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Bis(2,3,5-triphenyltetrazolium) tetrachloridocadmate(II)

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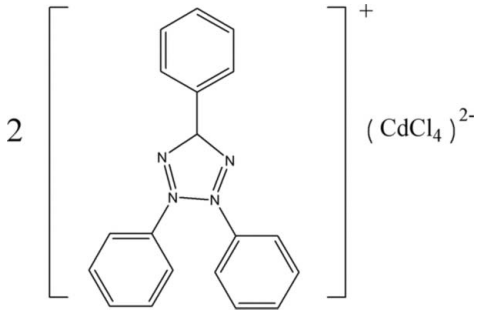
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 18.6.

The title compound, $(C_{19}H_{15}N_4)_2[CdCl_4]$, a salt comprising two 2,3,5-triphenyl-substituted tetrazolium cations and a tetrachloridocadmate(II) anion, was synthesized by hydrothermal methods. In the anion, the Cd^{II} ion is tetrahedrally coordinated by four chloride anions. In the crystal structure, four cations and two anions pack into inversion-related subunits linked by C—H···Cl and offset π-stacking interactions. Each of these subunits is surrounded by six others. Intermolecular π–π stacking interactions between phenyl rings are observed along the a axis, with perpendicular distances between the ring planes of 3.6015 and 3.6934 Å.

Related literature

For diagnostic applications of tetrazoles, see: Benon *et al.* (1980). For related structures, see: Předota *et al.* (1991) and Morsy *et al.* (2007).



Experimental

Crystal data

$(C_{19}H_{15}N_4)_2[CdCl_4]$
M_r = 852.90
Monoclinic, $P2_1/c$
a = 12.207 (2) Å
b = 15.254 (3) Å
c = 20.132 (4) Å
β = 90.73 (3)°
V = 3748.4 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 153 (2) K
0.24 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.812, T_{max} = 0.868
35919 measured reflections
8568 independent reflections
7790 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.09
8568 reflections
460 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···Cl3^{i}	0.93	2.81	3.6362 (19)	148
C37—H37A···Cl4^{ii}	0.93	2.71	3.5271 (18)	146

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2289).

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supplementary materials

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Bis(2,3,5-triphenyltetrazolium) tetrachloridocadmate(II)

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Comment

Tetrazole derivatives are frequently used as colour indicators for the detection of enzyme systems in which reduction equivalents are formed. Due to this feature, they are extremely useful tools in academic and clinical research as well as for many diagnostic applications (Benon *et al.*, 1980). The tetrazole derivatives most used in biochemistry and cell biology are aromatic derivatives of 1,2,3,4-tetrazole (substitution at positions 2, 3, and 5). So far 2, 3, 5-triphenyl-2*H*-tetrazolium salts have received a great deal of attention (Předota *et al.*, 1991). Here we report the crystal structure of the title compound a 2,3,5-triphenyl-2*H*-tetrazolium salt.

The title compound $(C_{19}H_{15}N_4)_2.(CdCl_4)$, a salt comprising two 2,3,5-triphenylsubstituted tetrazolium cations and a tetrachloridocadmate anion (Fig. 1) was synthesized by hydrothermal methods. Bond lengths and angles in the tetrazole unit, Table 1, are in good agreement with those reported previously (Morsy *et al.*, 2007). In the $[(CdCl_4)^{2-}]$ anion, the Cd (II) ion is tetra-coordinated by four chloride atoms, with the bond lengths from 2.4451 (6) to 2.4800 (6) Å and bond angles from 105.507 (18) to 117.232 (16) °.

Four cations and two anions pack into inversion related sub-units linked by C–H···Cl and offset π-stacking interactions, Fig. 2. Each of these sub-units is surrounded by six others, Figure 3. Intermolecular π-π stacking interactions between the C4 and C10 pyridyl rings (symmetry operation 1+x, 1/2-y, 1/2+z) are observed along the a axis, with a perpendicular distance between the ring planes of 3.6015 Å. Further π-π stacking interactions between the C8-pyridyl ring and its symmetry partner at (1-x,1-y,1-z) are also observed along the a axis, with a perpendicular distance between the ring planes of 3.6934 Å.

Experimental

The title compound was synthesized by a hydrothermal method. A mixture of 2,3,5-triphenyl-2 h-tetrazolium chloride (0.25 g), $CdCl_2.2.5H_2O$(0.144 g, 0.50 mmol), and H_2O (10 mL) was mechanically stirred at room temperature in air reaching a final pH of 5.0. The solution was then transferred to and sealed in a 37.5 mL Teflon-lined reactor which was heated at 443 K for 4 days. Then the reactor was opened to the air and after cooling to room temperature, colorless block-like crystals were isolated from the resulting mixture.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C).

