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The role of π–π stacking and hydrogen-bonding interactions in the assembly of a series of isostructural group IIB coordination compounds

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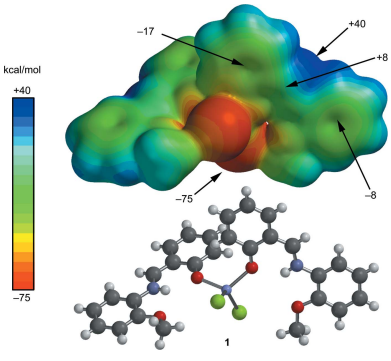
The supramolecular chemistry of coordination compounds has become an important research domain of modern inorganic chemistry. Herein, six isostructural group IIB coordination compounds containing a 2-{[(2-methoxyphenyl)imino]methyl}phenol ligand, namely dichloridobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)zinc(II), $[ZnCl_2(C_{28}H_{26}N_2O_4)]$, **1**, diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)-zinc(II), $[ZnI_2(C_{28}H_{26}N_2O_4)]$, **2**, dibromidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)cadmium(II), $[CdBr_2(C_{28}H_{26}N_2O_4)]$, **3**, diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)cadmium(II), $[CdI_2(C_{28}H_{26}N_2O_4)]$, **4**, dichloridobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)mercury(II), $[HgCl_2(C_{28}H_{26}N_2O_4)]$, **5**, and diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)-mercury(II), $[HgI_2(C_{28}H_{26}N_2O_4)]$, **6**, were synthesized and characterized by X-ray crystallography and spectroscopic techniques. All six compounds exhibit an infinite one-dimensional ladder in the solid state governed by the formation of hydrogen-bonding and π–π stacking interactions. The crystal structures of these compounds were studied using geometrical and Hirshfeld surface analyses. They have also been studied using M06-2X/def2-TZVP calculations and Bader's theory of 'atoms in molecules'. The energies associated with the interactions, including the contribution of the different forces, have been evaluated. In general, the π–π stacking interactions are stronger than those reported for conventional π–π complexes, which is attributed to the influence of the metal coordination, which is stronger for Zn than either Cd or Hg. The results reported herein might be useful for understanding the solid-state architecture of metal-containing materials that contain $M^{II}X_2$ subunits and aromatic organic ligands.



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1. Introduction

Over the last two decades, the supramolecular chemistry of metal-containing compounds has attracted intense attention, due not only to their fascinating structures (Holliday & Mirkin, 2001; Brammer, 2004), but also their potential applications in diverse fields such as medicine (McKinlay *et al.*, 2010; Reedijk, 2009), ion and molecular recognition (Custelcean *et al.*, 2012; Busschaert *et al.*, 2015) and catalysis (Wang *et al.*, 2013; Wiester *et al.*, 2011).

The ultimate goal of supramolecular chemistry is to understand the inherent complexities of the association mechanisms of molecular and ionic building blocks organized through noncovalent intermolecular interactions with prescribed properties and functions (Lehn, 1995; Steed &

Atwood, 2013). In the context of metallosupramolecular chemistry (Braga & Grepioni, 2000; Braga *et al.*, 1998), hydrogen bonding (Reedijk, 2013; Azhdari Tehrani *et al.*, 2016) and halogen bonding (Khavasi *et al.*, 2015; Khavasi & Azhdari Tehrani, 2013; Li *et al.*, 2016) have been widely used so far to drive the self-assembly of coordination compounds, because of their directionality and versatility (Politzer *et al.*, 2010; Desiraju, 1998). However, there are some reports that provide evidence suggesting the crucial role of nondirectional intermolecular interactions, such as π–π stacking (Khavasi & Azizpoor Fard, 2010; Janiak, 2000; Khavasi & Sadegh, 2014; Semeniuc *et al.*, 2010), for designing the supramolecular architecture of metal-containing species in the solid state. In this regard, supramolecular chemists and crystal engineers have explored and studied the use of noncovalent interactions as a key tool for constructing supramolecular architectures of metal-containing building units in the solid state in which X-ray crystallography could provide a detailed picture of the supramolecular structure (Desiraju, 2014; Blake *et al.*, 1999; Đaković *et al.*, 2018). These studies reveal an undeniable contribution of such noncovalent interactions to the organization and stabilization of the ultimate crystal structures. These studies also revealed that the ultimate supramolecular architecture of self-assembled metal-containing compounds could be affected by various factors, such as ligand and metal geometries (Khavasi *et al.*, 2012; Hajiashrafi *et al.*, 2013), counter-ions (Schottel *et al.*, 2006; Zeng *et al.*, 2010) and reaction conditions (Khavasi & Mohammad Sadegh, 2010; Mahata *et al.*, 2009).

In continuation of our research aimed at understanding the role of noncovalent interactions in the fabrication and self-assembly of metal-containing building blocks (Hajiashrafi *et al.*, 2013, 2016; Kielmann & Senge, 2018), a series of coordination compounds, namely $[ZnL_2Cl_2]$ (**1**), $[ZnL_2I_2]$ (**2**), $[CdL_2Br_2]$ (**3**), $[CdL_2I_2]$ (**4**), $[HgL_2Cl_2]$ (**5**) and $[HgL_2I_2]$ (**6**), where *L* is 2-{[(2-methoxyphenyl)azaniumylidene]methyl}-phenolate, have been synthesized and characterized using X-ray crystallography and different spectroscopic techniques (see Scheme 1). Geometrical, Hirshfeld surface analysis and theoretical calculations reveal the importance of π–π stacking interactions, as well as hydrogen bonding, in governing the crystal packing of this series of isostructural metal-containing compounds.

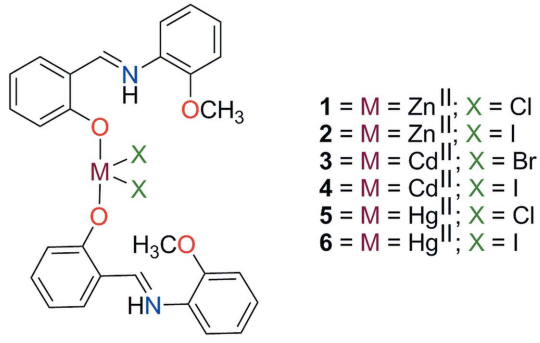
2. Experimental

2.1. Materials and apparatus

Chemicals and reagents were purchased from commercial sources. 2-Hydroxybenzaldehyde, 2-methoxyaniline and anhydrous M^{II} halides, where *M* is Zn, Cd and Hg, were purchased from Sigma–Aldrich and Merck, and used as received. The Schiff base ligand 2-{[(2-methoxyphenyl)imino]methyl}-phenol (*L*) was prepared according to a previously reported method (Song *et al.*, 2013). The IR spectra were recorded on a Nicolet FT–IR 100 spectrometer in the range 500–4000 cm^{-1} using the KBr disk technique. Elemental analyses (C, H and N) were performed using an ECS 4010 CHN-O made in Costech, Italy. Melting points were measured by an Electrothermal 9100 melting-point apparatus and corrected. The measurements were carried out using 10 mg of a powdered sample sealed in aluminium pans with a mechanical crimp.

2.2. Computational methods

The geometries of the complexes included in this study were computed at the M06-2X/def2-TZVP level of theory using the crystallographic coordinates within *TURBOMOLE 7.0* (Ahlrichs *et al.*, 1989). We have used the crystallographic coordinates instead of the optimized complexes because we are interested in estimating the binding energies of several assemblies as they stand in the crystal structure, instead of investigating the most favourable geometry for a given complex. The interaction energies were calculated with correction for the basis set superposition error (BSSE) by using the Boys–Bernardi counterpoise technique (Boys & Bernardi, 1970). The 'atoms-in-molecules' (AIM) analysis of the electron density was performed at the same level of theory using the *AIMAll* program (Keith, 2013).



Scheme 1

2.3. Synthesis and crystallization

The ligand 2-{[(2-methoxyphenyl)imino]methyl}phenol (*L*) was utilized previously for the preparation of a number of coordination compounds (Song *et al.*, 2013; Gong *et al.*, 2014; Reddy *et al.*, 2003*a*,*b*; Li & Yuan, 2012). *L* was synthesized by reacting 2-hydroxybenzaldehyde (0.53 ml, 5 mmol) with 2-methoxyaniline (0.56 ml, 5 mmol) in ethanol. After stirring for 30 min at 323 K, the ligand precipitated from the reaction mixture as an orange powder which was filtered off, washed several times with cold ethanol and normal hexane, and then dried under vacuum.

The six coordination compounds $[ZnL_2Cl_2]$ (**1**), $[ZnL_2I_2]$ (**2**), $[CdL_2Br_2]$ (**3**), $[CdL_2I_2]$ (**4**), $[HgL_2Cl_2]$ (**5**) and $[HgL_2I_2]$ (**6**) were synthesized by combining a solution of MX_2 (0.1 mmol; *M* = Zn, Cd or Hg and *X* = Cl, Br or I) in methanol (5 ml) and a solution of *L* (0.2 mmol) in methanol (5 ml) with stirring. Each mixture was heated at 333 K for about 30 min. Reduction of the solvent volume resulted in the formation of a yellow-to-orange precipitate. The precipitate was filtered off, washed with methanol (3 × 2 ml) and then dried *in vacuo*. The solid was subsequently dissolved in boiling methanol, ethanol or acetonitrile (10 ml) and filtered. Upon slow evaporation of

Table 1
Experimental details.

	1	**2**	**3**
Crystal data			
Chemical formula	$[ZnCl_2(C_{28}H_{26}N_2O_4)]$	$[ZnI_2(C_{28}H_{26}N_2O_4)]$	$[CdBr_2(C_{28}H_{26}N_2O_4)]$
M_r	590.78	773.68	726.73
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	100	100	100
a, b, c (Å)	9.1926 (2), 10.6101 (2), 14.8057 (3)	9.2709 (19), 10.020 (2), 16.248 (4)	9.2772 (3), 10.0935 (3), 16.1021 (5)
α, β, γ (°)	94.188 (1), 97.716 (1), 114.409 (1)	98.56 (4), 100.50 (4), 110.09 (3)	97.699 (2), 100.586 (2), 111.149 (2)
V (Å^3)	1289.80 (5)	1356.7 (6)	1348.92 (8)
Z	2	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.20	3.22	3.81
Crystal size (mm)	0.26 × 0.12 × 0.11	0.14 × 0.07 × 0.03	0.27 × 0.13 × 0.10
Data collection			
Diffractometer	Bruker SMART APEXII area detector	Bruker APEXII area detector	Bruker APEXII area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)	Multi-scan (*TWINABS*; Bruker, 2012)	Multi-scan (*TWINABS*; Bruker, 2012)
T_{min}, T_{max}	0.691, 0.747	0.612, 0.746	0.538, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	93163, 11965, 9331	7281, 7281, 4608	10130, 10130, 8342
R_{int}	0.053	0.116	0.020
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.822	0.606	0.634
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.084, 1.02	0.067, 0.195, 0.99	0.040, 0.126, 1.03
No. of reflections	11965	7281	10130
No. of parameters	336	337	337
No. of restraints	0	174	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.77, −0.71	2.19, −1.18	1.04, −0.70

	4	**5**	**6**
Crystal data			
Chemical formula	$[CdI_2(C_{28}H_{26}N_2O_4)]$	$[HgCl_2(C_{28}H_{26}N_2O_4)]$	$[HgI_2(C_{28}H_{26}N_2O_4)]$
M_r	820.71	726.00	908.90
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	100	100	100
a, b, c (Å)	9.3200 (3), 10.0498 (3), 16.6239 (5)	9.2456 (4), 10.1510 (4), 15.8499 (6)	9.2783 (14), 10.0060 (15), 16.695 (3)
α, β, γ (°)	99.140 (1), 100.528 (1), 109.332 (1)	96.5447 (15), 99.7441 (15), 112.6735 (14)	98.777 (1), 100.296 (1), 109.396 (1)
V (Å^3)	1403.58 (8)	1326.25 (9)	1400.4 (4)
Z	2	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	3.01	6.04	7.74
Crystal size (mm)	0.40 × 0.26 × 0.14	0.17 × 0.14 × 0.08	0.38 × 0.19 × 0.13
Data collection			
Diffractometer	Bruker SMART APEXII area detector	Bruker APEXII area detector	Bruker APEXII area detector
Absorption correction	Numerical (*SADABS*; Bruker, 2016)	Multi-scan (*TWINABS*; Bruker, 2012)	Multi-scan (*TWINABS*; Bruker, 2012)
T_{min}, T_{max}	0.416, 0.667	0.630, 0.746	0.441, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	110757, 13807, 10917	22779, 22779, 21098	11185, 11185, 10132
R_{int}	0.055	0.012	0.071
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.838	0.668	0.650
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.067, 1.03	0.022, 0.052, 1.03	0.032, 0.112, 1.08
No. of reflections	13807	22779	11185
No. of parameters	336	337	337
No. of restraints	0	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.04, −1.33	1.29, −0.60	1.48, −1.78

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*b*), *SHELXL2014* (Sheldrick, 2015*a*) and *OLEX2* (Dolomanov *et al.*, 2009).

the filtrate at room temperature, crystals of complexes **1**–**6** suitable for X-ray crystallography were obtained (Hope, 1994; Senge, 2000). The coordination compounds were characterized using X-ray crystallography, FT–IR spectroscopy and elemental analysis.

2.3.1. Analytical data for *L*. M.p. 330 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3445 (*w*, broad), 1246 (*s*), 3061 (*w*), 1615 (*s*), 792 (*s*), 849 (*m*).

2.3.2. Analytical data for 1. Yield 52%. M.p. 505–507 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3679 (*w*), 3447 (*w*), 1637 (*s*), 1525 (*m*), 1382 (*s*), 1025 (*m*), 800 (*m*), 750 (*m*). Analysis calculated for $C_{28}H_{26}Cl_2N_2O_4Zn$ (%): C 56.92, H 4.44, N 4.74; found: C 56.86, H 4.42, N 4.70.

2.3.3. Analytical data for 2. Yield 70%. M.p. 520–522 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3676 (*w*), 3447 (*w*), 1614 (*s*), 1542 (*m*), 1385 (*s*), 1019 (*m*), 805 (*m*), 754 (*m*). Analysis calculated for $C_{28}H_{26}I_2N_2O_4Zn$ (%): C 43.47, H 3.39, N 3.62; found: C 43.36, H 3.42, N 3.58.

2.3.4. Analytical data for 3. Yield 54%. M.p. 543–545 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3674 (*w*), 3445 (*m*), 1620 (*s*), 1530 (*m*), 1484 (*m*), 1383 (*s*), 1020 (*m*), 794 (*m*), 753 (*m*). Analysis calculated for $C_{28}H_{26}Br_2CdN_2O_4$ (%): C 46.28, H 3.61, N 3.85; found: C 46.24, H 3.40, N 3.82.

2.3.5. Analytical data for 4. Yield 46%. M.p. 461–463 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3679 (*w*), 3447 (*m*), 1637 (*s*), 1520 (*m*), 1380 (*m*), 1025 (*m*), 796 (*m*), 741 (*m*). Analysis calculated for $C_{28}H_{26}CdI_2N_2O_4$ (%): C 40.98, H 3.19, N 3.41; found: C 40.88, H 3.12, N 3.44.

2.3.6. Analytical data for 5. Yield 65%. M.p. 438–440 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3675 (*w*), 3435 (*m*), 1622 (*s*), 1534 (*m*), 1378 (*m*), 1028 (*m*), 794 (*m*), 750 (*m*). Analysis calculated for $C_{28}H_{26}Cl_2HgN_2O_4$ (%): C 46.32, H 3.61, N 3.86; found: C 46.28, H 3.62, N 3.92.

2.3.7. Analytical data for 6. Yield 70%. M.p. 383–385 K. FT–IR (KBr, ν/cm^{-1}, selected bands): 3675 (*w*), 3446 (*m*), 1630 (*s*), 1523 (*m*), 1382 (*m*), 1018 (*m*), 796 (*m*), 738 (*w*).

