .
Pt1 Cd1 N31 C32 33(2) no . . . .
Pt1 Cd1 N31 C36 -159.3(18) no . . . .
Pt1 Cd1 N41 C42 39.2(14) no . . . .
Pt1 Cd1 N41 C46 -134.9(17) no . . . .
Cl1 Cd1 Se42 Pt1 -51.3(2) no . . . .
Cl1 Cd1 Se42 C42 -166.5(3) no . . . .
Se42 Cd1 O51 C51 45(2) no . . . .
O51 Cd1 Se42 Pt1 170.6(10) no . . . .
O51 Cd1 Se42 C42 55.4(10) no . . . .
Se42 Cd1 O52 C51 -139.9(12) no . . . .
O52 Cd1 Se42 Pt1 -149.4(7) no . . . .
O52 Cd1 Se42 C42 95.4(7) no . . . .
Se42 Cd1 N31 C32 -6(3) no . . . .
Se42 Cd1 N31 C36 162.1(14) no . . . .
N31 Cd1 Se42 Pt1 55.6(8) no . . . .
N31 Cd1 Se42 C42 -59.6(8) no . . . .
Se42 Cd1 N41 C42 -2.9(11) no . . . .
Se42 Cd1 N41 C46 -177(2) no . . . .
N41 Cd1 Se42 Pt1 116.9(7) no . . . .
N41 Cd1 Se42 C42 1.7(7) no . . . .
Cl1 Cd1 O51 C51 -95.7(14) no . . . .
Cl1 Cd1 O52 C51 107.4(12) no . . . .
Cl1 Cd1 N31 C32 112(3) no . . . .
Cl1 Cd1 N31 C36 -80.3(17) no . . . .
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O52 Cd1 O51 C51 -6.1(13) no . . . .
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N31 Cd1 O51 C51 169.7(16) no . . . .
O51 Cd1 N41 C42 -147.0(16) no . . . .
O51 Cd1 N41 C46 38.9(18) no . . . .
N41 Cd1 O51 C51 88.5(15) no . . . .
O52 Cd1 N31 C32 -138.2(19) no . . . .
O52 Cd1 N31 C36 30(3) no . . . .
N31 Cd1 O52 C51 -2(3) no . . . .
O52 Cd1 N41 C42 -91.2(16) no . . . .
O52 Cd1 N41 C46 94.6(18) no . . . .
N41 Cd1 O52 C51 -80.9(14) no . . . .
N31 Cd1 N41 C42 123.6(16) no . . . .
N31 Cd1 N41 C46 -50.6(18) no . . . .
N41 Cd1 N31 C32 -55(3) no . . . .
N41 Cd1 N31 C36 112.5(19) no . . . .
Pt1 Se32 C32 N31 -31(3) no . . . .
Pt1 Se32 C32 C33 153(2) no . . . .
Pt1 Se42 C42 N41 -64(2) no . . . .
Pt1 Se42 C42 C43 119(2) no . . . .
Cd1 Se42 C42 N41 -3.2(17) no . . . .
Cd1 Se42 C42 C43 179(3) no . . . .
Pt1 P1 C1 C2 -61(2) no . . . .
Pt1 P1 C4 C5 90(3) no . . . .
Pt1 P1 C4 C9 -86(3) no . . . .
Pt1 P1 C10 C11 166.6(15) no . . . .
Pt1 P1 C10 C15 -11(3) no . . . .
C1 P1 C4 C5 -142(3) no . . . .
C1 P1 C4 C9 41(3) no . . . .
C4 P1 C1 C2 170.2(19) no . . . .
C1 P1 C10 C11 40(3) no . . . .
C1 P1 C10 C15 -138(2) no . . . .
C10 P1 C1 C2 64(2) no . . . .
C4 P1 C10 C11 -65(3) no . . . .
C4 P1 C10 C15 117(2) no . . . .
C10 P1 C4 C5 -35(3) no . . . .
C10 P1 C4 C9 149(3) no . . . .
Pt1 P2 C3 C2 55(3) no . . . .
Pt1 P2 C16 C17 -151.5(18) no . . . .
Pt1 P2 C16 C21 28(3) no . . . .
Pt1 P2 C22 C23 68(3) no . . . .
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C3 P2 C22 C27 117(3) no . . . .
C22 P2 C3 C2 -177(2) no . . . .
C16 P2 C22 C23 -169(3) no . . . .
C16 P2 C22 C27 5(4) no . . . .
C22 P2 C16 C17 80(3) no . . . .
C22 P2 C16 C21 -100(3) no . . . .
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Cd1 N31 C32 C33 168(3) no . . . .
Cd1 N31 C36 C35 -174(3) no . . . .
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C36 N31 C32 Se32 -175(3) no . . . .
C36 N31 C32 C33 -0(6) no . . . .
Cd1 N41 C42 Se42 4(3) no . . . .
Cd1 N41 C42 C43 -178.2(19) no . . . .
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# Additional structures and associated data_? identifiers
# should be added at this point if there is more than one
# structure analysis in the CIF.

#=============================================================================
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#     End of CIF
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