Figures

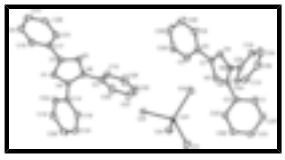


Fig. 1. View of the title compound, with displacement ellipsoids drawn at the 30 % probability level.

Fig. 2. View of the inversion related subunits of (I).

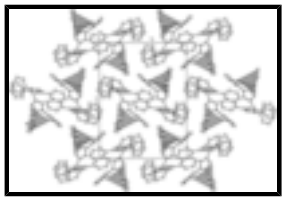


Fig. 3. Packing diagram for (I) viewed down the a axis.

Bis(2,3,5-triphenyltetrazolium) tetrachloridocadmate(II)

Crystal data

$(C_{19}H_{15}N_4)_2[CdCl_4]$	F_{000} = 1720
M_r = 852.90	D_x = 1.511 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 31115 reflections
a = 12.207 (2) Å	θ = 3.2–27.5º
b = 15.254 (3) Å	μ = 0.91 mm^{-1}
c = 20.132 (4) Å	T = 153 (2) K
β = 90.73 (3)º	Block, colorless
V = 3748.4 (13) Å^3	0.24 × 0.22 × 0.16 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	8568 independent reflections
Radiation source: fine-focus sealed tube	7790 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 153(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.812, T_{max} = 0.868	k = −19→19
35919 measured reflections	l = −26→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.058$

$S = 1.09$

8568 reflections

460 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.8818P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.95$ e Å^{-3}

$\Delta\rho_{min} = -0.45$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.714725 (9)	0.234715 (7)	0.156523 (5)	0.02065 (4)
Cl1	0.69331 (4)	0.07695 (3)	0.17345 (2)	0.03064 (9)
Cl2	0.90043 (3)	0.28875 (3)	0.12929 (2)	0.02984 (9)
Cl3	0.58886 (3)	0.28616 (2)	0.067656 (17)	0.02120 (7)
Cl4	0.66298 (3)	0.30323 (3)	0.262572 (17)	0.02458 (8)
N1	0.28772 (10)	0.78597 (8)	0.06939 (6)	0.0181 (2)
N2	0.46597 (11)	0.79913 (8)	0.09433 (6)	0.0196 (2)
N3	0.32786 (10)	0.70996 (8)	0.08724 (6)	0.0172 (2)
N4	1.16473 (11)	0.27541 (9)	0.03994 (6)	0.0211 (3)
N5	1.16603 (11)	0.22688 (8)	0.09388 (6)	0.0193 (2)
N6	0.43434 (10)	0.71756 (8)	0.10180 (6)	0.0181 (2)
N7	1.05604 (11)	0.15861 (8)	0.02597 (6)	0.0204 (3)
N8	1.10206 (10)	0.15691 (8)	0.08531 (6)	0.0184 (2)
C1	1.17519 (14)	0.04745 (11)	0.16212 (8)	0.0255 (3)
H1B	1.2460	0.0666	0.1536	0.031*
C2	0.50584 (12)	0.64480 (10)	0.11877 (8)	0.0207 (3)