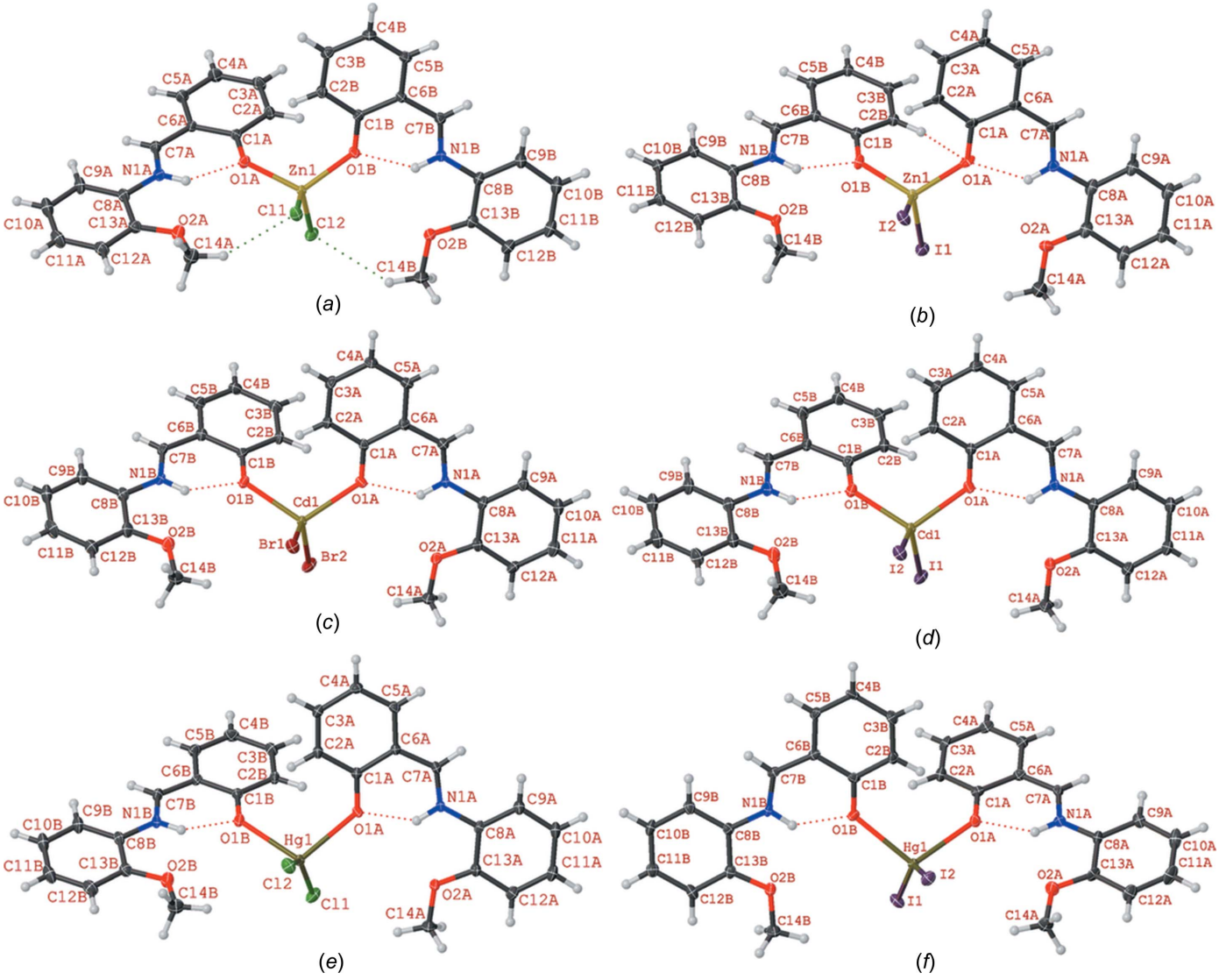


Figure 1
(*a*)–(*f*) The molecular structures of compounds **1**–**6**, respectively, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Selected bond lengths (Å) and angles (°) for compounds **1**–**6**.

Compound		**1**	**2**	**3**	**4**	**5**	**6**
Bond lengths	*M*1—*X*1	2.240 (4)	2.588 (3)	2.537 (1)	2.720 (1)	2.371 (1)	2.658 (1)
	*M*1—*X*2	2.243 (4)	2.568 (3)	2.545 (1)	2.710 (1)	2.369 (1)	2.654 (1)
	*M*1—O2*A*	1.985 (1)	1.990 (10)	2.216 (4)	2.231 (2)	2.259 (2)	2.387 (5)
	*M*1—O2*B*	1.983 (1)	1.990 (10)	2.225 (4)	2.216 (2)	2.356 (2)	2.378 (5)
Bond angles	*X*1—*M*1—*X*2	124.8 (2)	123.7 (1)	130.0 (1)	130.1 (1)	148.2 (1)	145.1 (1)
	O1*A*—*M*1—*X*1	103.9 (3)	104.0 (4)	104.4 (1)	103.7 (1)	98.3 (1)	102.0 (1)
	O1*A*—*M*1—*X*2	104.0 (3)	103.6 (4)	103.6 (1)	104.8 (1)	100.4 (1)	98.7 (1)
	O1*B*—*M*1—*X*1	105.5 (3)	106.2 (4)	104.8 (1)	102.9 (1)	98.8 (1)	98.6 (1)
	O1*B*—*M*1—*X*2	102.8 (3)	104.2 (4)	101.9 (1)	103.5 (1)	100.7 (1)	102.3 (1)
	O1*A*—*M*1—O1*B*	116.8 (4)	115.8 (5)	112.0 (2)	111.6 (1)	105.6 (1)	105.8 (2)

Analysis calculated for $C_{28}H_{26}HgI_2N_2O_4$ (%): C 37.00, H 2.88, N 3.08; found: C 36.94, H 2.80, N 3.10.

2.4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. C- and N-bound H atoms were placed in their expected calculated positions and refined as riding, with N—H = 0.88 Å and C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(N,C) otherwise. In the structure of **2**, the C and N atoms were restrained to have similar isotropic displacement parameters. Atoms N1*A*, N1*B* and C14*B* were restrained to have close to isotropic displacement parameters. The structure was solved as a rotational twin rotated from the first domain by 179.8° about the reciprocal axis 0.002 1.000 0.001 and the real axis 0.434 1.000 0.197. The twin law to convert *hkl* from the first to this domain (*SHELXL* TWIN matrix) was −0.999 0.004 −0.001, 0.866 0.998 0.395, 0.007 0.003 −0.999. The structure of **3** was solved as a rotational twin rotated from the first domain by 179.7° about the reciprocal axis −0.003 −0.997 1.000 and the real axis 0.311 1.000 −0.257. The twin law to convert *hkl* from the first to this domain (*SHELXL* TWIN matrix) was −1.001 0.001 −0.004, 0.498 0.590 −0.407, −0.487 −1.593 −0.589. The structure of **5** was solved as a rotational twin rotated from the first domain by 179.9° about the reciprocal axis −0.001 1.000 −0.999 and the real axis 0.345 1.000 −0.274. The twin law to convert *hkl* from the first to this domain (*SHELXL* TWIN matrix) was −1.000 −0.001 0.001, 0.541 0.570 −0.431, −0.543 −1.570 −0.570. The structure of **6** was solved as a rotational twin rotated from the first domain by 149.8° about the reciprocal axis 1.000 0.235 0.787 and the real axis 1.000 0.533 0.319. The twin law to convert *hkl* from the first to this domain (*SHELXL* TWIN matrix) was 0.534 0.949 0.308, 0.116 −0.693 0.359, 1.269 −0.145 −0.569.

3. Results and discussion

3.1. Crystal structure analysis

X-ray crystallography revealed that compounds **1**–**6** are isostructural and crystallize in the triclinic space group $P\overline{1}$ (Fig. 1 and Table 1). The asymmetric units of these structures contain two *L* ligands, two halide ions and a metal ion of group IIB. Crystal structure analysis reveals that in compounds **1**–**6**, the M^{II} ion is in a distorted trigonal pyramidal geometry, with four-coordinate geometry indices, τ_4 (Yang *et al.*, 2007), of 0.83, 0.85, 0.83, 0.84, 0.75, and 0.77, respectively. Selected bond lengths and angles are listed in Table 2 and are in agreement with the values reported for similar compounds (Shkol'nikova *et al.*, 1970; Gong *et al.*, 2014). The trigonal pyramidal geometry around M^{II} is made up of two halide ions and two phenolate O atoms from two different *L* ligands. It should be noted that *N*-salicylideneanilines may exist in different tautomeric forms and the tautomeric isomerization reaction between the enol and keto forms is accompanied by intra- and intermolecular proton transfer (Dürr & Bouas-Laurent, 2003; Cohen & Schmidt, 1962; Cohen *et al.*, 1964; Tsuchimoto *et al.*, 2016). The Schiff base ligand *L* shows a self-isomerization induced by an intramolecular proton transfer from the hydroxy O to the imine N atom through an O—H···N hydrogen bond (Hoshino *et al.*, 1988; Alarcón *et al.*, 1999). Thus, the ligand is a zwitterion with the negative and positive charges located at atoms O1*B* and N1*B*, respectively (Charland *et al.*, 1989; Redshaw *et al.*, 2013; Tsuchimoto *et al.*, 2016; Kargili *et al.*, 2014). This is supported by the geometry of the ligand and the unambiguous location of the H atom attached to atom N1*B*. The ligand almost keeps it coplanarity upon coordination; the dihedral angles between the planes of the two aromatic rings of ligand *L* lie in the range 4.10–10.68° for compounds **1**–**6** (see supporting information), which is a consequence of intramolecular N—H···O hydrogen bonding. In this form, *L* can act as a monodentate ligand, where it is coordinated to the metal ion *via* the phenolate O atom. It should be noted that at basic pH, the *L* ligand may act as a tridentate ligand through the imine N, phenolate O and methoxy O atoms (Gong *et al.*, 2014; Song *et al.*, 2013; Reddy *et al.*, 2003*a*).

As shown in Fig. 2, the crystal packing of compounds **1**–**6** consists of mononuclear units which are connected in the crystallographic *a* direction through a combination of π–π stacking interactions involving the C═N group of the ligand and C—H···π interactions. These units are then linked to other units *via* C—H···*X* (*X* = Cl, Br and I) hydrogen-bonding interactions in the *bc* plane. The intermolecular contacts involved in the crystal packing of compounds **1**–**6** can be quantified *via* Hirshfeld surface analysis (Spackman & Jayatilaka, 2009; Mackenzie *et al.*, 2017). The analysis shows that in compounds **1**–**6**, the H···H interactions have the

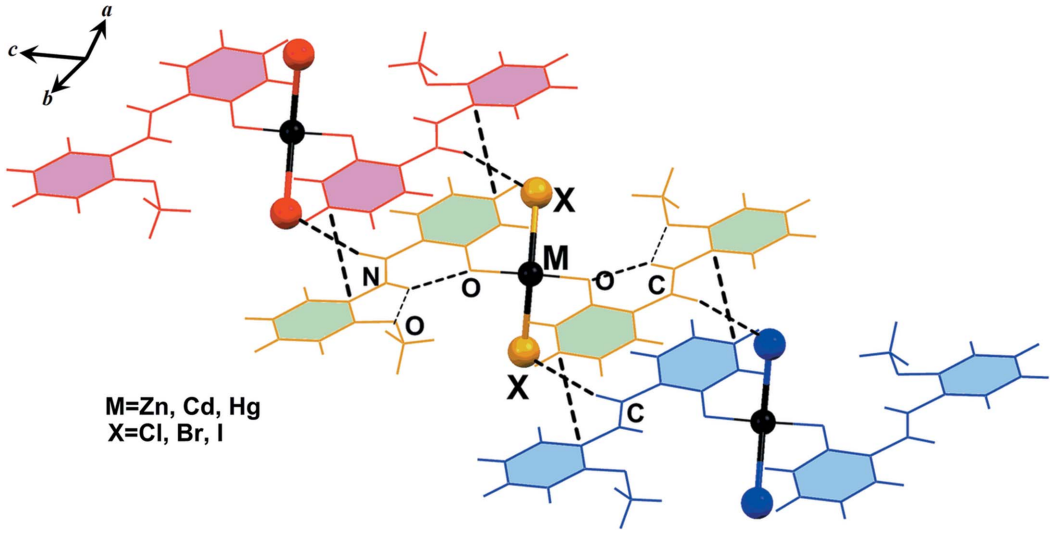


Figure 2
Representation of the self-assembly of compounds **1**–**6**, showing the association of discrete units through π–π stacking interactions in the crystallographic *a* direction and C—H···*X* (*X* = Cl, Br and I) hydrogen bonding in the *bc* plane.

highest priority (the highest contribution to the Hirshfeld surface) and the C—H···π, *M*—*X*···H and π–π interactions have the next highest priorities, respectively. Also, it has been found that the probability of hydrogen-bonding *M*—*X*···H interactions involving metal-bound halogen increases for a given metal on going from a lighter to a heavier halogen atom. Selected contribution percentages are shown as a histogram in Fig. 3.

3.2. Theoretical study

Six ML_2X_2 (*M* = Zn, Cd or Hg and *X* = Cl, Br or I) complexes have been synthesized and characterized by X-ray diffraction analysis (see Fig. 1). The ligand is mono-coordinated to the metal centre and presents an extended π-system that comprises two phenyl rings and an imino group that connects both aromatic moieties.

The solid-state architecture of all six structures is governed by the formation of π-stacking interactions between the aromatic ligands. In particular, each ligand forms infinite one-dimensional (1D) ladders in the crystal packing, as detailed for compounds **1**, **3** and **5** in Fig. 4 as representative systems.

We have focused the theoretical study on a comparison of the energetic features shown by the π-stacking and hydrogen-bonding interactions (depending on the type of metal) observed in the crystal packing of compounds **1**–**6** described above. In particular, we have analyzed the π–π and C—H···*X* noncovalent interactions that are crucial to understanding

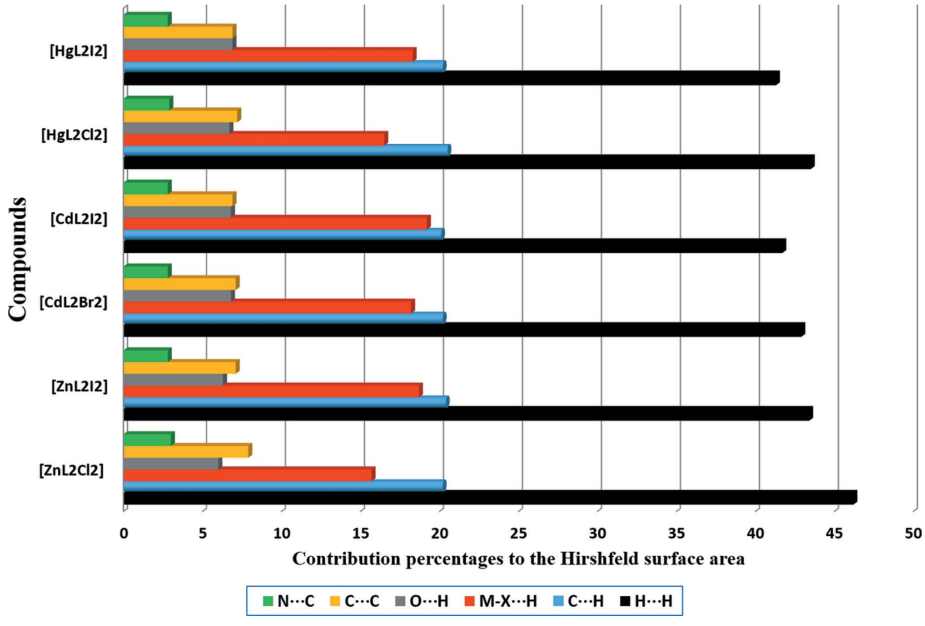


Figure 3
Relative contributions of the various noncovalent contacts to the Hirshfeld surface area in complexes **1**–**6**.

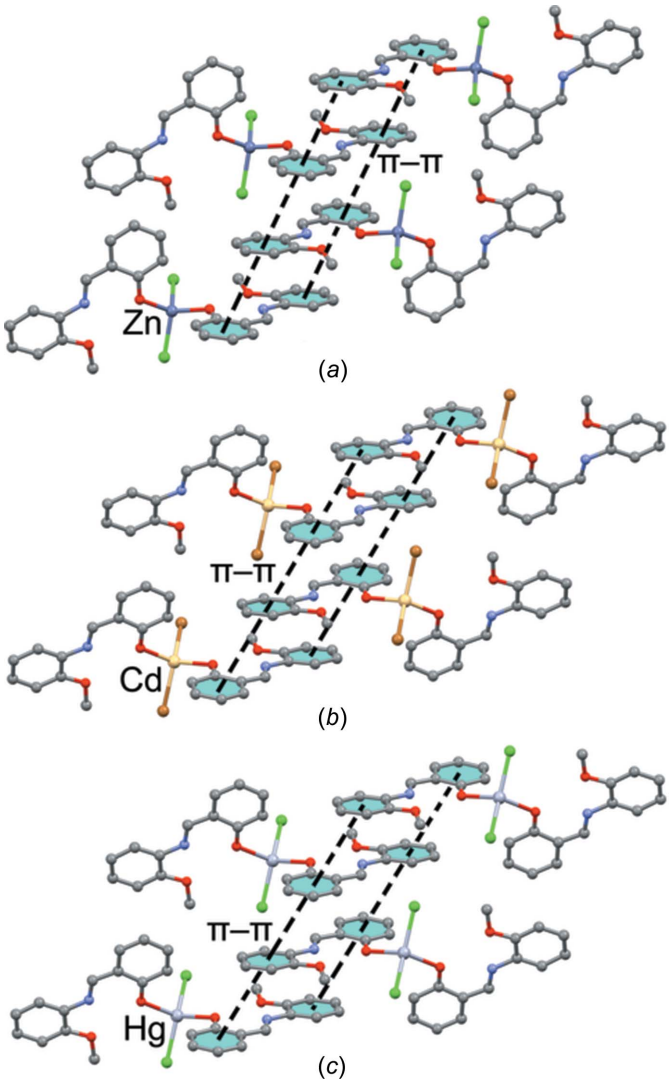


Figure 4
Partial view of the X-ray crystal structures in compounds (*a*) **1** (Zn), (*b*) **3** (Cd) and (*c*) **5** (Hg).

their solid-state architectures. First of all, in order to study the donor–acceptor ability of the ML_2X_2 complexes, we have computed the molecular electrostatic potential (MEP) surface of a model system (compound **1**), which is shown in Fig. 5. As expected, the most negative electrostatic potential corresponds to the region of the Cl ligands (−75 kcal mol^{-1}). The MEP surface also reveals that the N—H group is totally inaccessible since it is involved in an intramolecular hydrogen bond with the O atom of the ligand. Consequently, the most positive part is located in the region of the exocyclic C—H group at the molecular plane, also influenced by the aromatic C—H groups (40 kcal mol^{-1}). Therefore, hydrogen-bonding interactions between these groups (C—H$\cdots X$) should be electrostatically favoured. Furthermore, perpendicular to the molecular plane, we found that each aromatic ring presents negative MEP values (−17 and −8 kcal mol^{-1}); therefore, face-to-face π–π stacking interactions are not electrostatically favoured (electrostatic repulsion). Remarkably, the electrostatic potential over the π-system of the linker (C═N) is positive, thus explaining the large displacement observed in the antiparallel π-stacking interactions highlighted in Fig. 4 and further discussed below.