C3	1.08506 (13)	0.08649 (10)	0.13188 (7)	0.0194 (3)
C4	0.97900 (13)	0.22698 (11)	−0.10237 (8)	0.0249 (3)
H4B	0.9470	0.1756	−0.0870	0.030*
C5	0.37427 (12)	0.84022 (9)	0.07391 (7)	0.0179 (3)
C6	1.06337 (13)	0.26663 (10)	−0.06641 (7)	0.0214 (3)
C7	1.09531 (13)	0.23275 (10)	−0.00113 (7)	0.0201 (3)
C8	0.28952 (15)	1.04843 (11)	−0.00965 (8)	0.0287 (4)
H8A	0.2389	1.0673	−0.0415	0.034*
C9	1.11354 (16)	0.34246 (11)	−0.09007 (8)	0.0295 (4)
H9A	1.1711	0.3681	−0.0664	0.035*
C10	0.20113 (15)	0.50241 (12)	0.14217 (10)	0.0332 (4)
H10A	0.2009	0.4649	0.1786	0.040*
C11	0.36276 (15)	1.10763 (11)	0.01861 (9)	0.0299 (4)
H11A	0.3613	1.1661	0.0055	0.036*
C12	0.54656 (14)	0.59573 (11)	0.06708 (8)	0.0284 (3)
H12A	0.5310	0.6102	0.0231	0.034*
C13	1.21644 (15)	0.29460 (12)	0.26792 (8)	0.0291 (4)
H13A	1.1795	0.2988	0.3079	0.035*
C14	0.26513 (12)	0.62984 (9)	0.08774 (7)	0.0192 (3)
C15	1.32978 (13)	0.28155 (11)	0.14890 (9)	0.0262 (3)
H15A	1.3668	0.2766	0.1090	0.031*
C16	0.29176 (13)	0.96112 (10)	0.00953 (8)	0.0233 (3)
H16A	0.2424	0.9214	−0.0091	0.028*
C17	0.36847 (12)	0.93340 (10)	0.05690 (7)	0.0188 (3)
C18	0.13693 (14)	0.53840 (12)	0.03213 (9)	0.0315 (4)
H18A	0.0933	0.5250	−0.0047	0.038*
C19	0.26649 (14)	0.57716 (11)	0.14365 (8)	0.0262 (3)
H19A	0.3093	0.5911	0.1807	0.031*
C20	0.94289 (15)	0.26472 (13)	−0.16149 (9)	0.0313 (4)
H20A	0.8865	0.2386	−0.1859	0.038*
C21	0.44200 (13)	0.99264 (10)	0.08539 (8)	0.0232 (3)
H21A	0.4932	0.9738	0.1169	0.028*
C22	0.20176 (13)	0.61304 (11)	0.03161 (8)	0.0233 (3)
H22A	0.2027	0.6503	−0.0049	0.028*
C23	0.97874 (13)	0.05929 (10)	0.14174 (8)	0.0231 (3)
H23A	0.9203	0.0862	0.1197	0.028*
C24	1.16301 (14)	0.26143 (11)	0.21197 (8)	0.0234 (3)
H24A	1.0901	0.2440	0.2135	0.028*
C25	1.22195 (12)	0.25521 (10)	0.15412 (7)	0.0193 (3)
C26	0.61160 (16)	0.52405 (12)	0.08323 (10)	0.0365 (4)
H26A	0.6406	0.4895	0.0497	0.044*
C27	0.59140 (17)	0.55454 (14)	0.19931 (10)	0.0410 (5)
H27A	0.6067	0.5401	0.2433	0.049*
C28	0.13662 (15)	0.48343 (11)	0.08718 (11)	0.0357 (4)
H28A	0.0927	0.4336	0.0870	0.043*
C29	1.07672 (18)	0.37922 (13)	−0.14926 (9)	0.0373 (4)
H29A	1.1098	0.4296	−0.1656	0.045*
C30	0.99065 (17)	0.34099 (13)	−0.18406 (8)	0.0357 (4)
H30A	0.9648	0.3669	−0.2230	0.043*

C31	1.05005 (16)	−0.04896 (11)	0.21749 (8)	0.0309 (4)
H31A	1.0381	−0.0945	0.2472	0.037*
C32	0.52652 (15)	0.62680 (12)	0.18486 (9)	0.0322 (4)
H32A	0.4981	0.6617	0.2184	0.039*
C33	0.63346 (16)	0.50377 (12)	0.14888 (10)	0.0379 (4)
H33A	0.6769	0.4555	0.1593	0.045*
C34	1.38103 (14)	0.31553 (12)	0.20490 (9)	0.0324 (4)
H34A	1.4533	0.3345	0.2028	0.039*
C35	0.96171 (15)	−0.00952 (11)	0.18556 (8)	0.0282 (3)
H35A	0.8910	−0.0292	0.1935	0.034*
C36	0.43818 (14)	1.08006 (11)	0.06637 (9)	0.0290 (4)
H36A	0.4862	1.1202	0.0857	0.035*
C37	1.15587 (15)	−0.02118 (11)	0.20551 (9)	0.0301 (4)
H37A	1.2145	−0.0488	0.2267	0.036*
C38	1.32453 (15)	0.32131 (12)	0.26427 (9)	0.0320 (4)
H38A	1.3598	0.3434	0.3019	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02031 (6)	0.02291 (6)	0.01869 (6)	−0.00040 (4)	−0.00164 (4)	0.00029 (4)
Cl1	0.0350 (2)	0.02315 (19)	0.0337 (2)	−0.00084 (16)	−0.00361 (17)	0.00242 (16)
Cl2	0.02000 (18)	0.0354 (2)	0.0341 (2)	−0.00039 (15)	0.00095 (16)	0.00203 (17)
Cl3	0.02154 (17)	0.02392 (17)	0.01808 (15)	−0.00071 (13)	−0.00155 (13)	0.00113 (13)
Cl4	0.02743 (19)	0.02940 (19)	0.01689 (16)	−0.00481 (15)	−0.00084 (14)	−0.00108 (14)
N1	0.0201 (6)	0.0165 (6)	0.0176 (6)	0.0021 (5)	0.0020 (5)	−0.0004 (5)
N2	0.0218 (6)	0.0173 (6)	0.0197 (6)	0.0004 (5)	0.0008 (5)	−0.0016 (5)
N3	0.0163 (6)	0.0167 (6)	0.0185 (6)	0.0012 (5)	0.0004 (5)	−0.0008 (5)
N4	0.0227 (6)	0.0218 (6)	0.0189 (6)	0.0014 (5)	0.0022 (5)	0.0021 (5)
N5	0.0196 (6)	0.0194 (6)	0.0188 (6)	0.0001 (5)	0.0002 (5)	0.0005 (5)
N6	0.0175 (6)	0.0164 (6)	0.0202 (6)	0.0007 (5)	−0.0012 (5)	−0.0017 (5)
N7	0.0214 (6)	0.0221 (6)	0.0178 (6)	0.0027 (5)	−0.0014 (5)	0.0000 (5)
N8	0.0181 (6)	0.0201 (6)	0.0172 (5)	0.0008 (5)	0.0007 (5)	0.0002 (5)
C1	0.0259 (8)	0.0231 (8)	0.0273 (8)	0.0038 (6)	−0.0036 (6)	−0.0010 (6)
C2	0.0186 (7)	0.0172 (7)	0.0263 (7)	0.0023 (6)	−0.0031 (6)	0.0000 (6)
C3	0.0248 (7)	0.0165 (7)	0.0169 (6)	0.0009 (6)	0.0009 (6)	0.0007 (5)
C4	0.0233 (8)	0.0300 (8)	0.0216 (7)	0.0061 (6)	0.0029 (6)	0.0002 (6)
C5	0.0193 (7)	0.0186 (7)	0.0159 (6)	0.0012 (5)	0.0016 (5)	−0.0026 (5)
C6	0.0244 (8)	0.0229 (7)	0.0169 (7)	0.0063 (6)	0.0037 (6)	0.0001 (6)
C7	0.0203 (7)	0.0207 (7)	0.0194 (7)	0.0029 (6)	0.0022 (6)	−0.0011 (6)
C8	0.0333 (9)	0.0262 (8)	0.0268 (8)	0.0099 (7)	0.0060 (7)	0.0045 (7)
C9	0.0388 (10)	0.0265 (8)	0.0231 (7)	−0.0007 (7)	0.0036 (7)	0.0011 (6)
C10	0.0320 (9)	0.0222 (8)	0.0458 (10)	0.0033 (7)	0.0089 (8)	0.0111 (7)
C11	0.0354 (9)	0.0173 (7)	0.0374 (9)	0.0050 (7)	0.0158 (7)	0.0034 (7)
C12	0.0309 (9)	0.0263 (8)	0.0278 (8)	0.0070 (7)	−0.0020 (7)	−0.0023 (7)
C13	0.0369 (9)	0.0293 (8)	0.0211 (7)	−0.0005 (7)	−0.0007 (7)	−0.0008 (6)
C14	0.0179 (7)	0.0148 (6)	0.0250 (7)	−0.0001 (5)	0.0026 (6)	−0.0020 (6)
C15	0.0195 (7)	0.0295 (8)	0.0296 (8)	0.0011 (6)	0.0032 (6)	−0.0025 (7)

C16	0.0250 (8)	0.0225 (7)	0.0224 (7)	0.0028 (6)	0.0018 (6)	−0.0011 (6)
C17	0.0197 (7)	0.0168 (7)	0.0201 (7)	0.0019 (5)	0.0061 (6)	−0.0004 (5)
C18	0.0237 (8)	0.0304 (9)	0.0405 (9)	−0.0048 (7)	0.0015 (7)	−0.0114 (7)
C19	0.0260 (8)	0.0235 (8)	0.0291 (8)	0.0037 (6)	0.0005 (7)	0.0046 (6)
C20	0.0292 (9)	0.0418 (10)	0.0228 (8)	0.0128 (7)	−0.0022 (7)	−0.0038 (7)
C21	0.0204 (7)	0.0208 (7)	0.0286 (8)	0.0008 (6)	0.0045 (6)	−0.0030 (6)
C22	0.0208 (7)	0.0250 (8)	0.0243 (7)	−0.0002 (6)	0.0028 (6)	−0.0026 (6)
C23	0.0231 (7)	0.0208 (7)	0.0255 (7)	0.0005 (6)	0.0000 (6)	0.0003 (6)
C24	0.0230 (8)	0.0250 (8)	0.0221 (7)	−0.0015 (6)	−0.0003 (6)	0.0009 (6)
C25	0.0186 (7)	0.0197 (7)	0.0196 (7)	0.0010 (5)	−0.0019 (6)	−0.0010 (5)
C26	0.0379 (10)	0.0277 (9)	0.0436 (10)	0.0125 (8)	−0.0036 (8)	−0.0102 (8)
C27	0.0471 (11)	0.0392 (11)	0.0364 (10)	0.0108 (9)	−0.0153 (9)	0.0054 (8)
C28	0.0286 (9)	0.0189 (8)	0.0598 (12)	−0.0049 (7)	0.0064 (8)	−0.0030 (8)
C29	0.0576 (12)	0.0276 (9)	0.0269 (8)	0.0049 (8)	0.0054 (8)	0.0071 (7)
C30	0.0506 (11)	0.0370 (10)	0.0194 (7)	0.0202 (9)	0.0027 (7)	0.0041 (7)
C31	0.0490 (11)	0.0177 (7)	0.0258 (8)	−0.0013 (7)	−0.0022 (7)	0.0014 (6)
C32	0.0346 (9)	0.0346 (9)	0.0273 (8)	0.0100 (8)	−0.0074 (7)	−0.0031 (7)
C33	0.0375 (10)	0.0241 (9)	0.0517 (11)	0.0107 (7)	−0.0127 (9)	0.0012 (8)
C34	0.0213 (8)	0.0337 (9)	0.0421 (10)	−0.0011 (7)	−0.0068 (7)	−0.0041 (8)
C35	0.0323 (9)	0.0209 (8)	0.0316 (8)	−0.0052 (7)	0.0043 (7)	0.0008 (7)
C36	0.0254 (8)	0.0195 (8)	0.0425 (9)	−0.0030 (6)	0.0099 (7)	−0.0049 (7)
C37	0.0391 (10)	0.0218 (8)	0.0292 (8)	0.0071 (7)	−0.0099 (7)	0.0011 (7)
C38	0.0348 (9)	0.0311 (9)	0.0298 (8)	0.0002 (7)	−0.0135 (7)	−0.0037 (7)