In isostructural Zn compounds **1**–**3**, we have computed the interaction energies of the self-assembled π-stacked dimers (shown in Fig. 6*a*) that are responsible for the formation of the 1D ladders shown in Fig. 3. The self-assembled dimers are stabilized by a combination of hydrogen bonds and π–π stacking interactions involving the C═N group of the ligand. The dimerization energies in **1** and **2** ($\Delta E1$ = −33.0 kcal mol^{-1} and $\Delta E2$ = −31.4 kcal mol^{-1}, respectively) are very large due to the contribution of both hydrogen-bonding (red dashed lines in Fig. 6) and π–π interactions (blue dashed lines in Fig. 6), where the former involves the most positive (C—H groups, see Fig. 5) and the most negative (belts of the halide ligands) potential regions of the metal compound. In an effort to calculate the contribution of the different forces that govern the formation of the self-assembled dimers, we have computed additional theoretical models where the halide ligands that establish the hydrogen bonds have been replaced by hydride ligands (see Fig. 6*b*) and consequently the hydrogen-bonding interactions between the halide ligands and the C—H groups are not formed. As a result, the interaction energies are reduced to $\Delta E3$ = −24.8 kcal mol^{-1} and $\Delta E4$ = −22.5 kcal mol^{-1} in **1** and **2**, respectively. Therefore, the contribution of both symmetrically equivalent hydrogen-bonding interactions can be roughly estimated by the difference (they are −8.2 and 8.9 kcal mol^{-1} for **1** and **2**, respectively) and it is similar in both compounds. Furthermore, we have used additional dimers where the $ZnCl_2$ group in **1** or the ZnI_2 group in **2** has been removed (see Fig. 6*c*) in order to evaluate the influence of the metal coordination on the interaction energy. The resulting interaction energies are

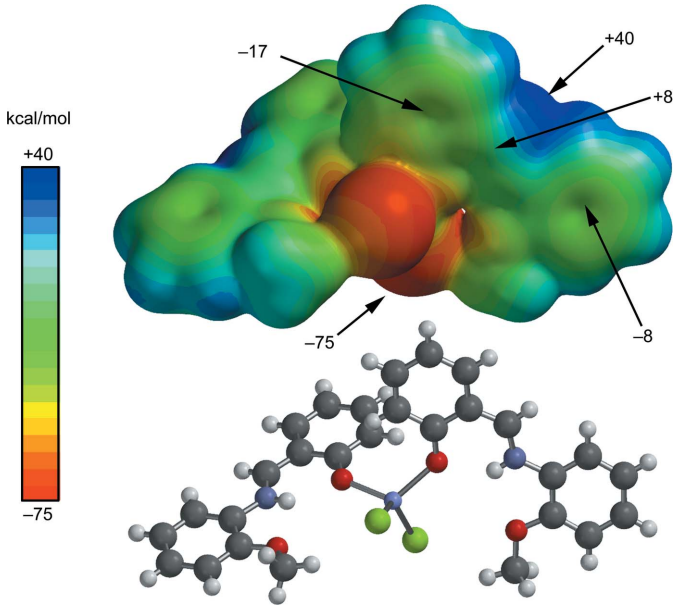


Figure 5
MEP surface of compound **1**. The MEP values at selected points are given in kcal mol^{-1}.

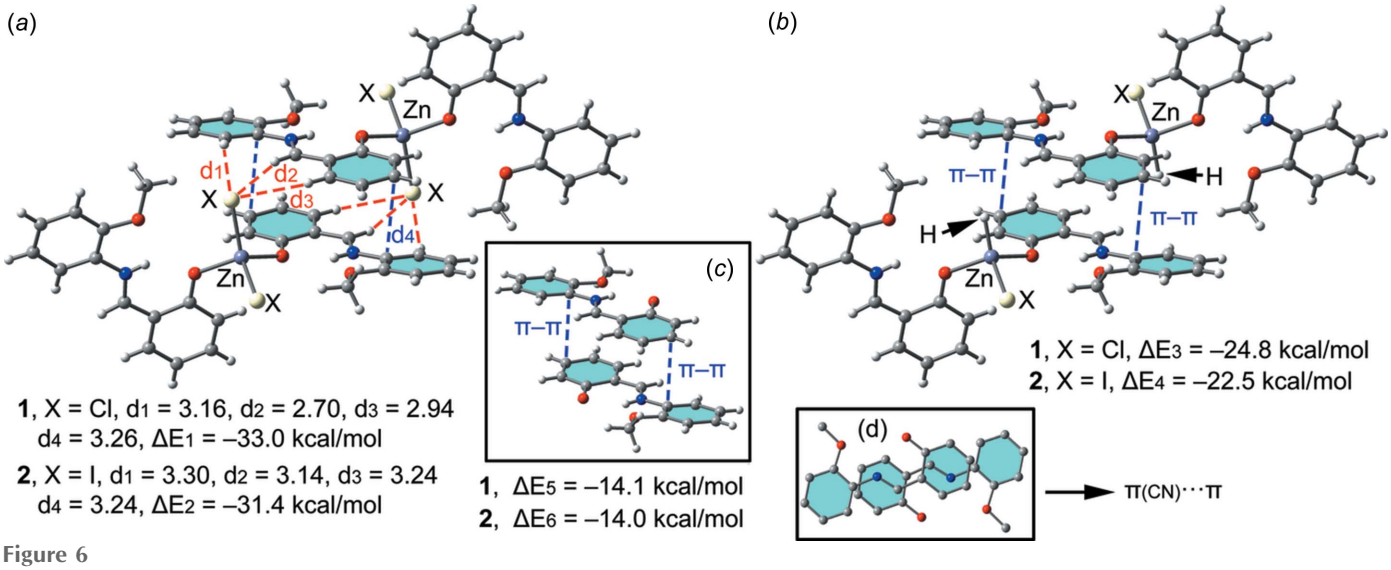


Figure 6
(*a*) Interaction energies of the self-assembled π-stacked dimers observed in the solid state of compounds **1** and **2**. (*b*)/(*c*) Interaction energies in several theoretical models of **1** and **2**. (*d*) On-top representation of the π-stacking interaction. All distances are in Å.

almost identical for both complexes ($\Delta E5 = -14.0$ kcal mol^{-1} and $\Delta E6 = -14.1$ kcal mol^{-1} for **1** and **2**, respectively) and reveal the strong influence of the metal coordination on the π–π stacking interaction. This is likely due to the stronger dipole–dipole interaction in the antiparallel arrangement of the assembly. It is also worthy to mention that the π–π interaction energy computed for these compounds is large compared to other π-stacking interactions (*i.e.* benzene dimer). This is due to the special arrangement of the two π-systems where the C═N bond is located over the aromatic ring (see the on-top representation in Fig. 6). This fact is in very good agreement with the MEP surface represented in Fig. 5 and explains the large interaction energy since two electrostatically enhanced π(CN)$\cdots\pi$ interactions are established.

In Cd compounds **3** and **4**, the π-stacking binding mode is very similar to that described before for **1** and **2**. As mentioned above, hydrogen-bonding and π–π interactions control the dimer formation (see Fig. 7*a*). The computed interaction energies of the self-assembled dimers are almost identical ($\Delta E7 = -30.9$ kcal mol^{-1} and $\Delta E8 = -29.9$ kcal mol^{-1} for **3** and **4**, respectively), indicating that the halide (Br or I) has a minimal influence on the binding energy. Compared to **1** and **2**, the interaction energies are less favourable, thus revealing a larger influence of the Zn ion on the binding energy of the assembly compared to Cd. Also, in both compounds, we have computed theoretical models where the Br or I ligands have been replaced by H atoms and consequently the hydrogen bonds are not formed (see Fig. 7*b*). As a result, the interaction energies are reduced to $\Delta E9 = -22.7$ kcal mol^{-1} and $\Delta E10 =$

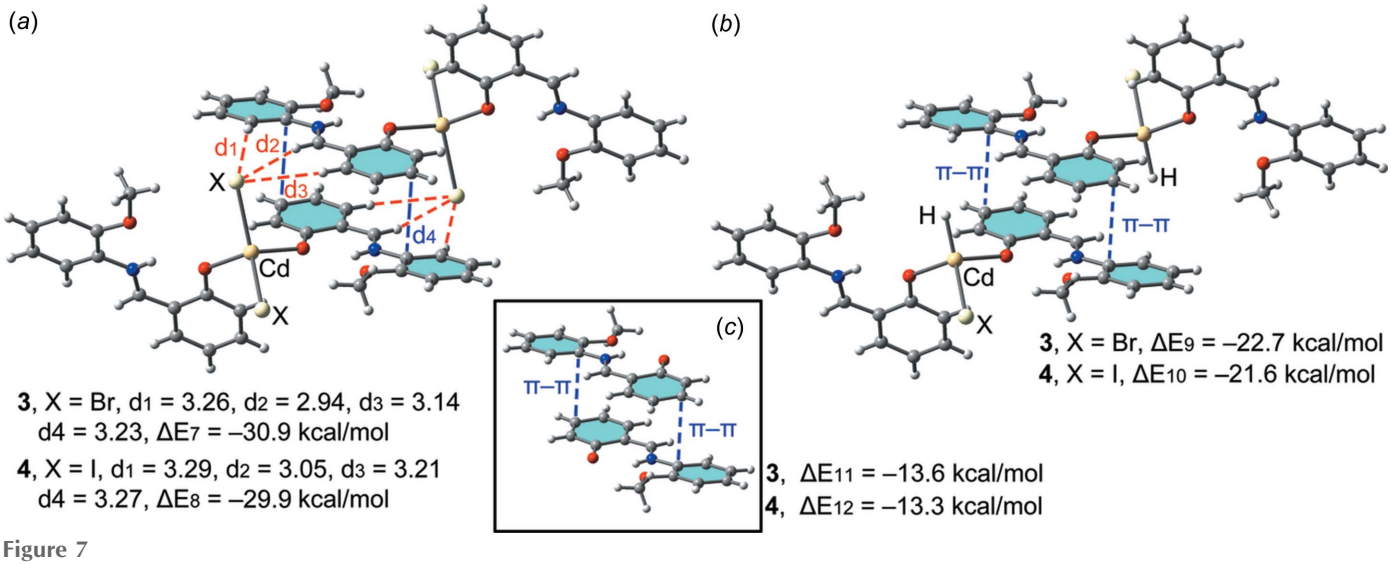


Figure 7
(*a*) Interaction energies of the self-assembled π-stacked dimers observed in the solid state of compounds **3** and **4**. (*b*)/(*c*) Interaction energies in several theoretical models of **3** and **4**. All distances are in Å.

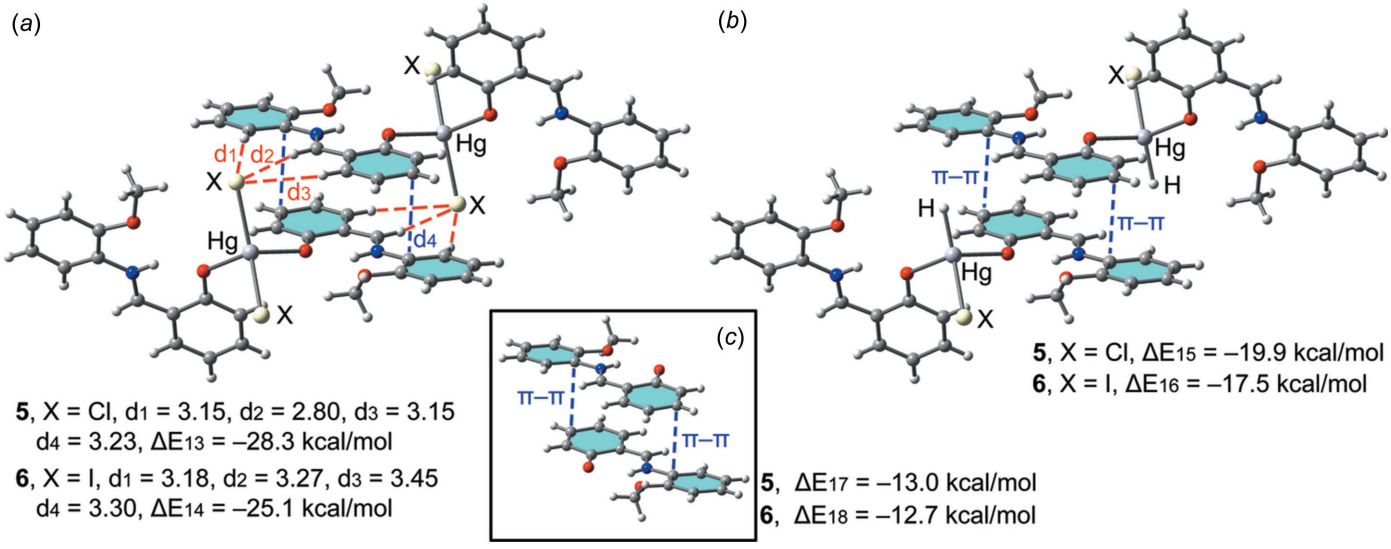


Figure 8
(*a*) Interaction energies of the self-assembled π-stacked dimers observed in the solid state of compounds **5** and **6**. (*b*)/(*c*) Interaction energies in several theoretical models of **5** and **6**. All distances are in Å.

-21.6 kcal mol^{-1} in **3** and **4**, respectively. Therefore, this contribution (both hydrogen bonds) can be roughly estimated by the difference (-8.2 and -8.3 kcal mol^{-1} for **3** and **4**, respectively). These values are very close to those found for compounds **1** and **2**, thus indicating that the contribution of the hydrogen bonds is not influenced by the type of transition metal (Zn or Cd). Furthermore, we have used an additional dimer, where the $CdBr_2$ and CdI_2 groups have been removed. The interaction energies are further reduced to $\Delta E9 = -13.3$ kcal mol^{-1} and $\Delta E6 = -13.6$ kcal mol^{-1} for **3** and **4**, respectively, which is in agreement with the Zn complexes, revealing a strong influence of the metal coordination on the strength of the π-stacking interaction.

For Hg compounds **5** and **6**, we have performed an equivalent study (see Fig. 8). The computed interaction energies of the self-assembled dimers are almost identical ($\Delta E13 = -28.3$ kcal mol^{-1} and $\Delta E14 = -25.1$ kcal mol^{-1} for **5** and **6**, respectively), indicating that Hg has a smaller effect on the interaction energy than Cd and Zn. Also, in both Hg compounds, we have computed theoretical models where the Cl^- or I^- ligands have been replaced by H^- ligands and consequently the hydrogen bonds are not formed (see Fig. 8*b*). As a result, the interaction energies are reduced to $\Delta E15 = -19.9$ kcal mol^{-1} and $\Delta E16 = -17.5$ kcal mol^{-1} in **5** and **6**, respectively. Therefore, this contribution (both hydrogen bonds) can be roughly estimated as -8.4 and -7.6 kcal mol^{-1}

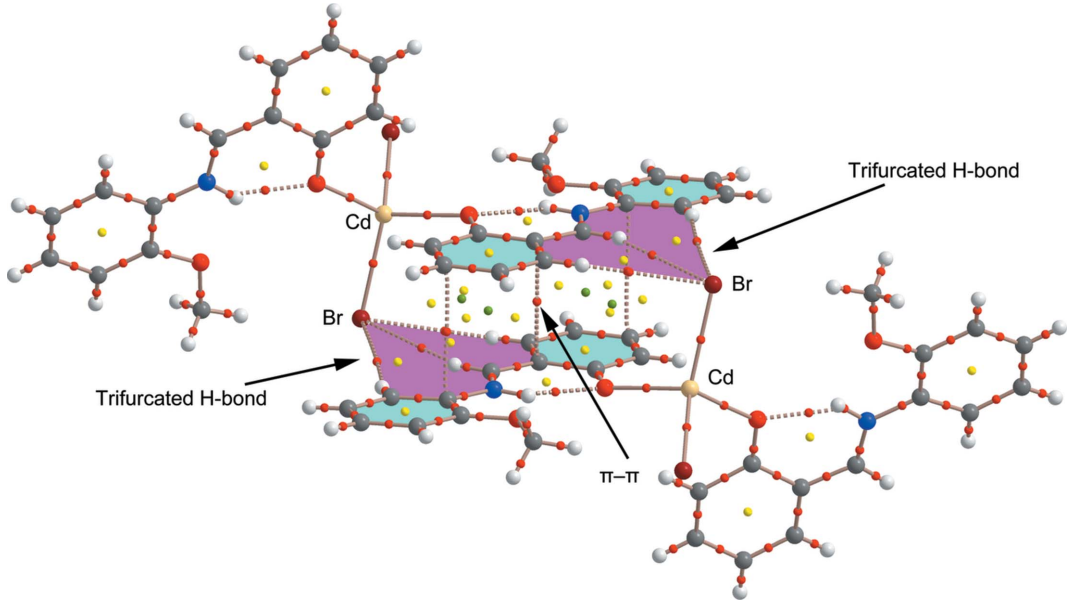


Figure 9
AIM analysis of the self-assembled dimers retrieved from the X-ray structure of compound **3**. Bond, ring and cage critical points are represented by red, yellow and green spheres, respectively. The bond paths connecting bond critical points are also represented by dashed lines.

for **5** and **6**, respectively. These values are in agreement with those found for compounds **1**–**4**, thus confirming that the interaction energy of the hydrogen bonds is not influenced by the type of transition metal (Zn/Cd/Hg). Furthermore, we have used an additional dimer, where the $HgCl_2$ and HgI_2 groups have been eliminated. Consequently, the interaction energies are further reduced to $\Delta E17 = -13.0$ kcal mol^{-1} and $\Delta E18 = -12.7$ kcal mol^{-1} for **5** and **6**, respectively; which is in agreement to the rest of complexes commented on above and confirms the strong influence of the metal coordination on the strength of the π-stacking interaction.