Geometric parameters (Å, °)

Cd1—Cl1	2.4450 (6)	C13—C24	1.390 (2)
Cd1—Cl4	2.4666 (6)	C13—H13A	0.9300
Cd1—Cl3	2.4712 (8)	C14—C19	1.383 (2)
Cd1—Cl2	2.4801 (6)	C14—C22	1.385 (2)
N1—N3	1.3073 (18)	C15—C25	1.382 (2)
N1—C5	1.3442 (19)	C15—C34	1.383 (2)
N2—N6	1.3120 (18)	C15—H15A	0.9300
N2—C5	1.3428 (19)	C16—C17	1.394 (2)
N3—N6	1.3339 (17)	C16—H16A	0.9300
N3—C14	1.4424 (19)	C17—C21	1.392 (2)
N4—N5	1.3142 (18)	C18—C22	1.387 (2)
N4—C7	1.344 (2)	C18—C28	1.390 (3)
N5—N8	1.3323 (18)	C18—H18A	0.9300
N5—C25	1.4498 (19)	C19—H19A	0.9300
N6—C2	1.4500 (19)	C20—C30	1.381 (3)
N7—N8	1.3139 (17)	C20—H20A	0.9300
N7—C7	1.346 (2)	C21—C36	1.388 (2)
N8—C3	1.4425 (19)	C21—H21A	0.9300
C1—C3	1.385 (2)	C22—H22A	0.9300
C1—C37	1.386 (2)	C23—C35	1.388 (2)
C1—H1B	0.9300	C23—H23A	0.9300
C2—C32	1.379 (2)	C24—C25	1.380 (2)
C2—C12	1.380 (2)	C24—H24A	0.9300

C3—C23	1.379 (2)	C26—C33	1.380 (3)
C4—C20	1.389 (2)	C26—H26A	0.9300
C4—C6	1.390 (2)	C27—C33	1.381 (3)
C4—H4B	0.9300	C27—C32	1.386 (3)
C5—C17	1.464 (2)	C27—H27A	0.9300
C6—C9	1.395 (2)	C28—H28A	0.9300
C6—C7	1.461 (2)	C29—C30	1.384 (3)
C8—C16	1.387 (2)	C29—H29A	0.9300
C8—C11	1.388 (3)	C30—H30A	0.9300
C8—H8A	0.9300	C31—C37	1.384 (3)
C9—C29	1.387 (2)	C31—C35	1.386 (3)
C9—H9A	0.9300	C31—H31A	0.9300
C10—C28	1.381 (3)	C32—H32A	0.9300
C10—C19	1.392 (2)	C33—H33A	0.9300
C10—H10A	0.9300	C34—C38	1.390 (3)
C11—C36	1.388 (3)	C34—H34A	0.9300
C11—H11A	0.9300	C35—H35A	0.9300
C12—C26	1.387 (2)	C36—H36A	0.9300
C12—H12A	0.9300	C37—H37A	0.9300
C13—C38	1.384 (3)	C38—H38A	0.9300
Cl1—Cd1—Cl4	105.508 (18)	C8—C16—H16A	120.2
Cl1—Cd1—Cl3	110.297 (15)	C17—C16—H16A	120.2
Cl4—Cd1—Cl3	109.17 (2)	C21—C17—C16	120.60 (14)
Cl1—Cd1—Cl2	117.232 (16)	C21—C17—C5	120.33 (14)
Cl4—Cd1—Cl2	107.18 (3)	C16—C17—C5	119.00 (14)
Cl3—Cd1—Cl2	107.22 (2)	C22—C18—C28	120.58 (17)
N3—N1—C5	103.64 (12)	C22—C18—H18A	119.7
N6—N2—C5	103.44 (12)	C28—C18—H18A	119.7
N1—N3—N6	110.12 (12)	C14—C19—C10	117.25 (16)
N1—N3—C14	123.80 (12)	C14—C19—H19A	121.4
N6—N3—C14	126.02 (12)	C10—C19—H19A	121.4
N5—N4—C7	103.67 (13)	C30—C20—C4	120.04 (18)
N4—N5—N8	110.08 (12)	C30—C20—H20A	120.0
N4—N5—C25	121.59 (13)	C4—C20—H20A	120.0
N8—N5—C25	128.02 (12)	C36—C21—C17	119.39 (15)
N2—N6—N3	110.16 (12)	C36—C21—H21A	120.3
N2—N6—C2	125.16 (13)	C17—C21—H21A	120.3
N3—N6—C2	124.55 (12)	C14—C22—C18	117.29 (16)
N8—N7—C7	103.58 (12)	C14—C22—H22A	121.4
N7—N8—N5	110.18 (12)	C18—C22—H22A	121.4
N7—N8—C3	122.84 (12)	C3—C23—C35	117.88 (15)
N5—N8—C3	126.96 (12)	C3—C23—H23A	121.1
C3—C1—C37	117.46 (16)	C35—C23—H23A	121.1
C3—C1—H1B	121.3	C25—C24—C13	117.69 (15)
C37—C1—H1B	121.3	C25—C24—H24A	121.2
C32—C2—C12	123.82 (15)	C13—C24—H24A	121.2
C32—C2—N6	118.82 (14)	C24—C25—C15	123.48 (15)
C12—C2—N6	117.34 (14)	C24—C25—N5	118.78 (14)
C23—C3—C1	123.43 (15)	C15—C25—N5	117.51 (14)

C23—C3—N8	117.45 (13)	C33—C26—C12	120.27 (17)
C1—C3—N8	119.06 (14)	C33—C26—H26A	119.9
C20—C4—C6	119.40 (17)	C12—C26—H26A	119.9
C20—C4—H4B	120.3	C33—C27—C32	120.56 (17)
C6—C4—H4B	120.3	C33—C27—H27A	119.7
N2—C5—N1	112.63 (13)	C32—C27—H27A	119.7
N2—C5—C17	124.24 (13)	C10—C28—C18	120.36 (16)
N1—C5—C17	123.12 (13)	C10—C28—H28A	119.8
C4—C6—C9	120.57 (15)	C18—C28—H28A	119.8
C4—C6—C7	120.14 (15)	C30—C29—C9	120.02 (18)
C9—C6—C7	119.15 (15)	C30—C29—H29A	120.0
N4—C7—N7	112.47 (13)	C9—C29—H29A	120.0
N4—C7—C6	122.75 (14)	C20—C30—C29	120.62 (16)
N7—C7—C6	124.71 (14)	C20—C30—H30A	119.7
C16—C8—C11	120.04 (16)	C29—C30—H30A	119.7
C16—C8—H8A	120.0	C37—C31—C35	120.57 (16)
C11—C8—H8A	120.0	C37—C31—H31A	119.7
C29—C9—C6	119.32 (17)	C35—C31—H31A	119.7
C29—C9—H9A	120.3	C2—C32—C27	117.26 (17)
C6—C9—H9A	120.3	C2—C32—H32A	121.4
C28—C10—C19	120.64 (17)	C27—C32—H32A	121.4
C28—C10—H10A	119.7	C26—C33—C27	120.60 (17)
C19—C10—H10A	119.7	C26—C33—H33A	119.7
C8—C11—C36	120.33 (15)	C27—C33—H33A	119.7
C8—C11—H11A	119.8	C15—C34—C38	120.02 (16)
C36—C11—H11A	119.8	C15—C34—H34A	120.0
C2—C12—C26	117.48 (16)	C38—C34—H34A	120.0
C2—C12—H12A	121.3	C31—C35—C23	120.08 (16)
C26—C12—H12A	121.3	C31—C35—H35A	120.0
C38—C13—C24	120.14 (16)	C23—C35—H35A	120.0
C38—C13—H13A	119.9	C11—C36—C21	120.12 (16)
C24—C13—H13A	119.9	C11—C36—H36A	119.9
C19—C14—C22	123.87 (15)	C21—C36—H36A	119.9
C19—C14—N3	119.81 (14)	C31—C37—C1	120.55 (16)
C22—C14—N3	116.23 (13)	C31—C37—H37A	119.7
C25—C15—C34	117.94 (16)	C1—C37—H37A	119.7
C25—C15—H15A	121.0	C13—C38—C34	120.71 (16)
C34—C15—H15A	121.0	C13—C38—H38A	119.6
C8—C16—C17	119.51 (15)	C34—C38—H38A	119.6
C5—N1—N3—N6	−0.19 (15)	N6—N3—C14—C22	−130.16 (15)
C5—N1—N3—C14	−177.63 (13)	C11—C8—C16—C17	−0.5 (2)
C7—N4—N5—N8	1.30 (16)	C8—C16—C17—C21	0.5 (2)
C7—N4—N5—C25	−172.82 (13)	C8—C16—C17—C5	−176.49 (14)
C5—N2—N6—N3	−0.66 (15)	N2—C5—C17—C21	−26.7 (2)
C5—N2—N6—C2	175.24 (13)	N1—C5—C17—C21	154.71 (14)
N1—N3—N6—N2	0.56 (16)	N2—C5—C17—C16	150.37 (14)
C14—N3—N6—N2	177.93 (13)	N1—C5—C17—C16	−28.3 (2)
N1—N3—N6—C2	−175.37 (13)	C22—C14—C19—C10	1.0 (2)
C14—N3—N6—C2	2.0 (2)	N3—C14—C19—C10	177.61 (14)