In order to provide additional evidence for the existence of the C—H$\cdots X$ hydrogen-bond and π–π stacking interactions, we have analyzed the self-assembled π-stacked dimer of compound **3** (as an exemplifying model) using Bader's theory of 'atoms in molecules' (AIM) (Bader, 1991), which provides an unambiguous definition of chemical bonding. The AIM theory has been successfully used to characterize and understand a great variety of interactions, including those described herein. In Fig. 9 we show the AIM analysis of compound **3**. It can be observed that the π–π interaction is characterized by the presence of three bond critical points that interconnect three C atoms of each aromatic ligand. The interaction is further characterized by several ring and cage critical points. Furthermore, the distribution of critical points reveals the existence of two symmetrically disposed sets of C—H$\cdots$Br hydrogen-bonding interactions. Each one is characterized by a bond critical point and a bond path connecting one H atom of the C—H groups with the Br^- ligand, thus confirming the formation of the trifurcated hydrogen bonds. The value of the Laplacian at the bond critical points is positive, as is common in closed-shell interactions.

4. Conclusion

We herein reported the syntheses and structural characterization of six new metal complexes based on the 2-{[(2-methoxyphenyl)imino]methyl}phenol ligand. All compounds exhibited an infinite 1D ladder in the solid state governed by the formation of hydrogen-bonding and π–π stacking interactions in the solid state. The crystal structure of these compounds was studied using geometrical and Hirshfeld surface analyses. They have also been studied using M06-2X/def2-TZVP calculations and Bader's theory of 'atoms in molecules'. The energies associated with the interactions, including the contribution of the different forces, have been evaluated. In general, the π–π stacking interactions are stronger than those reported for conventional π–π complexes, that is attributed to the influence of the metal coordination, which is stronger for Zn than for either Cd or Hg. The results reported herein might be useful for understanding the solid-state architecture of metal-containing materials that contain $M^{II}X_2$ subunits and organic aromatic ligands.

Acknowledgements

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References

Ahlrichs, R., Bär, M., Häser, M., Horn, H. & Kölmel, C. (1989). *Chem. Phys. Lett.* **162**, 165–169.
Alarcón, S., Pagani, D., Bacigalupo, J. & Olivieri, A. (1999). *J. Mol. Struct.* **475**, 233–240.
Azhdari Tehrani, A., Abedi, S. & Morsali, A. (2016). *Cryst. Growth Des.* **17**, 255–261.
Bader, R. F. (1991). *Chem. Rev.* **91**, 893–928.
Blake, A. J., Champness, N. R., Hubberstey, P., Li, W.-S., Withersby, M. A. & Schröder, M. (1999). *Coord. Chem. Rev.* **183**, 117–138.
Boys, S. F. & Bernardi, F. D. (1970). *Mol. Phys.* **19**, 553–566.
Braga, D. & Grepioni, F. (2000). *Acc. Chem. Res.* **33**, 601–608.
Braga, D., Grepioni, F. & Desiraju, G. R. (1998). *Chem. Rev.* **98**, 1375–1406.
Brammer, L. (2004). *Chem. Soc. Rev.* **33**, 476–489.
Bruker (2012). *TWINABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2015). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2016). *APEX3* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Busschaert, N., Caltagirone, C., Van Rossom, W. & Gale, P. A. (2015). *Chem. Rev.* **115**, 8038–8155.
Charland, J., Gabe, E., Khoo, L. & Smith, F. (1989). *Polyhedron*, **8**, 1897–1901.
Cohen, M. & Schmidt, G. (1962). *J. Phys. Chem.* **66**, 2442–2446.
Cohen, M., Schmidt, G. & Flavian, S. (1964). *J. Chem. Soc*. pp. 2041–2051.
Custelcean, R., Bonnesen, P. V., Duncan, N. C., Zhang, X., Watson, L. A., Van Berkel, G., Parson, W. B. & Hay, B. P. (2012). *J. Am. Chem. Soc.* **134**, 8525–8534.
Đaković, M., Soldin, Ž., Kukovec, B.-M., Kodrin, I., Aakeröy, C. B., Baus, N. & Rinkovec, T. (2018). *IUCrJ*, **5**, 13–21.
Desiraju, G. (1998). *Chem. Commun.* pp. 891–892.
Desiraju, G. R. (2014). *Angew. Chem. Int. Ed.* **53**, 604–605.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Dürr, H. & Bouas-Laurent, H. (2003). In *Photochromism: Molecules and Systems*. Amsterdam: Elsevier.
Gong, D., Wang, B., Jia, X. & Zhang, X. (2014). *Dalton Trans.* **43**, 4169–4178.
Hajiashrafi, T., Kharat, A. N., Love, J. A. & Patrick, B. O. (2013). *Polyhedron*, **60**, 30–38.
Hajiashrafi, T., Ziarani, G. M., Kubicki, M., Fadaei, F. T. & Schenk, K. J. (2016). *Polyhedron*, **119**, 260–266.
Holliday, B. J. & Mirkin, C. A. (2001). *Angew. Chem. Int. Ed.* **40**, 2022–2043.
Hope, H. (1994). *Prog. Inorg. Chem.* **41**, 1–19.
Hoshino, N., Inabe, T., Mitani, T. & Maruyama, Y. (1988). *Bull. Chem. Soc. Jpn*, **61**, 4207–4214.
Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
Kargili, H., Alpaslan, G., Macit, M., Erdönmez, A. & Büyükgüngör, O. (2014). *Opt. Spectrosc.* **116**, 179–186.
Keith, T. A. (2013). *AIMAll*. Version 13.05.06. TK Gristmill Software, Overland Park, KS, USA.
Khavasi, H. R. & Azhdari Tehrani, A. (2013). *Inorg. Chem.* **52**, 2891–2905.

Khavasi, H. R. & Azizpoor Fard, M. (2010). *Cryst. Growth Des.* **10**, 1892–1896.
Khavasi, H. R., Barforoush, M. M. & Fard, M. A. (2012). *CrystEngComm*, **14**, 7236–7244.
Khavasi, H. R. & Mohammad Sadegh, B. M. (2010). *Inorg. Chem.* **49**, 5356–5358.
Khavasi, H. R., Norouzi, F. & Azhdari Tehrani, A. (2015). *Cryst. Growth Des.* **15**, 2579–2583.
Khavasi, H. R. & Sadegh, B. M. M. (2014). *Dalton Trans.* **43**, 5564–5573.
Kielmann, M. & Senge, M. O. (2018). *Angew. Chem. Int. Ed.* **58**, 418–441.
Lehn, J.-M. (1995). In *Supramolecular Chemistry*. Weinheim: VCH.
Li, B., Zang, S.-Q., Wang, L.-Y. & Mak, T. C. (2016). *Coord. Chem. Rev.* **308**, 1–21.
Li, L. & Yuan, F. (2012). *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **42**, 994–998.
Mackenzie, C. F., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *IUCrJ*, **4**, 575–587.
Mahata, P., Prabu, M. & Natarajan, S. (2009). *Cryst. Growth Des.* **9**, 3683–3691.
McKinlay, A. C., Morris, R. E., Horcajada, P., Férey, G., Gref, R., Couvreur, P. & Serre, C. (2010). *Angew. Chem. Int. Ed.* **49**, 6260–6266.
Politzer, P., Murray, J. S. & Clark, T. (2010). *Phys. Chem. Chem. Phys.* **12**, 7748–7757.
Reddy, P. A., Nethaji, M. & Chakravarty, A. R. (2003*a*). *Eur. J. Inorg. Chem.* pp. 2318–2324.
Reddy, P. A., Nethaji, M. & Chakravarty, A. R. (2003*b*). *Inorg. Chem. Commun.* **6**, 698–701.
Redshaw, C., Walton, M., Clowes, L., Hughes, D. L., Fuller, A. M., Chao, Y., Walton, A., Sumerin, V., Elo, P. & Soshnikov, I. (2013). *Chem. Eur. J.* **19**, 8884–8899.
Reedijk, J. (2009). *Eur. J. Inorg. Chem.* pp. 1303–1312.
Reedijk, J. (2013). *Chem. Soc. Rev.* **42**, 1776–1783.
Schottel, B. L., Chifotides, H. T., Shatruk, M., Chouai, A., Pérez, L. M., Bacsa, J. & Dunbar, K. R. (2006). *J. Am. Chem. Soc.* **128**, 5895–5912.
Semeniuc, R. F., Reamer, T. J. & Smith, M. D. (2010). *New J. Chem.* **34**, 439–452.
Senge, M. O. (2000). *Z. Naturforsch. Teil B*, **55**, 336–344.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* C**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* A**71**, 3–8.
Shkol'nikova, L., Obodovskaya, A. & Shugam, E. (1970). *J. Struct. Chem.* **11**, 47–53.
Song, X., Wang, Z., Zhao, J. & Hor, T. A. (2013). *Chem. Commun.* **49**, 4992–4994.
Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
Steed, J. W. & Atwood, J. L. (2013). In *Supramolecular Chemistry*. London: John Wiley & Sons.
Tsuchimoto, M., Yoshida, N., Sugimoto, A., Teramoto, N. & Nakajima, K. (2016). *J. Mol. Struct.* **1105**, 152–158.
Wang, Z. J., Clary, K. N., Bergman, R. G., Raymond, K. N. & Toste, F. D. (2013). *Nat. Chem.* **5**, 100–103.
Wiester, M. J., Ulmann, P. A. & Mirkin, C. A. (2011). *Angew. Chem. Int. Ed.* **50**, 114–137.
Yang, L., Powell, D. R. & Houser, R. P. (2007). *Dalton Trans.* pp. 955–964.
Zeng, F., Ni, J., Wang, Q., Ding, Y., Ng, S. W., Zhu, W. & Xie, Y. (2010). *Cryst. Growth Des.* **10**, 1611–1622.

supporting information

Acta Cryst. (2019). C**75**, 178-188 [https://doi.org/10.1107/S2053229618018314]

The role of π–π stacking and hydrogen-bonding interactions in the assembly of a series of isostructural group IIB coordination compounds

Taraneh Hajiashrafi, Roghayeh Zekriazadeh, Keith J. Flanagan, Farnoush Kia, Antonio Bauzá, Antonio Frontera and Mathias O. Senge

Computing details

For all structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015b); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015a); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Dichloridobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κO)zinc(II) (Compound_1)

Crystal data

$[ZnCl_2(C_{28}H_{26}N_2O_4)]$
M_r = 590.78
Triclinic, $P\overline{1}$
a = 9.1926 (2) Å
b = 10.6101 (2) Å
c = 14.8057 (3) Å
α = 94.188 (1)°
β = 97.716 (1)°
γ = 114.409 (1)°
V = 1289.80 (5) Å^3
Z = 2
$F(000)$ = 608
D_x = 1.521 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9828 reflections
θ = 2.5–34.0°
μ = 1.20 mm^{-1}
T = 100 K
Block, yellow
0.26 × 0.12 × 0.11 mm

Data collection

Bruker SMART APEXII area detector diffractometer
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.691, T_{max} = 0.747
93163 measured reflections
11965 independent reflections
9331 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 35.7°, θ_{min} = 2.1°
h = −15→15
k = −17→17
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.084
S = 1.02
11965 reflections
336 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.6038P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.78269 (2)	0.33923 (2)	0.71660 (2)	0.01225 (4)
Cl1	0.58971 (4)	0.39395 (3)	0.64597 (2)	0.01828 (6)
Cl2	1.05003 (4)	0.46074 (3)	0.72121 (2)	0.01983 (6)
O1A	0.75873 (12)	0.35079 (10)	0.84784 (6)	0.01486 (16)
O1B	0.73799 (11)	0.15246 (9)	0.65301 (6)	0.01458 (16)
O2B	1.01441 (12)	0.27418 (10)	0.49592 (7)	0.01827 (18)
O2A	0.63225 (13)	0.63174 (11)	0.84985 (7)	0.02096 (19)
N1B	0.78530 (13)	0.02994 (11)	0.50462 (7)	0.01276 (17)
H1B	0.8193	0.1044	0.5463	0.015*
N1A	0.73008 (13)	0.51596 (11)	0.97988 (8)	0.01443 (18)
H1A	0.7160	0.4892	0.9204	0.017*
C1B	0.60814 (15)	0.03742 (12)	0.65300 (8)	0.01257 (19)
C1A	0.81909 (14)	0.29733 (12)	0.91128 (8)	0.01229 (19)
C6A	0.83502 (15)	0.34584 (12)	1.00664 (8)	0.01243 (19)
C6B	0.56362 (15)	−0.08101 (12)	0.58464 (8)	0.01256 (19)
C7B	0.65395 (15)	−0.07798 (13)	0.51344 (8)	0.0135 (2)
H7B	0.6165	−0.1596	0.4695	0.016*
C2A	0.87012 (16)	0.19149 (13)	0.89030 (9)	0.0161 (2)
H2A	0.8635	0.1585	0.8278	0.019*
C2B	0.50596 (15)	0.02403 (13)	0.71897 (9)	0.0149 (2)
H2B	0.5319	0.1006	0.7653	0.018*
C7A	0.79231 (15)	0.45396 (13)	1.03586 (8)	0.0141 (2)
H7A	0.8099	0.4833	1.1001	0.017*
C5B	0.42209 (15)	−0.20542 (13)	0.58441 (9)	0.0150 (2)
H5B	0.3934	−0.2833	0.5386	0.018*
C9B	0.85462 (16)	−0.07663 (14)	0.37295 (9)	0.0168 (2)
H9B	0.7741	−0.1668	0.3771	0.020*
C5A	0.89772 (16)	0.28629 (14)	1.07591 (9)	0.0168 (2)
H5A	0.9085	0.3192	1.1390	0.020*
C10B	0.95009 (17)	−0.05883 (16)	0.30531 (9)	0.0210 (3)
H10B	0.9365	−0.1372	0.2639	0.025*
C13B	0.99865 (15)	0.17174 (14)	0.42983 (8)	0.0152 (2)
C8B	0.87793 (15)	0.03839 (13)	0.43438 (8)	0.0137 (2)
C3B	0.36930 (16)	−0.09889 (14)	0.71670 (9)	0.0159 (2)
H3B	0.3030	−0.1051	0.7617	0.019*
C9A	0.68435 (16)	0.66509 (15)	1.09870 (9)	0.0191 (2)

H9A	0.7179	0.6228	1.1467	0.023*
C4B	0.32585 (15)	−0.21493 (13)	0.64943 (9)	0.0157 (2)
H4B	0.2314	−0.2986	0.6489	0.019*
C8A	0.68327 (16)	0.62282 (13)	1.00706 (9)	0.0156 (2)
C12A	0.58437 (17)	0.79013 (15)	0.95712 (11)	0.0212 (3)
H12A	0.5507	0.8329	0.9095	0.025*
C12B	1.09137 (17)	0.18984 (16)	0.36023 (9)	0.0190 (2)
H12B	1.1710	0.2799	0.3551	0.023*
C4A	0.94279 (18)	0.18186 (15)	1.05275 (10)	0.0200 (2)
H4A	0.9826	0.1412	1.0994	0.024*
C11B	1.06531 (17)	0.07378 (17)	0.29848 (9)	0.0212 (3)
H11B	1.1275	0.0856	0.2508	0.025*
C13A	0.63154 (16)	0.68325 (14)	0.93594 (9)	0.0171 (2)
C14B	1.1425 (2)	0.41087 (15)	0.49745 (11)	0.0254 (3)
H14A	1.1247	0.4457	0.4394	0.038*
H14B	1.2472	0.4054	0.5051	0.038*
H14C	1.1428	0.4747	0.5489	0.038*
C3A	0.92945 (18)	0.13554 (14)	0.95946 (10)	0.0197 (2)
H3A	0.9620	0.0640	0.9435	0.024*
C11A	0.58748 (18)	0.83271 (16)	1.04881 (11)	0.0243 (3)
H11A	0.5563	0.9055	1.0636	0.029*
C14A	0.54557 (19)	0.66647 (16)	0.77481 (10)	0.0231 (3)
H14D	0.5446	0.6152	0.7167	0.035*
H14E	0.5994	0.7672	0.7726	0.035*
H14F	0.4337	0.6407	0.7839	0.035*
C10A	0.63522 (18)	0.77081 (16)	1.11873 (11)	0.0244 (3)
H10A	0.6347	0.8003	1.1808	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01434 (7)	0.01084 (6)	0.01021 (6)	0.00409 (5)	0.00255 (5)	0.00064 (4)
Cl1	0.02136 (14)	0.01873 (13)	0.01582 (13)	0.01077 (12)	0.00027 (10)	0.00101 (10)
Cl2	0.01624 (13)	0.02080 (14)	0.01455 (12)	0.00027 (11)	0.00358 (10)	0.00072 (10)
O1A	0.0187 (4)	0.0185 (4)	0.0116 (4)	0.0114 (3)	0.0037 (3)	0.0040 (3)
O1B	0.0136 (4)	0.0111 (4)	0.0169 (4)	0.0030 (3)	0.0049 (3)	−0.0005 (3)
O2B	0.0204 (5)	0.0149 (4)	0.0175 (4)	0.0043 (3)	0.0078 (3)	0.0018 (3)
O2A	0.0278 (5)	0.0268 (5)	0.0172 (4)	0.0195 (4)	0.0053 (4)	0.0057 (4)
N1B	0.0133 (4)	0.0133 (4)	0.0120 (4)	0.0061 (4)	0.0028 (3)	0.0009 (3)
N1A	0.0143 (5)	0.0150 (4)	0.0158 (4)	0.0079 (4)	0.0033 (4)	0.0015 (4)
C1B	0.0127 (5)	0.0121 (5)	0.0132 (5)	0.0058 (4)	0.0018 (4)	0.0015 (4)
C1A	0.0118 (5)	0.0129 (5)	0.0123 (5)	0.0052 (4)	0.0029 (4)	0.0020 (4)
C6A	0.0133 (5)	0.0133 (5)	0.0120 (5)	0.0068 (4)	0.0024 (4)	0.0021 (4)
C6B	0.0132 (5)	0.0108 (4)	0.0131 (5)	0.0048 (4)	0.0018 (4)	0.0010 (4)
C7B	0.0142 (5)	0.0130 (5)	0.0130 (5)	0.0060 (4)	0.0016 (4)	0.0012 (4)
C2A	0.0188 (6)	0.0161 (5)	0.0157 (5)	0.0101 (4)	0.0034 (4)	0.0001 (4)
C2B	0.0147 (5)	0.0153 (5)	0.0152 (5)	0.0068 (4)	0.0037 (4)	0.0008 (4)
C7A	0.0140 (5)	0.0144 (5)	0.0138 (5)	0.0060 (4)	0.0030 (4)	0.0007 (4)