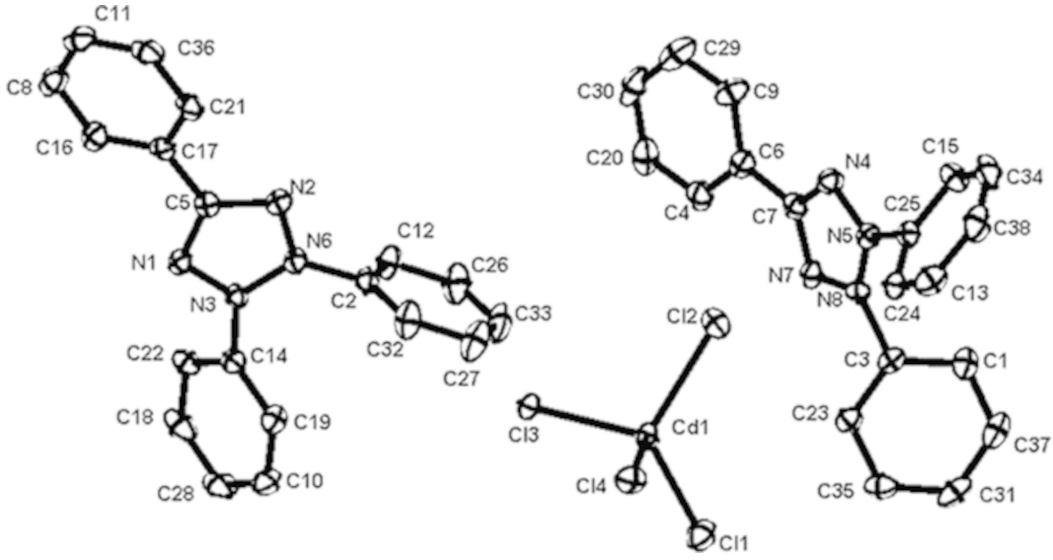
C7—N7—N8—N5	0.16 (16)	C28—C10—C19—C14	−1.1 (3)
C7—N7—N8—C3	−178.37 (13)	C6—C4—C20—C30	0.0 (2)
N4—N5—N8—N7	−0.96 (16)	C16—C17—C21—C36	0.2 (2)
C25—N5—N8—N7	172.67 (13)	C5—C17—C21—C36	177.18 (14)
N4—N5—N8—C3	177.49 (13)	C19—C14—C22—C18	−0.5 (2)
C25—N5—N8—C3	−8.9 (2)	N3—C14—C22—C18	−177.18 (14)
N2—N6—C2—C32	87.7 (2)	C28—C18—C22—C14	0.0 (2)
N3—N6—C2—C32	−96.95 (19)	C1—C3—C23—C35	1.6 (2)
N2—N6—C2—C12	−94.28 (18)	N8—C3—C23—C35	178.84 (14)
N3—N6—C2—C12	81.1 (2)	C38—C13—C24—C25	1.0 (2)
C37—C1—C3—C23	−1.5 (2)	C13—C24—C25—C15	−1.2 (2)
C37—C1—C3—N8	−178.68 (14)	C13—C24—C25—N5	−175.56 (14)
N7—N8—C3—C23	−47.3 (2)	C34—C15—C25—C24	0.3 (3)
N5—N8—C3—C23	134.40 (16)	C34—C15—C25—N5	174.74 (15)
N7—N8—C3—C1	130.06 (15)	N4—N5—C25—C24	122.90 (16)
N5—N8—C3—C1	−48.2 (2)	N8—N5—C25—C24	−50.1 (2)
N6—N2—C5—N1	0.56 (16)	N4—N5—C25—C15	−51.8 (2)
N6—N2—C5—C17	−178.19 (13)	N8—N5—C25—C15	135.22 (16)
N3—N1—C5—N2	−0.24 (16)	C2—C12—C26—C33	0.1 (3)
N3—N1—C5—C17	178.53 (13)	C19—C10—C28—C18	0.7 (3)
C20—C4—C6—C9	−1.6 (2)	C22—C18—C28—C10	−0.1 (3)
C20—C4—C6—C7	174.10 (14)	C6—C9—C29—C30	0.3 (3)
N5—N4—C7—N7	−1.23 (17)	C4—C20—C30—C29	1.8 (3)
N5—N4—C7—C6	176.06 (14)	C9—C29—C30—C20	−2.0 (3)
N8—N7—C7—N4	0.68 (17)	C12—C2—C32—C27	−0.6 (3)
N8—N7—C7—C6	−176.56 (14)	N6—C2—C32—C27	177.31 (17)
C4—C6—C7—N4	−170.09 (15)	C33—C27—C32—C2	0.4 (3)
C9—C6—C7—N4	5.7 (2)	C12—C26—C33—C27	−0.2 (3)
C4—C6—C7—N7	6.9 (2)	C32—C27—C33—C26	0.0 (3)
C9—C6—C7—N7	−177.36 (15)	C25—C15—C34—C38	0.8 (3)
C4—C6—C9—C29	1.5 (3)	C37—C31—C35—C23	−0.9 (3)
C7—C6—C9—C29	−174.30 (16)	C3—C23—C35—C31	−0.4 (2)
C16—C8—C11—C36	−0.3 (2)	C8—C11—C36—C21	1.1 (3)
C32—C2—C12—C26	0.3 (3)	C17—C21—C36—C11	−1.0 (2)
N6—C2—C12—C26	−177.60 (16)	C35—C31—C37—C1	1.0 (3)
N1—N3—C14—C19	−129.97 (16)	C3—C1—C37—C31	0.1 (2)
N6—N3—C14—C19	53.0 (2)	C24—C13—C38—C34	0.1 (3)
N1—N3—C14—C22	46.9 (2)	C15—C34—C38—C13	−1.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12A···Cl3^{i}	0.93	2.81	3.6362 (19)	148
C37—H37A···Cl4^{ii}	0.93	2.71	3.5271 (18)	146