C5B	0.0147 (5)	0.0122 (5)	0.0158 (5)	0.0041 (4)	0.0010 (4)	0.0021 (4)
C9B	0.0158 (5)	0.0206 (6)	0.0147 (5)	0.0096 (5)	0.0010 (4)	−0.0012 (4)
C5A	0.0198 (6)	0.0176 (5)	0.0136 (5)	0.0089 (5)	0.0016 (4)	0.0035 (4)
C10B	0.0192 (6)	0.0312 (7)	0.0146 (5)	0.0143 (5)	0.0016 (4)	−0.0030 (5)
C13B	0.0143 (5)	0.0192 (5)	0.0132 (5)	0.0082 (4)	0.0028 (4)	0.0029 (4)
C8B	0.0129 (5)	0.0187 (5)	0.0112 (5)	0.0085 (4)	0.0022 (4)	0.0020 (4)
C3B	0.0143 (5)	0.0183 (5)	0.0173 (5)	0.0080 (4)	0.0056 (4)	0.0056 (4)
C9A	0.0158 (6)	0.0238 (6)	0.0177 (6)	0.0104 (5)	0.0012 (4)	−0.0054 (5)
C4B	0.0134 (5)	0.0139 (5)	0.0188 (5)	0.0043 (4)	0.0029 (4)	0.0050 (4)
C8A	0.0139 (5)	0.0150 (5)	0.0185 (5)	0.0073 (4)	0.0026 (4)	−0.0005 (4)
C12A	0.0190 (6)	0.0178 (6)	0.0290 (7)	0.0099 (5)	0.0053 (5)	0.0019 (5)
C12B	0.0176 (6)	0.0262 (6)	0.0154 (5)	0.0103 (5)	0.0058 (4)	0.0064 (5)
C4A	0.0253 (7)	0.0199 (6)	0.0188 (6)	0.0141 (5)	0.0008 (5)	0.0057 (5)
C11B	0.0182 (6)	0.0344 (7)	0.0134 (5)	0.0137 (6)	0.0041 (4)	0.0020 (5)
C13A	0.0157 (5)	0.0161 (5)	0.0205 (6)	0.0075 (4)	0.0048 (4)	0.0018 (4)
C14B	0.0284 (7)	0.0163 (6)	0.0260 (7)	0.0018 (5)	0.0122 (6)	0.0035 (5)
C3A	0.0240 (6)	0.0175 (6)	0.0222 (6)	0.0137 (5)	0.0030 (5)	0.0025 (5)
C11A	0.0191 (6)	0.0202 (6)	0.0334 (8)	0.0105 (5)	0.0020 (5)	−0.0050 (5)
C14A	0.0273 (7)	0.0262 (7)	0.0217 (6)	0.0167 (6)	0.0044 (5)	0.0074 (5)
C10A	0.0199 (6)	0.0273 (7)	0.0247 (7)	0.0124 (6)	−0.0001 (5)	−0.0094 (5)

Geometric parameters (Å, º)

Zn1—Cl1	2.2404 (4)	C9B—C10B	1.3912 (19)
Zn1—Cl2	2.2427 (4)	C9B—C8B	1.3899 (18)
Zn1—O1A	1.9854 (9)	C5A—H5A	0.9500
Zn1—O1B	1.9832 (9)	C5A—C4A	1.3707 (19)
O1A—C1A	1.3076 (14)	C10B—H10B	0.9500
O1B—C1B	1.3078 (15)	C10B—C11B	1.389 (2)
O2B—C13B	1.3550 (16)	C13B—C8B	1.4050 (18)
O2B—C14B	1.4376 (17)	C13B—C12B	1.3981 (18)
O2A—C13A	1.3516 (16)	C3B—H3B	0.9500
O2A—C14A	1.4387 (17)	C3B—C4B	1.4053 (18)
N1B—H1B	0.8800	C9A—H9A	0.9500
N1B—C7B	1.3067 (16)	C9A—C8A	1.3949 (18)
N1B—C8B	1.4152 (16)	C9A—C10A	1.399 (2)
N1A—H1A	0.8800	C4B—H4B	0.9500
N1A—C7A	1.3077 (16)	C8A—C13A	1.4008 (19)
N1A—C8A	1.4197 (16)	C12A—H12A	0.9500
C1B—C6B	1.4314 (17)	C12A—C13A	1.4012 (19)
C1B—C2B	1.4187 (17)	C12A—C11A	1.392 (2)
C1A—C6A	1.4338 (17)	C12B—H12B	0.9500
C1A—C2A	1.4147 (17)	C12B—C11B	1.394 (2)
C6A—C7A	1.4151 (17)	C4A—H4A	0.9500
C6A—C5A	1.4213 (17)	C4A—C3A	1.404 (2)
C6B—C7B	1.4212 (17)	C11B—H11B	0.9500
C6B—C5B	1.4191 (17)	C14B—H14A	0.9800
C7B—H7B	0.9500	C14B—H14B	0.9800

C2A—H2A	0.9500	C14B—H14C	0.9800
C2A—C3A	1.3802 (19)	C3A—H3A	0.9500
C2B—H2B	0.9500	C11A—H11A	0.9500
C2B—C3B	1.3814 (18)	C11A—C10A	1.382 (2)
C7A—H7A	0.9500	C14A—H14D	0.9800
C5B—H5B	0.9500	C14A—H14E	0.9800
C5B—C4B	1.3742 (18)	C14A—H14F	0.9800
C9B—H9B	0.9500	C10A—H10A	0.9500

Cl1—Zn1—Cl2	124.837 (14)	O2B—C13B—C12B	125.28 (12)
O1A—Zn1—Cl1	103.90 (3)	C12B—C13B—C8B	119.56 (12)
O1A—Zn1—Cl2	104.04 (3)	C9B—C8B—N1B	123.25 (12)
O1B—Zn1—Cl1	105.46 (3)	C9B—C8B—C13B	120.69 (11)
O1B—Zn1—Cl2	102.79 (3)	C13B—C8B—N1B	116.05 (11)
O1B—Zn1—O1A	116.75 (4)	C2B—C3B—H3B	119.2
C1A—O1A—Zn1	125.54 (8)	C2B—C3B—C4B	121.66 (12)
C1B—O1B—Zn1	125.06 (8)	C4B—C3B—H3B	119.2
C13B—O2B—C14B	117.28 (11)	C8A—C9A—H9A	120.6
C13A—O2A—C14A	117.02 (11)	C8A—C9A—C10A	118.83 (14)
C7B—N1B—H1B	116.9	C10A—C9A—H9A	120.6
C7B—N1B—C8B	126.13 (11)	C5B—C4B—C3B	118.97 (12)
C8B—N1B—H1B	116.9	C5B—C4B—H4B	120.5
C7A—N1A—H1A	117.3	C3B—C4B—H4B	120.5
C7A—N1A—C8A	125.41 (11)	C9A—C8A—N1A	122.96 (12)
C8A—N1A—H1A	117.3	C9A—C8A—C13A	120.83 (12)
O1B—C1B—C6B	120.27 (11)	C13A—C8A—N1A	116.19 (11)
O1B—C1B—C2B	122.41 (11)	C13A—C12A—H12A	120.5
C2B—C1B—C6B	117.32 (11)	C11A—C12A—H12A	120.5
O1A—C1A—C6A	119.79 (11)	C11A—C12A—C13A	119.10 (14)
O1A—C1A—C2A	122.76 (11)	C13B—C12B—H12B	120.5
C2A—C1A—C6A	117.45 (11)	C11B—C12B—C13B	119.03 (13)
C7A—C6A—C1A	122.46 (11)	C11B—C12B—H12B	120.5
C7A—C6A—C5A	117.50 (11)	C5A—C4A—H4A	120.3
C5A—C6A—C1A	120.04 (11)	C5A—C4A—C3A	119.33 (12)
C7B—C6B—C1B	122.20 (11)	C3A—C4A—H4A	120.3
C5B—C6B—C1B	120.17 (11)	C10B—C11B—C12B	121.24 (13)
C5B—C6B—C7B	117.60 (11)	C10B—C11B—H11B	119.4
N1B—C7B—C6B	124.13 (11)	C12B—C11B—H11B	119.4
N1B—C7B—H7B	117.9	O2A—C13A—C8A	115.56 (11)
C6B—C7B—H7B	117.9	O2A—C13A—C12A	124.76 (13)
C1A—C2A—H2A	119.6	C8A—C13A—C12A	119.68 (13)
C3A—C2A—C1A	120.85 (12)	O2B—C14B—H14A	109.5
C3A—C2A—H2A	119.6	O2B—C14B—H14B	109.5
C1B—C2B—H2B	119.6	O2B—C14B—H14C	109.5
C3B—C2B—C1B	120.87 (12)	H14A—C14B—H14B	109.5
C3B—C2B—H2B	119.6	H14A—C14B—H14C	109.5
N1A—C7A—C6A	124.08 (11)	H14B—C14B—H14C	109.5
N1A—C7A—H7A	118.0	C2A—C3A—C4A	121.56 (12)

C6A—C7A—H7A	118.0	C2A—C3A—H3A	119.2
C6B—C5B—H5B	119.5	C4A—C3A—H3A	119.2
C4B—C5B—C6B	121.01 (12)	C12A—C11A—H11A	119.4
C4B—C5B—H5B	119.5	C10A—C11A—C12A	121.10 (13)
C10B—C9B—H9B	120.2	C10A—C11A—H11A	119.4
C8B—C9B—H9B	120.2	O2A—C14A—H14D	109.5
C8B—C9B—C10B	119.53 (13)	O2A—C14A—H14E	109.5
C6A—C5A—H5A	119.6	O2A—C14A—H14F	109.5
C4A—C5A—C6A	120.74 (12)	H14D—C14A—H14E	109.5
C4A—C5A—H5A	119.6	H14D—C14A—H14F	109.5
C9B—C10B—H10B	120.1	H14E—C14A—H14F	109.5
C11B—C10B—C9B	119.87 (13)	C9A—C10A—H10A	119.8
C11B—C10B—H10B	120.1	C11A—C10A—C9A	120.43 (14)
O2B—C13B—C8B	115.16 (11)	C11A—C10A—H10A	119.8

Zn1—O1A—C1A—C6A	161.78 (9)	C2B—C1B—C6B—C5B	0.11 (17)
Zn1—O1A—C1A—C2A	−18.43 (17)	C2B—C3B—C4B—C5B	0.01 (19)
Zn1—O1B—C1B—C6B	161.25 (9)	C7A—N1A—C8A—C9A	−6.4 (2)
Zn1—O1B—C1B—C2B	−18.45 (16)	C7A—N1A—C8A—C13A	174.92 (12)
O1A—C1A—C6A—C7A	−2.03 (18)	C7A—C6A—C5A—C4A	−179.52 (13)
O1A—C1A—C6A—C5A	178.83 (11)	C5B—C6B—C7B—N1B	179.18 (12)
O1A—C1A—C2A—C3A	−178.39 (13)	C9B—C10B—C11B—C12B	2.1 (2)
O1B—C1B—C6B—C7B	−1.78 (18)	C5A—C6A—C7A—N1A	−178.46 (12)
O1B—C1B—C6B—C5B	−179.60 (11)	C5A—C4A—C3A—C2A	−0.8 (2)
O1B—C1B—C2B—C3B	179.73 (12)	C10B—C9B—C8B—N1B	179.37 (12)
O2B—C13B—C8B—N1B	2.38 (16)	C10B—C9B—C8B—C13B	−1.12 (19)
O2B—C13B—C8B—C9B	−177.17 (11)	C13B—C12B—C11B—C10B	−0.4 (2)
O2B—C13B—C12B—C11B	177.94 (12)	C8B—N1B—C7B—C6B	−179.17 (11)
N1A—C8A—C13A—O2A	0.17 (17)	C8B—C9B—C10B—C11B	−1.3 (2)
N1A—C8A—C13A—C12A	−179.56 (12)	C8B—C13B—C12B—C11B	−2.06 (19)
C1B—C6B—C7B—N1B	1.32 (19)	C9A—C8A—C13A—O2A	−178.54 (12)
C1B—C6B—C5B—C4B	−0.20 (18)	C9A—C8A—C13A—C12A	1.7 (2)
C1B—C2B—C3B—C4B	−0.1 (2)	C8A—N1A—C7A—C6A	178.78 (12)
C1A—C6A—C7A—N1A	2.4 (2)	C8A—C9A—C10A—C11A	−0.4 (2)
C1A—C6A—C5A—C4A	−0.3 (2)	C12A—C11A—C10A—C9A	1.1 (2)
C1A—C2A—C3A—C4A	−0.5 (2)	C12B—C13B—C8B—N1B	−177.62 (11)
C6A—C1A—C2A—C3A	1.40 (19)	C12B—C13B—C8B—C9B	2.83 (19)
C6A—C5A—C4A—C3A	1.2 (2)	C13A—C12A—C11A—C10A	−0.4 (2)
C6B—C1B—C2B—C3B	0.03 (18)	C14B—O2B—C13B—C8B	176.51 (12)
C6B—C5B—C4B—C3B	0.14 (19)	C14B—O2B—C13B—C12B	−3.48 (19)
C7B—N1B—C8B—C9B	−10.54 (19)	C11A—C12A—C13A—O2A	179.28 (13)
C7B—N1B—C8B—C13B	169.93 (12)	C11A—C12A—C13A—C8A	−1.0 (2)
C7B—C6B—C5B—C4B	−178.11 (12)	C14A—O2A—C13A—C8A	165.83 (12)
C2A—C1A—C6A—C7A	178.17 (12)	C14A—O2A—C13A—C12A	−14.5 (2)
C2A—C1A—C6A—C5A	−0.96 (18)	C10A—C9A—C8A—N1A	−179.64 (13)
C2B—C1B—C6B—C7B	177.93 (11)	C10A—C9A—C8A—C13A	−1.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*B*—H1*B*···O1*B*	0.88	1.96	2.6481 (14)	134
N1*A*—H1*A*···O1*A*	0.88	1.96	2.6424 (14)	134
C7*B*—H7*B*···Cl1^{i}	0.95	2.70	3.6118 (13)	160
C7*A*—H7*A*···Cl2^{ii}	0.95	2.69	3.5913 (13)	159
C14*B*—H14*C*···Cl2	0.98	2.79	3.5845 (16)	138
C14*A*—H14*D*···Cl1	0.98	2.71	3.5406 (16)	143

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

Diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κ*O*)zinc(II) (Compound_2)

Crystal data

$[ZnI_2(C_{28}H_{26}N_2O_4)]$
M_r = 773.68
Triclinic, $P\overline{1}$
a = 9.2709 (19) Å
b = 10.020 (2) Å
c = 16.248 (4) Å
α = 98.56 (4)°
β = 100.50 (4)°
γ = 110.09 (3)°
V = 1356.7 (6) Å^3
Z = 2
F(000) = 752
D_x = 1.894 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 4135 reflections
θ = 4.4–51.3°
μ = 3.22 mm^{-1}
T = 100 K
Plate, yellow
0.14 × 0.07 × 0.03 mm

Data collection

Bruker APEXII area detector diffractometer
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (TWINABS; Bruker, 2012)
T_{min} = 0.612, T_{max} = 0.746
7281 measured reflections
7281 independent reflections
4608 reflections with $I > 2\sigma(I)$
R_{int} = 0.116
θ_{max} = 25.5°, θ_{min} = 2.2°
h = −10→10
k = −12→12
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.195
S = 0.99
7281 reflections
337 parameters
174 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1055P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.19 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

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. The carbon and nitrogen atoms were fixed using the similarity restraint for Uij (SIMU). Atoms N1A, N1B, and C14B were fixed using the ISOR restraint. The structure was solved as a rotational twin rotated from first domain by 179.8 degrees about reciprocal axis 0.002 1.000 0.001 and real axis 0.434 1.000 0.197. Twin law to convert hkl from first to this domain (SHELXL TWIN matrix): -0.999 0.004 -0.001, 0.866 0.998 0.395, 0.007 0.003 -0.999.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.334 (2)	0.3133 (16)	0.8865 (11)	0.0165 (17)
C1B	0.130 (2)	0.0695 (17)	0.6410 (10)	0.0129 (15)
C2A	0.396 (2)	0.2136 (16)	0.8566 (11)	0.0167 (17)
H2A	0.3964	0.1941	0.7976	0.020*
C2B	0.035 (2)	0.0640 (17)	0.7007 (10)	0.0131 (16)
H2B	0.0540	0.1491	0.7425	0.016*
C3A	0.457 (2)	0.1434 (17)	0.9096 (11)	0.0166 (17)
H3A	0.4988	0.0757	0.8867	0.020*
C3B	−0.086 (2)	−0.0684 (17)	0.6971 (10)	0.0129 (16)
H3B	−0.1476	−0.0722	0.7380	0.015*
C4A	0.461 (2)	0.1669 (17)	0.9945 (12)	0.0164 (17)
H4A	0.5043	0.1156	1.0299	0.020*
C4B	−0.120 (2)	−0.1964 (18)	0.6350 (10)	0.0125 (16)
H4B	−0.2036	−0.2844	0.6340	0.015*
C5A	0.402 (2)	0.2647 (16)	1.0300 (11)	0.0165 (17)
H5A	0.4031	0.2802	1.0893	0.020*
C5B	−0.030 (2)	−0.1933 (18)	0.5759 (10)	0.0126 (15)
H5B	−0.0511	−0.2793	0.5342	0.015*
C6A	0.339 (2)	0.3415 (16)	0.9766 (11)	0.0164 (16)
C6B	0.095 (2)	−0.0591 (17)	0.5779 (10)	0.0127 (15)
C7A	0.286 (2)	0.4453 (16)	1.0157 (12)	0.0165 (18)
H7A	0.2929	0.4567	1.0755	0.020*
C7B	0.179 (2)	−0.0640 (17)	0.5121 (10)	0.0127 (17)
H7B	0.1475	−0.1546	0.4723	0.015*
C8A	0.172 (2)	0.6273 (19)	1.0156 (12)	0.0191 (17)
C8B	0.373 (2)	0.0414 (18)	0.4378 (11)	0.0155 (17)
C9A	0.165 (2)	0.6426 (19)	1.1017 (11)	0.0191 (17)
H9A	0.1964	0.5837	1.1361	0.023*
C9B	0.347 (2)	−0.0865 (18)	0.3801 (11)	0.0156 (17)
H9B	0.2717	−0.1770	0.3831	0.019*
C10A	0.110 (2)	0.7469 (18)	1.1353 (12)	0.0195 (17)
H10A	0.0986	0.7564	1.1925	0.023*
C10B	0.430 (2)	−0.0809 (17)	0.3198 (11)	0.0158 (17)
H10B	0.4100	−0.1677	0.2791	0.019*
C11A	0.073 (2)	0.8366 (19)	1.0856 (11)	0.0193 (17)
H11A	0.0415	0.9105	1.1105	0.023*
C11B	0.544 (2)	0.0498 (17)	0.3160 (11)	0.0155 (17)
H11B	0.6030	0.0498	0.2740	0.019*
C12A	0.081 (2)	0.8227 (18)	1.0019 (12)	0.0193 (17)
H12A	0.0504	0.8825	0.9680	0.023*

C12B	0.573 (2)	0.1793 (17)	0.3719 (10)	0.0154 (17)
H12B	0.6483	0.2691	0.3679	0.018*
C13A	0.137 (2)	0.7151 (18)	0.9662 (11)	0.0193 (17)
C13B	0.489 (2)	0.1732 (17)	0.4339 (10)	0.0153 (17)
C14A	0.098 (3)	0.776 (2)	0.8298 (12)	0.037 (6)
H14A	0.1086	0.7446	0.7719	0.056*
H14B	0.1618	0.8807	0.8517	0.056*
H14C	−0.0139	0.7584	0.8274	0.056*
C14B	0.637 (2)	0.4251 (17)	0.5024 (11)	0.017 (4)
H14D	0.6157	0.4646	0.4518	0.026*
H14E	0.7343	0.4063	0.5057	0.026*
H14F	0.6489	0.4959	0.5544	0.026*
I1	0.06551 (14)	0.45980 (12)	0.65185 (7)	0.0183 (3)
I2	0.58382 (14)	0.53025 (12)	0.73369 (7)	0.0185 (3)
N1A	0.2297 (17)	0.5259 (14)	0.9761 (9)	0.015 (3)
H1A	0.2267	0.5179	0.9211	0.018*
N1B	0.2921 (16)	0.0437 (13)	0.5033 (8)	0.010 (3)
H1B	0.3227	0.1268	0.5411	0.012*
O1A	0.2721 (14)	0.3821 (12)	0.8366 (8)	0.017 (3)
O1B	0.2479 (14)	0.1894 (12)	0.6433 (7)	0.015 (3)
O2A	0.1519 (15)	0.6952 (12)	0.8862 (8)	0.021 (3)
O2B	0.5048 (13)	0.2897 (11)	0.4952 (7)	0.014 (3)
Zn1	0.2884 (3)	0.38214 (19)	0.71687 (14)	0.0131 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.021 (4)	0.006 (3)	0.021 (4)	0.002 (3)	0.008 (3)	0.004 (3)
C1B	0.011 (4)	0.015 (3)	0.013 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C2A	0.021 (4)	0.006 (3)	0.022 (4)	0.002 (3)	0.008 (3)	0.004 (3)
C2B	0.011 (4)	0.015 (3)	0.013 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C3A	0.021 (4)	0.006 (3)	0.022 (4)	0.002 (3)	0.008 (3)	0.005 (3)
C3B	0.011 (4)	0.015 (3)	0.012 (3)	0.006 (3)	0.002 (3)	0.001 (3)
C4A	0.021 (4)	0.006 (3)	0.022 (4)	0.002 (3)	0.009 (3)	0.004 (3)
C4B	0.011 (4)	0.014 (3)	0.012 (3)	0.006 (3)	0.002 (3)	0.002 (3)
C5A	0.021 (4)	0.006 (3)	0.021 (4)	0.002 (3)	0.009 (3)	0.004 (3)
C5B	0.011 (4)	0.014 (3)	0.012 (3)	0.006 (3)	0.002 (3)	0.001 (3)
C6A	0.021 (4)	0.006 (3)	0.021 (4)	0.002 (3)	0.009 (3)	0.005 (3)
C6B	0.011 (4)	0.014 (3)	0.013 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C7A	0.021 (4)	0.007 (3)	0.021 (4)	0.002 (3)	0.008 (3)	0.005 (3)
C7B	0.011 (4)	0.014 (3)	0.013 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C8A	0.011 (4)	0.023 (4)	0.022 (4)	0.010 (3)	0.002 (3)	−0.001 (3)
C8B	0.016 (4)	0.017 (3)	0.014 (4)	0.007 (3)	0.005 (3)	0.004 (3)
C9A	0.011 (4)	0.023 (4)	0.022 (4)	0.010 (3)	0.002 (3)	−0.002 (3)
C9B	0.016 (4)	0.017 (3)	0.014 (4)	0.006 (3)	0.005 (3)	0.004 (3)
C10A	0.012 (4)	0.024 (4)	0.023 (4)	0.010 (3)	0.002 (3)	−0.002 (3)
C10B	0.017 (4)	0.017 (3)	0.014 (4)	0.007 (3)	0.005 (3)	0.003 (3)
C11A	0.012 (4)	0.023 (4)	0.023 (4)	0.010 (3)	0.002 (3)	−0.002 (3)

C11B	0.016 (4)	0.017 (3)	0.014 (4)	0.007 (3)	0.005 (3)	0.004 (3)
C12A	0.012 (4)	0.023 (4)	0.023 (4)	0.010 (3)	0.002 (3)	−0.001 (3)
C12B	0.016 (4)	0.017 (3)	0.014 (4)	0.007 (3)	0.005 (3)	0.004 (3)
C13A	0.012 (4)	0.023 (4)	0.023 (4)	0.010 (3)	0.002 (3)	−0.001 (3)
C13B	0.016 (4)	0.017 (3)	0.013 (4)	0.007 (3)	0.005 (3)	0.004 (3)
C14A	0.063 (17)	0.032 (11)	0.027 (11)	0.026 (12)	0.016 (12)	0.009 (9)
C14B	0.018 (4)	0.016 (4)	0.018 (4)	0.007 (3)	0.005 (3)	0.002 (3)
I1	0.0170 (7)	0.0182 (6)	0.0184 (7)	0.0077 (5)	0.0005 (6)	0.0024 (5)
I2	0.0132 (7)	0.0233 (7)	0.0141 (6)	0.0012 (5)	0.0029 (5)	0.0044 (5)
N1A	0.015 (3)	0.014 (3)	0.015 (3)	0.0062 (17)	0.0030 (15)	0.0032 (14)
N1B	0.009 (3)	0.010 (3)	0.009 (3)	0.0029 (16)	0.0028 (14)	0.0020 (14)
O1A	0.011 (7)	0.013 (6)	0.027 (7)	0.008 (5)	0.000 (6)	0.002 (5)
O1B	0.010 (7)	0.013 (6)	0.016 (6)	0.003 (5)	0.002 (5)	−0.004 (5)
O2A	0.029 (8)	0.016 (6)	0.020 (7)	0.008 (6)	0.007 (6)	0.008 (5)
O2B	0.015 (7)	0.007 (5)	0.020 (6)	0.000 (5)	0.013 (6)	0.001 (5)
Zn1	0.0137 (10)	0.0132 (10)	0.0115 (9)	0.0043 (9)	0.0032 (7)	0.0021 (7)

Geometric parameters (Å, º)

C1A—C2A	1.39 (2)	C8B—N1B	1.41 (2)
C1A—C6A	1.44 (2)	C9A—H9A	0.9500
C1A—O1A	1.31 (2)	C9A—C10A	1.39 (2)
C1B—C2B	1.42 (2)	C9B—H9B	0.9500
C1B—C6B	1.42 (2)	C9B—C10B	1.35 (2)
C1B—O1B	1.307 (19)	C10A—H10A	0.9500
C2A—H2A	0.9500	C10A—C11A	1.38 (2)
C2A—C3A	1.35 (2)	C10B—H10B	0.9500
C2B—H2B	0.9500	C10B—C11B	1.39 (2)
C2B—C3B	1.40 (2)	C11A—H11A	0.9500
C3A—H3A	0.9500	C11A—C12A	1.36 (2)
C3A—C4A	1.36 (2)	C11B—H11B	0.9500
C3B—H3B	0.9500	C11B—C12B	1.38 (2)
C3B—C4B	1.41 (2)	C12A—H12A	0.9500
C4A—H4A	0.9500	C12A—C13A	1.44 (2)
C4A—C5A	1.38 (2)	C12B—H12B	0.9500
C4B—H4B	0.9500	C12B—C13B	1.38 (2)
C4B—C5B	1.38 (2)	C13A—O2A	1.32 (2)
C5A—H5A	0.9500	C13B—O2B	1.362 (18)
C5A—C6A	1.42 (2)	C14A—H14A	0.9800
C5B—H5B	0.9500	C14A—H14B	0.9800
C5B—C6B	1.43 (2)	C14A—H14C	0.9800
C6A—C7A	1.41 (2)	C14A—O2A	1.44 (2)
C6B—C7B	1.44 (2)	C14B—H14D	0.9800
C7A—H7A	0.9500	C14B—H14E	0.9800
C7A—N1A	1.29 (2)	C14B—H14F	0.9800
C7B—H7B	0.9500	C14B—O2B	1.453 (18)
C7B—N1B	1.27 (2)	I1—Zn1	2.558 (3)
C8A—C9A	1.40 (2)	I2—Zn1	2.568 (3)

C8A—C13A	1.35 (2)	N1A—H1A	0.8800
C8A—N1A	1.43 (2)	N1B—H1B	0.8800
C8B—C9B	1.39 (2)	O1A—Zn1	1.979 (12)
C8B—C13B	1.41 (2)	O1B—Zn1	1.988 (11)
C2A—C1A—C6A	117.4 (16)	C10B—C9B—H9B	120.4
O1A—C1A—C2A	123.1 (16)	C9A—C10A—H10A	120.0
O1A—C1A—C6A	119.4 (15)	C11A—C10A—C9A	120.1 (17)
C2B—C1B—C6B	118.5 (15)	C11A—C10A—H10A	120.0
O1B—C1B—C2B	121.5 (15)	C9B—C10B—H10B	119.4
O1B—C1B—C6B	120.0 (14)	C9B—C10B—C11B	121.1 (16)
C1A—C2A—H2A	119.2	C11B—C10B—H10B	119.4
C3A—C2A—C1A	121.5 (17)	C10A—C11A—H11A	118.9
C3A—C2A—H2A	119.2	C12A—C11A—C10A	122.1 (17)
C1B—C2B—H2B	120.5	C12A—C11A—H11A	118.9
C3B—C2B—C1B	119.1 (15)	C10B—C11B—H11B	119.3
C3B—C2B—H2B	120.5	C12B—C11B—C10B	121.5 (16)
C2A—C3A—H3A	119.0	C12B—C11B—H11B	119.3
C2A—C3A—C4A	121.9 (17)	C11A—C12A—H12A	120.8
C4A—C3A—H3A	119.0	C11A—C12A—C13A	118.4 (16)
C2B—C3B—H3B	118.8	C13A—C12A—H12A	120.8
C2B—C3B—C4B	122.3 (16)	C11B—C12B—H12B	121.4
C4B—C3B—H3B	118.8	C11B—C12B—C13B	117.3 (15)
C3A—C4A—H4A	119.7	C13B—C12B—H12B	121.4
C3A—C4A—C5A	120.6 (17)	C8A—C13A—C12A	118.6 (16)
C5A—C4A—H4A	119.7	O2A—C13A—C8A	118.3 (15)
C3B—C4B—H4B	120.2	O2A—C13A—C12A	123.0 (16)
C5B—C4B—C3B	119.6 (16)	C12B—C13B—C8B	121.4 (15)
C5B—C4B—H4B	120.2	O2B—C13B—C8B	113.5 (14)
C4A—C5A—H5A	120.5	O2B—C13B—C12B	125.1 (14)
C4A—C5A—C6A	119.0 (16)	H14A—C14A—H14B	109.5
C6A—C5A—H5A	120.5	H14A—C14A—H14C	109.5
C4B—C5B—H5B	120.3	H14B—C14A—H14C	109.5
C4B—C5B—C6B	119.4 (15)	O2A—C14A—H14A	109.5
C6B—C5B—H5B	120.3	O2A—C14A—H14B	109.5
C5A—C6A—C1A	119.5 (15)	O2A—C14A—H14C	109.5
C7A—C6A—C1A	123.0 (16)	H14D—C14B—H14E	109.5
C7A—C6A—C5A	117.5 (16)	H14D—C14B—H14F	109.5
C1B—C6B—C5B	121.1 (15)	H14E—C14B—H14F	109.5
C1B—C6B—C7B	123.0 (15)	O2B—C14B—H14D	109.5
C5B—C6B—C7B	115.9 (15)	O2B—C14B—H14E	109.5
C6A—C7A—H7A	117.6	O2B—C14B—H14F	109.5
N1A—C7A—C6A	124.8 (17)	C7A—N1A—C8A	124.4 (15)
N1A—C7A—H7A	117.6	C7A—N1A—H1A	117.8
C6B—C7B—H7B	117.5	C8A—N1A—H1A	117.8
N1B—C7B—C6B	124.9 (16)	C7B—N1B—C8B	125.5 (14)
N1B—C7B—H7B	117.5	C7B—N1B—H1B	117.2
C9A—C8A—N1A	121.8 (15)	C8B—N1B—H1B	117.2

C13A—C8A—C9A	122.8 (16)	C1A—O1A—Zn1	124.5 (11)
C13A—C8A—N1A	115.1 (15)	C1B—O1B—Zn1	123.4 (10)
C9B—C8B—C13B	119.5 (15)	C13A—O2A—C14A	118.8 (13)
C9B—C8B—N1B	122.4 (14)	C13B—O2B—C14B	116.2 (12)
C13B—C8B—N1B	118.1 (15)	I1—Zn1—I2	123.65 (7)
C8A—C9A—H9A	121.1	O1A—Zn1—I1	104.0 (4)
C10A—C9A—C8A	117.8 (17)	O1A—Zn1—I2	103.6 (4)
C10A—C9A—H9A	121.1	O1A—Zn1—O1B	115.8 (4)
C8B—C9B—H9B	120.4	O1B—Zn1—I1	106.2 (4)
C10B—C9B—C8B	119.2 (16)	O1B—Zn1—I2	104.2 (3)