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, *y*−1/2, −*z*+1/2.

Fig. 1


C11
C36
C8
C21
C16
C17
N2
C5
N6
C12
N1
C26
N3
C2
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C22
C14
C27
C18
C19
C28
C10
C29
C30
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C20
C6
N4
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C25
N5
C38
N7
C13
N8
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C1
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C37
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C31
Cl2
Cd1
Cl3
Cl4
Cl1

Fig. 2

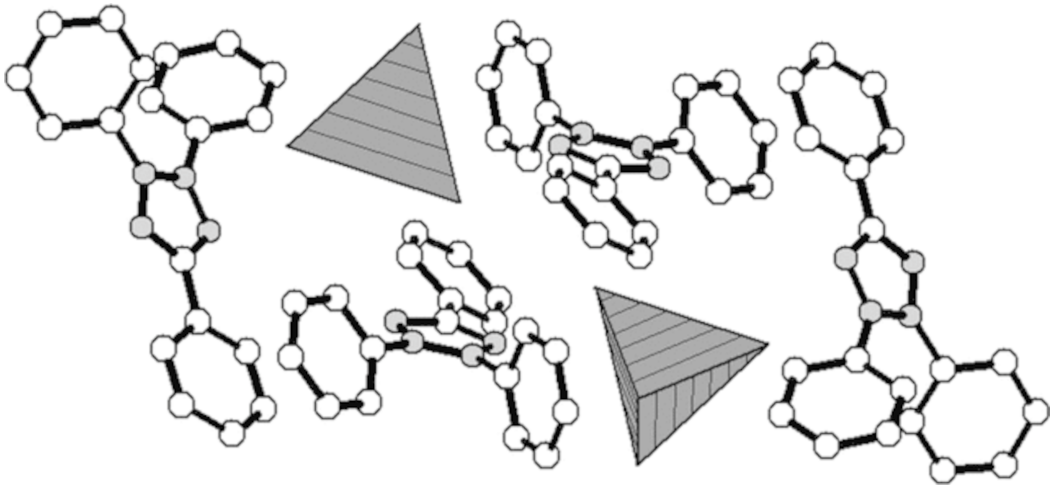

Fig. 3