C1A—C2A—C3A—C4A	0 (3)	C9A—C8A—C13A—O2A	177.8 (17)
C1A—C6A—C7A—N1A	0 (3)	C9A—C8A—N1A—C7A	−3 (3)
C1B—C2B—C3B—C4B	−1 (2)	C9A—C10A—C11A—C12A	3 (3)
C1B—C6B—C7B—N1B	0 (3)	C9B—C8B—C13B—C12B	2 (3)
C2A—C1A—C6A—C5A	−2 (2)	C9B—C8B—C13B—O2B	−178.7 (15)
C2A—C1A—C6A—C7A	176.9 (16)	C9B—C8B—N1B—C7B	−7 (3)
C2A—C1A—O1A—Zn1	−11 (2)	C9B—C10B—C11B—C12B	−2 (3)
C2A—C3A—C4A—C5A	0 (3)	C10A—C11A—C12A—C13A	−3 (3)
C2B—C1B—C6B—C5B	−2 (2)	C10B—C11B—C12B—C13B	2 (3)
C2B—C1B—C6B—C7B	177.3 (16)	C11A—C12A—C13A—C8A	3 (3)
C2B—C1B—O1B—Zn1	−9 (2)	C11A—C12A—C13A—O2A	−178.6 (17)
C2B—C3B—C4B—C5B	1 (2)	C11B—C12B—C13B—C8B	−2 (3)
C3A—C4A—C5A—C6A	−1 (3)	C11B—C12B—C13B—O2B	178.6 (16)
C3B—C4B—C5B—C6B	−1 (2)	C12A—C13A—O2A—C14A	−5 (3)
C4A—C5A—C6A—C1A	2 (2)	C12B—C13B—O2B—C14B	−9 (2)
C4A—C5A—C6A—C7A	−177.2 (15)	C13A—C8A—C9A—C10A	4 (3)
C4B—C5B—C6B—C1B	2 (2)	C13A—C8A—N1A—C7A	171.6 (17)
C4B—C5B—C6B—C7B	−178.0 (15)	C13B—C8B—C9B—C10B	−2 (3)
C5A—C6A—C7A—N1A	178.4 (16)	C13B—C8B—N1B—C7B	175.7 (16)
C5B—C6B—C7B—N1B	179.6 (16)	N1A—C8A—C9A—C10A	178.3 (16)
C6A—C1A—C2A—C3A	1 (3)	N1A—C8A—C13A—C12A	−178.6 (16)
C6A—C1A—O1A—Zn1	169.1 (11)	N1A—C8A—C13A—O2A	3 (2)
C6A—C7A—N1A—C8A	177.8 (16)	N1B—C8B—C9B—C10B	−179.3 (16)
C6B—C1B—C2B—C3B	2 (2)	N1B—C8B—C13B—C12B	179.8 (16)
C6B—C1B—O1B—Zn1	170.6 (11)	N1B—C8B—C13B—O2B	−1 (2)
C6B—C7B—N1B—C8B	−178.3 (16)	O1A—C1A—C2A—C3A	−179.1 (16)
C8A—C9A—C10A—C11A	−4 (3)	O1A—C1A—C6A—C5A	178.3 (15)
C8A—C13A—O2A—C14A	172.8 (17)	O1A—C1A—C6A—C7A	−3 (3)
C8B—C9B—C10B—C11B	2 (3)	O1B—C1B—C2B—C3B	−177.9 (15)
C8B—C13B—O2B—C14B	171.9 (14)	O1B—C1B—C6B—C5B	177.7 (15)
C9A—C8A—C13A—C12A	−4 (3)	O1B—C1B—C6B—C7B	−3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2*B*—H2*B*···O1*A*	0.95	2.54	3.34 (2)	143
N1*A*—H1*A*···O1*A*	0.88	1.99	2.666 (18)	133

N1*B*—H1*B*···O1*B*	0.88	2.01	2.690 (16)	133

Dibromidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κ*O*)cadmium(II) (Compound_3)

Crystal data

$[CdBr_2(C_{28}H_{26}N_2O_4)]$
M_r = 726.73
Triclinic, $P\overline{1}$
a = 9.2772 (3) Å
b = 10.0935 (3) Å
c = 16.1021 (5) Å
α = 97.699 (2)°
β = 100.586 (2)°
γ = 111.149 (2)°
V = 1348.92 (8) Å^3
Z = 2
$F(000)$ = 716
D_x = 1.789 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9888 reflections
θ = 4.4–53.3°
μ = 3.81 mm^{-1}
T = 100 K
Fragment, orange
0.27 × 0.13 × 0.10 mm

Data collection

Bruker APEXII area detector diffractometer
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (TWINABS; Bruker, 2012)
T_{min} = 0.538, T_{max} = 0.745
10130 measured reflections
10130 independent reflections
8342 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 26.8°, θ_{min} = 2.2°
h = −11→11
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.126
S = 1.03
10130 reflections
337 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.1296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

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. The structure was solved as a rotational twin. Rotated from first domain by 179.7 degrees about reciprocal axis -0.003 -0.997 1.000 and real axis 0.311 1.000 -0.257. Twin law to convert hkl from first to this domain (SHELXL TWIN matrix) -1.001 0.001 -0.004, 0.498 0.590 -0.407, -0.487 -1.593 -0.589.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.29206 (5)	0.39716 (4)	0.71100 (3)	0.01298 (12)
Br2	0.59152 (7)	0.53416 (7)	0.73453 (4)	0.02186 (16)
Br1	0.06225 (7)	0.45851 (6)	0.64168 (4)	0.01971 (15)
O1B	0.2700 (5)	0.3889 (4)	0.8457 (2)	0.0146 (8)

O1A	0.2436 (5)	0.1800 (4)	0.6336 (3)	0.0147 (8)
O2A	0.5041 (5)	0.2829 (4)	0.4950 (3)	0.0171 (8)
O2B	0.1460 (5)	0.6818 (4)	0.8836 (3)	0.0218 (9)
N1A	0.2869 (5)	0.0342 (5)	0.4984 (3)	0.0124 (9)
H1A	0.3168	0.1169	0.5359	0.015*
N1B	0.2287 (5)	0.5245 (5)	0.9842 (3)	0.0133 (9)
H1B	0.2207	0.5120	0.9281	0.016*
C13A	0.4882 (6)	0.1700 (6)	0.4328 (3)	0.0141 (11)
C13B	0.1329 (7)	0.7125 (6)	0.9656 (4)	0.0183 (12)
C6A	0.0867 (6)	−0.0710 (6)	0.5738 (3)	0.0139 (11)
C7B	0.2879 (7)	0.4445 (6)	1.0253 (4)	0.0156 (11)
H7B	0.2977	0.4569	1.0859	0.019*
C1B	0.3292 (7)	0.3179 (6)	0.8939 (3)	0.0131 (11)
C7A	0.1681 (6)	−0.0769 (6)	0.5082 (3)	0.0133 (11)
H7A	0.1344	−0.1673	0.4687	0.016*
C3A	−0.0890 (7)	−0.0731 (6)	0.6974 (4)	0.0172 (12)
H3A	−0.1492	−0.0739	0.7393	0.021*
C6B	0.3379 (6)	0.3411 (6)	0.9855 (3)	0.0144 (11)
C5A	−0.0396 (7)	−0.2009 (6)	0.5771 (4)	0.0152 (11)
H5A	−0.0644	−0.2882	0.5363	0.018*
C4B	0.4565 (7)	0.1660 (6)	1.0034 (4)	0.0195 (12)
H4B	0.4980	0.1138	1.0391	0.023*
C8B	0.1770 (7)	0.6279 (6)	1.0205 (4)	0.0164 (11)
C9B	0.1653 (7)	0.6496 (6)	1.1060 (4)	0.0182 (12)
H9B	0.1929	0.5919	1.1429	0.022*
C8A	0.3719 (6)	0.0354 (6)	0.4343 (3)	0.0146 (11)
C2A	0.0323 (7)	0.0545 (6)	0.6965 (4)	0.0156 (11)
H2A	0.0543	0.1403	0.7378	0.019*
C4A	−0.1254 (7)	−0.2027 (6)	0.6372 (4)	0.0172 (12)
H4A	−0.2091	−0.2904	0.6386	0.021*
C12B	0.0820 (8)	0.8187 (6)	0.9980 (4)	0.0224 (13)
H12B	0.0537	0.8771	0.9619	0.027*
C11A	0.5502 (7)	0.0530 (7)	0.3122 (4)	0.0208 (13)
H11A	0.6087	0.0586	0.2693	0.025*
C10A	0.4388 (7)	−0.0804 (6)	0.3155 (4)	0.0193 (12)
H10A	0.4241	−0.1658	0.2760	0.023*
C9A	0.3486 (7)	−0.0901 (6)	0.3759 (4)	0.0165 (11)
H9A	0.2714	−0.1817	0.3776	0.020*
C5B	0.4009 (7)	0.2633 (6)	1.0369 (4)	0.0178 (12)
H5B	0.4047	0.2792	1.0969	0.021*
C2B	0.3900 (6)	0.2169 (6)	0.8608 (4)	0.0146 (11)
H2B	0.3884	0.1993	0.8011	0.017*
C11B	0.0733 (8)	0.8379 (7)	1.0833 (4)	0.0256 (14)
H11B	0.0385	0.9102	1.1052	0.031*
C12A	0.5773 (7)	0.1788 (6)	0.3712 (3)	0.0173 (12)
H12A	0.6556	0.2696	0.3695	0.021*
C1A	0.1259 (6)	0.0609 (5)	0.6349 (3)	0.0123 (10)
C14B	0.0889 (8)	0.7543 (7)	0.8220 (4)	0.0242 (13)

H14A	0.1000	0.7187	0.7648	0.036*
H14B	0.1516	0.8595	0.8404	0.036*
H14C	−0.0238	0.7339	0.8189	0.036*
C3B	0.4512 (7)	0.1445 (6)	0.9144 (4)	0.0183 (12)
H3B	0.4912	0.0777	0.8906	0.022*
C14A	0.6346 (7)	0.4188 (6)	0.5035 (4)	0.0210 (12)
H14D	0.6140	0.4601	0.4531	0.032*
H14E	0.7334	0.4026	0.5071	0.032*
H14F	0.6456	0.4865	0.5563	0.032*
C10B	0.1136 (7)	0.7551 (7)	1.1377 (4)	0.0218 (13)
H10B	0.1061	0.7699	1.1960	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0152 (2)	0.0125 (2)	0.0107 (2)	0.00478 (16)	0.00380 (14)	0.00165 (14)
Br2	0.0161 (3)	0.0281 (3)	0.0152 (3)	0.0012 (3)	0.0051 (2)	0.0049 (2)
Br1	0.0196 (3)	0.0194 (3)	0.0196 (3)	0.0099 (2)	0.0008 (2)	0.0017 (2)
O1B	0.019 (2)	0.0186 (19)	0.0107 (19)	0.0105 (17)	0.0059 (16)	0.0051 (15)
O1A	0.015 (2)	0.0108 (18)	0.018 (2)	0.0044 (16)	0.0058 (16)	0.0015 (15)
O2A	0.016 (2)	0.0156 (19)	0.016 (2)	0.0007 (16)	0.0073 (17)	0.0018 (16)
O2B	0.030 (2)	0.025 (2)	0.016 (2)	0.0160 (19)	0.0051 (18)	0.0050 (17)
N1A	0.014 (2)	0.014 (2)	0.010 (2)	0.0072 (19)	0.0032 (19)	−0.0014 (18)
N1B	0.014 (2)	0.017 (2)	0.010 (2)	0.0059 (19)	0.0056 (18)	0.0033 (18)
C13A	0.012 (3)	0.017 (3)	0.011 (3)	0.007 (2)	−0.001 (2)	−0.001 (2)
C13B	0.017 (3)	0.021 (3)	0.014 (3)	0.007 (2)	0.002 (2)	−0.001 (2)
C6A	0.015 (3)	0.014 (3)	0.013 (3)	0.007 (2)	0.002 (2)	0.002 (2)
C7B	0.015 (3)	0.018 (3)	0.013 (3)	0.004 (2)	0.007 (2)	0.003 (2)
C1B	0.014 (3)	0.012 (2)	0.013 (3)	0.003 (2)	0.006 (2)	0.004 (2)
C7A	0.012 (3)	0.014 (3)	0.014 (3)	0.006 (2)	0.000 (2)	0.002 (2)
C3A	0.016 (3)	0.021 (3)	0.017 (3)	0.008 (2)	0.010 (2)	0.005 (2)
C6B	0.010 (3)	0.016 (3)	0.015 (3)	0.004 (2)	0.002 (2)	0.002 (2)
C5A	0.014 (3)	0.011 (3)	0.018 (3)	0.004 (2)	0.001 (2)	0.003 (2)
C4B	0.024 (3)	0.014 (3)	0.021 (3)	0.008 (2)	0.006 (3)	0.005 (2)
C8B	0.013 (3)	0.018 (3)	0.020 (3)	0.009 (2)	0.006 (2)	0.002 (2)
C9B	0.014 (3)	0.025 (3)	0.016 (3)	0.010 (2)	0.002 (2)	0.000 (2)
C8A	0.013 (3)	0.022 (3)	0.011 (3)	0.009 (2)	0.004 (2)	0.003 (2)
C2A	0.019 (3)	0.016 (3)	0.014 (3)	0.008 (2)	0.008 (2)	0.002 (2)
C4A	0.014 (3)	0.012 (3)	0.021 (3)	0.000 (2)	0.005 (2)	0.003 (2)
C12B	0.024 (3)	0.019 (3)	0.025 (3)	0.010 (3)	0.006 (3)	0.002 (3)
C11A	0.017 (3)	0.030 (3)	0.016 (3)	0.011 (3)	0.005 (2)	0.002 (3)
C10A	0.020 (3)	0.025 (3)	0.014 (3)	0.013 (3)	0.002 (2)	−0.002 (2)
C9A	0.016 (3)	0.018 (3)	0.017 (3)	0.007 (2)	0.006 (2)	0.001 (2)
C5B	0.022 (3)	0.018 (3)	0.012 (3)	0.006 (2)	0.004 (2)	0.004 (2)
C2B	0.013 (3)	0.018 (3)	0.012 (3)	0.006 (2)	0.004 (2)	0.000 (2)
C11B	0.024 (3)	0.023 (3)	0.033 (4)	0.017 (3)	0.007 (3)	−0.002 (3)
C12A	0.017 (3)	0.020 (3)	0.014 (3)	0.005 (2)	0.006 (2)	0.007 (2)
C1A	0.014 (3)	0.012 (2)	0.013 (3)	0.008 (2)	0.004 (2)	0.002 (2)

C14B	0.035 (4)	0.024 (3)	0.022 (3)	0.020 (3)	0.006 (3)	0.010 (3)
C3B	0.016 (3)	0.015 (3)	0.026 (3)	0.007 (2)	0.006 (3)	0.005 (2)
C14A	0.024 (3)	0.015 (3)	0.020 (3)	0.002 (2)	0.008 (3)	0.003 (2)
C10B	0.017 (3)	0.029 (3)	0.017 (3)	0.011 (3)	0.002 (2)	−0.005 (2)

Geometric parameters (Å, º)

Cd1—Br2	2.5445 (7)	C5A—C4A	1.361 (7)
Cd1—Br1	2.5374 (7)	C4B—H4B	0.9500
Cd1—O1B	2.225 (4)	C4B—C5B	1.360 (8)
Cd1—O1A	2.216 (4)	C4B—C3B	1.410 (8)
O1B—C1B	1.302 (6)	C8B—C9B	1.394 (8)
O1A—C1A	1.306 (6)	C9B—H9B	0.9500
O2A—C13A	1.358 (6)	C9B—C10B	1.392 (8)
O2A—C14A	1.434 (6)	C8A—C9A	1.394 (8)
O2B—C13B	1.354 (7)	C2A—H2A	0.9500
O2B—C14B	1.441 (6)	C2A—C1A	1.426 (7)
N1A—H1A	0.8800	C4A—H4A	0.9500
N1A—C7A	1.310 (7)	C12B—H12B	0.9500
N1A—C8A	1.409 (7)	C12B—C11B	1.383 (9)
N1B—H1B	0.8800	C11A—H11A	0.9500
N1B—C7B	1.312 (7)	C11A—C10A	1.385 (8)
N1B—C8B	1.400 (7)	C11A—C12A	1.391 (8)
C13A—C8A	1.403 (8)	C10A—H10A	0.9500
C13A—C12A	1.397 (7)	C10A—C9A	1.387 (8)
C13B—C8B	1.414 (8)	C9A—H9A	0.9500
C13B—C12B	1.397 (8)	C5B—H5B	0.9500
C6A—C7A	1.414 (7)	C2B—H2B	0.9500
C6A—C5A	1.423 (7)	C2B—C3B	1.374 (8)
C6A—C1A	1.429 (7)	C11B—H11B	0.9500
C7B—H7B	0.9500	C11B—C10B	1.381 (9)
C7B—C6B	1.413 (7)	C12A—H12A	0.9500
C1B—C6B	1.444 (7)	C14B—H14A	0.9800
C1B—C2B	1.422 (7)	C14B—H14B	0.9800
C7A—H7A	0.9500	C14B—H14C	0.9800
C3A—H3A	0.9500	C3B—H3B	0.9500
C3A—C2A	1.375 (8)	C14A—H14D	0.9800
C3A—C4A	1.409 (8)	C14A—H14E	0.9800
C6B—C5B	1.404 (8)	C14A—H14F	0.9800
C5A—H5A	0.9500	C10B—H10B	0.9500

Br1—Cd1—Br2	130.04 (2)	C9A—C8A—N1A	122.9 (5)
O1B—Cd1—Br2	101.88 (11)	C9A—C8A—C13A	120.1 (5)
O1B—Cd1—Br1	104.78 (10)	C3A—C2A—H2A	119.2
O1A—Cd1—Br2	103.56 (10)	C3A—C2A—C1A	121.5 (5)
O1A—Cd1—Br1	104.40 (10)	C1A—C2A—H2A	119.2
O1A—Cd1—O1B	111.99 (12)	C3A—C4A—H4A	120.3
C1B—O1B—Cd1	124.1 (3)	C5A—C4A—C3A	119.3 (5)

C1A—O1A—Cd1	123.5 (3)	C5A—C4A—H4A	120.3
C13A—O2A—C14A	116.8 (4)	C13B—C12B—H12B	120.4
C13B—O2B—C14B	117.8 (4)	C11B—C12B—C13B	119.2 (6)
C7A—N1A—H1A	116.5	C11B—C12B—H12B	120.4
C7A—N1A—C8A	127.0 (5)	C10A—C11A—H11A	119.6
C8A—N1A—H1A	116.5	C10A—C11A—C12A	120.8 (5)
C7B—N1B—H1B	116.7	C12A—C11A—H11A	119.6
C7B—N1B—C8B	126.6 (5)	C11A—C10A—H10A	119.8
C8B—N1B—H1B	116.7	C11A—C10A—C9A	120.5 (5)
O2A—C13A—C8A	114.6 (5)	C9A—C10A—H10A	119.8
O2A—C13A—C12A	125.5 (5)	C8A—C9A—H9A	120.3
C12A—C13A—C8A	119.9 (5)	C10A—C9A—C8A	119.5 (5)
O2B—C13B—C8B	114.9 (5)	C10A—C9A—H9A	120.3
O2B—C13B—C12B	125.3 (5)	C6B—C5B—H5B	119.0
C12B—C13B—C8B	119.8 (5)	C4B—C5B—C6B	122.0 (5)
C7A—C6A—C5A	118.1 (5)	C4B—C5B—H5B	119.0
C7A—C6A—C1A	121.9 (5)	C1B—C2B—H2B	119.7
C5A—C6A—C1A	119.9 (5)	C3B—C2B—C1B	120.5 (5)
N1B—C7B—H7B	117.8	C3B—C2B—H2B	119.7
N1B—C7B—C6B	124.4 (5)	C12B—C11B—H11B	119.0
C6B—C7B—H7B	117.8	C10B—C11B—C12B	122.0 (6)
O1B—C1B—C6B	120.5 (5)	C10B—C11B—H11B	119.0
O1B—C1B—C2B	122.7 (5)	C13A—C12A—H12A	120.4
C2B—C1B—C6B	116.8 (5)	C11A—C12A—C13A	119.2 (5)
N1A—C7A—C6A	124.3 (5)	C11A—C12A—H12A	120.4
N1A—C7A—H7A	117.8	O1A—C1A—C6A	120.4 (5)
C6A—C7A—H7A	117.8	O1A—C1A—C2A	122.8 (5)
C2A—C3A—H3A	119.5	C2A—C1A—C6A	116.8 (5)
C2A—C3A—C4A	121.0 (5)	O2B—C14B—H14A	109.5
C4A—C3A—H3A	119.5	O2B—C14B—H14B	109.5
C7B—C6B—C1B	121.0 (5)	O2B—C14B—H14C	109.5
C5B—C6B—C7B	118.9 (5)	H14A—C14B—H14B	109.5
C5B—C6B—C1B	120.1 (5)	H14A—C14B—H14C	109.5
C6A—C5A—H5A	119.3	H14B—C14B—H14C	109.5
C4A—C5A—C6A	121.4 (5)	C4B—C3B—H3B	118.9
C4A—C5A—H5A	119.3	C2B—C3B—C4B	122.2 (5)
C5B—C4B—H4B	120.8	C2B—C3B—H3B	118.9
C5B—C4B—C3B	118.4 (5)	O2A—C14A—H14D	109.5
C3B—C4B—H4B	120.8	O2A—C14A—H14E	109.5
N1B—C8B—C13B	116.8 (5)	O2A—C14A—H14F	109.5
C9B—C8B—N1B	123.8 (5)	H14D—C14A—H14E	109.5
C9B—C8B—C13B	119.3 (5)	H14D—C14A—H14F	109.5
C8B—C9B—H9B	119.7	H14E—C14A—H14F	109.5
C10B—C9B—C8B	120.6 (5)	C9B—C10B—H10B	120.4
C10B—C9B—H9B	119.7	C11B—C10B—C9B	119.1 (6)
C13A—C8A—N1A	116.9 (5)	C11B—C10B—H10B	120.4
Cd1—O1B—C1B—C6B	167.5 (4)	C3A—C2A—C1A—O1A	−178.7 (5)

Cd1—O1B—C1B—C2B	−11.5 (7)	C3A—C2A—C1A—C6A	0.6 (8)
Cd1—O1A—C1A—C6A	170.3 (4)	C6B—C1B—C2B—C3B	1.0 (8)
Cd1—O1A—C1A—C2A	−10.4 (7)	C5A—C6A—C7A—N1A	−179.5 (5)
O1B—C1B—C6B—C7B	−2.2 (8)	C5A—C6A—C1A—O1A	178.6 (5)
O1B—C1B—C6B—C5B	179.5 (5)	C5A—C6A—C1A—C2A	−0.7 (8)
O1B—C1B—C2B—C3B	−179.9 (5)	C8B—N1B—C7B—C6B	179.8 (5)
O2A—C13A—C8A—N1A	0.4 (7)	C8B—C13B—C12B—C11B	−1.0 (9)
O2A—C13A—C8A—C9A	−177.4 (5)	C8B—C9B—C10B—C11B	0.2 (9)
O2A—C13A—C12A—C11A	178.7 (5)	C8A—N1A—C7A—C6A	−179.6 (5)
O2B—C13B—C8B—N1B	0.2 (7)	C8A—C13A—C12A—C11A	−0.5 (8)
O2B—C13B—C8B—C9B	−179.0 (5)	C2A—C3A—C4A—C5A	−0.4 (9)
O2B—C13B—C12B—C11B	179.6 (6)	C4A—C3A—C2A—C1A	0.0 (9)
N1A—C8A—C9A—C10A	−179.0 (5)	C12B—C13B—C8B—N1B	−179.3 (5)
N1B—C7B—C6B—C1B	1.1 (9)	C12B—C13B—C8B—C9B	1.5 (8)
N1B—C7B—C6B—C5B	179.3 (5)	C12B—C11B—C10B—C9B	0.3 (9)
N1B—C8B—C9B—C10B	179.7 (5)	C11A—C10A—C9A—C8A	−0.7 (9)
C13A—C8A—C9A—C10A	−1.3 (8)	C10A—C11A—C12A—C13A	−1.4 (9)
C13B—C8B—C9B—C10B	−1.1 (9)	C5B—C4B—C3B—C2B	−0.9 (9)
C13B—C12B—C11B—C10B	0.0 (10)	C2B—C1B—C6B—C7B	176.9 (5)
C6A—C5A—C4A—C3A	0.2 (8)	C2B—C1B—C6B—C5B	−1.4 (8)
C7B—N1B—C8B—C13B	173.6 (5)	C12A—C13A—C8A—N1A	179.7 (5)
C7B—N1B—C8B—C9B	−7.2 (9)	C12A—C13A—C8A—C9A	1.9 (8)
C7B—C6B—C5B—C4B	−177.6 (5)	C12A—C11A—C10A—C9A	2.1 (9)
C1B—C6B—C5B—C4B	0.6 (9)	C1A—C6A—C7A—N1A	1.7 (8)
C1B—C2B—C3B—C4B	0.1 (9)	C1A—C6A—C5A—C4A	0.3 (8)
C7A—N1A—C8A—C13A	175.8 (5)	C14B—O2B—C13B—C8B	174.3 (5)
C7A—N1A—C8A—C9A	−6.4 (9)	C14B—O2B—C13B—C12B	−6.2 (8)
C7A—C6A—C5A—C4A	−178.6 (5)	C3B—C4B—C5B—C6B	0.5 (9)
C7A—C6A—C1A—O1A	−2.5 (8)	C14A—O2A—C13A—C8A	172.3 (5)
C7A—C6A—C1A—C2A	178.1 (5)	C14A—O2A—C13A—C12A	−7.0 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O1*A*	0.88	1.94	2.638 (5)	135
N1*B*—H1*B*···O1*B*	0.88	1.93	2.621 (5)	135

Diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]\ methyl}phenolato-κ*O*)cadmium(II) (Compound_4)

Crystal data

$[CdI_2(C_{28}H_{26}N_2O_4)]$
M_r = 820.71
Triclinic, $P\overline{1}$
a = 9.3200 (3) Å
b = 10.0498 (3) Å
c = 16.6239 (5) Å
α = 99.140 (1)°
β = 100.528 (1)°
γ = 109.332 (1)°
V = 1403.58 (8) Å^3

Z = 2
$F(000)$ = 788
D_x = 1.942 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9951 reflections
θ = 2.3–35.6°
μ = 3.01 mm^{-1}
T = 100 K
Block, yellow
0.40 × 0.26 × 0.14 mm

Data collection

Bruker SMART APEXII area detector diffractometer
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: numerical (SADABS; Bruker, 2016)
T_{min} = 0.416, T_{max} = 0.667
110757 measured reflections
13807 independent reflections
10917 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 36.6°, θ_{min} = 2.2°
h = −15→15
k = −16→16
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.067
S = 1.03
13807 reflections
336 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0166P)^2 + 3.1202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −1.33 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.61219 (2)	0.54498 (2)	0.73702 (2)	0.02004 (3)
I2	0.05336 (2)	0.47473 (2)	0.64793 (2)	0.01951 (3)
Cd1	0.29815 (2)	0.40341 (2)	0.71415 (2)	0.01333 (3)
O1A	0.25028 (19)	0.18582 (17)	0.63597 (10)	0.0163 (3)
O1B	0.27608 (19)	0.39367 (18)	0.84469 (9)	0.0159 (3)
O2A	0.5029 (2)	0.28450 (17)	0.49378 (10)	0.0180 (3)
O2B	0.1482 (2)	0.6984 (2)	0.89037 (11)	0.0228 (3)
N1A	0.2908 (2)	0.03889 (19)	0.49969 (11)	0.0131 (3)
H1A	0.3210	0.1219	0.5369	0.016*
N1B	0.2263 (2)	0.5284 (2)	0.98053 (12)	0.0165 (3)
H1B	0.2193	0.5175	0.9262	0.020*
C1B	0.3350 (2)	0.3223 (2)	0.89094 (13)	0.0137 (3)
C6B	0.3388 (3)	0.3444 (2)	0.97888 (13)	0.0142 (3)
C3A	−0.0776 (3)	−0.0639 (2)	0.69293 (13)	0.0167 (4)
H3A	−0.1377	−0.0639	0.7334	0.020*
C1A	0.1349 (2)	0.0682 (2)	0.63543 (12)	0.0130 (3)
C2A	0.0430 (3)	0.0625 (2)	0.69497 (13)	0.0156 (4)
H2A	0.0649	0.1474	0.7371	0.019*
C7B	0.2850 (3)	0.4472 (2)	1.01879 (13)	0.0159 (4)
H7B	0.2922	0.4578	1.0774	0.019*

C2B	0.3980 (3)	0.2205 (2)	0.85860 (13)	0.0162 (4)
H2B	0.3978	0.2028	0.8007	0.019*
C6A	0.0955 (2)	−0.0632 (2)	0.57291 (12)	0.0129 (3)
C13A	0.4846 (3)	0.1676 (2)	0.43338 (13)	0.0146 (3)
C12A	0.5678 (3)	0.1712 (3)	0.37140 (14)	0.0181 (4)
H12A	0.6428	0.2604	0.3687	0.022*
C4B	0.4605 (3)	0.1683 (3)	0.99513 (15)	0.0194 (4)
H4B	0.5016	0.1155	1.0293	0.023*
C8A	0.3722 (2)	0.0350 (2)	0.43590 (13)	0.0140 (3)
C4A	−0.1135 (3)	−0.1924 (2)	0.63230 (14)	0.0181 (4)
H4A	−0.1955	−0.2790	0.6324	0.022*
C8B	0.1726 (3)	0.6332 (2)	1.01955 (14)	0.0174 (4)
C11A	0.5404 (3)	0.0439 (3)	0.31378 (14)	0.0195 (4)
H11A	0.5967	0.0467	0.2715	0.023*
C9B	0.1589 (3)	0.6470 (3)	1.10236 (14)	0.0196 (4)
H9B	0.1849	0.5850	1.1351	0.024*
C5B	0.4016 (3)	0.2664 (3)	1.02921 (14)	0.0186 (4)
H5B	0.4031	0.2818	1.0873	0.022*
C13B	0.1315 (3)	0.7227 (3)	0.97039 (14)	0.0195 (4)
C10A	0.4318 (3)	−0.0876 (3)	0.31701 (14)	0.0198 (4)
H10A	0.4154	−0.1741	0.2776	0.024*
C9A	0.3468 (3)	−0.0925 (2)	0.37816 (13)	0.0166 (4)
H9A	0.2722	−0.1822	0.3804	0.020*
C5A	−0.0285 (3)	−0.1913 (2)	0.57292 (13)	0.0165 (4)
H5A	−0.0532	−0.2776	0.5313	0.020*
C7A	0.1750 (2)	−0.0698 (2)	0.50829 (13)	0.0145 (3)
H7A	0.1416	−0.1598	0.4684	0.017*
C14A	0.6310 (3)	0.4168 (3)	0.49940 (15)	0.0205 (4)
H14A	0.6113	0.4513	0.4481	0.031*
H14B	0.7290	0.3987	0.5056	0.031*
H14C	0.6399	0.4906	0.5483	0.031*
C3B	0.4596 (3)	0.1470 (2)	0.90986 (14)	0.0180 (4)
H3B	0.5022	0.0805	0.8867	0.022*
C10B	0.1064 (3)	0.7531 (3)	1.13657 (16)	0.0249 (5)
H10B	0.0978	0.7643	1.1931	0.030*
C12B	0.0790 (3)	0.8278 (3)	1.00523 (17)	0.0250 (5)
H12B	0.0517	0.8893	0.9726	0.030*
C14B	0.1026 (4)	0.7842 (3)	0.83660 (17)	0.0271 (5)
H14D	0.1236	0.7587	0.7817	0.041*
H14E	0.1630	0.8874	0.8624	0.041*
H14F	−0.0098	0.7649	0.8291	0.041*
C11B	0.0670 (3)	0.8420 (3)	1.08820 (17)	0.0272 (5)
H11B	0.0313	0.9137	1.1119	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01512 (6)	0.02635 (7)	0.01340 (6)	0.00091 (5)	0.00337 (5)	0.00530 (5)

I2	0.01838 (7)	0.01849 (6)	0.01998 (6)	0.00879 (5)	0.00003 (5)	0.00123 (5)
Cd1	0.01452 (6)	0.01302 (6)	0.01137 (6)	0.00434 (5)	0.00314 (5)	0.00176 (4)
O1A	0.0159 (7)	0.0135 (6)	0.0174 (7)	0.0031 (5)	0.0065 (5)	0.0002 (5)
O1B	0.0183 (7)	0.0204 (7)	0.0127 (6)	0.0104 (6)	0.0054 (5)	0.0049 (5)
O2A	0.0198 (7)	0.0154 (7)	0.0171 (7)	0.0040 (6)	0.0080 (6)	0.0010 (5)
O2B	0.0323 (10)	0.0245 (8)	0.0160 (7)	0.0171 (8)	0.0047 (7)	0.0040 (6)
N1A	0.0129 (7)	0.0136 (7)	0.0133 (7)	0.0058 (6)	0.0045 (6)	0.0012 (6)
N1B	0.0166 (8)	0.0190 (8)	0.0156 (7)	0.0091 (7)	0.0049 (6)	0.0023 (6)
C1B	0.0132 (8)	0.0145 (8)	0.0130 (8)	0.0044 (7)	0.0043 (6)	0.0030 (6)
C6B	0.0161 (9)	0.0159 (8)	0.0117 (8)	0.0070 (7)	0.0046 (7)	0.0027 (6)
C3A	0.0154 (9)	0.0200 (9)	0.0154 (8)	0.0060 (8)	0.0064 (7)	0.0050 (7)
C1A	0.0119 (8)	0.0138 (8)	0.0128 (8)	0.0047 (7)	0.0027 (6)	0.0026 (6)
C2A	0.0154 (9)	0.0178 (9)	0.0145 (8)	0.0070 (7)	0.0057 (7)	0.0027 (7)
C7B	0.0174 (9)	0.0173 (9)	0.0138 (8)	0.0077 (7)	0.0046 (7)	0.0019 (7)
C2B	0.0176 (9)	0.0178 (9)	0.0130 (8)	0.0074 (7)	0.0044 (7)	0.0009 (7)
C6A	0.0124 (8)	0.0127 (8)	0.0131 (8)	0.0046 (6)	0.0030 (6)	0.0022 (6)
C13A	0.0151 (9)	0.0160 (9)	0.0128 (8)	0.0063 (7)	0.0033 (7)	0.0028 (7)
C12A	0.0188 (10)	0.0213 (10)	0.0166 (9)	0.0081 (8)	0.0075 (7)	0.0057 (7)
C4B	0.0254 (11)	0.0167 (9)	0.0185 (9)	0.0102 (8)	0.0059 (8)	0.0048 (7)
C8A	0.0131 (8)	0.0173 (9)	0.0119 (8)	0.0065 (7)	0.0036 (6)	0.0022 (6)
C4A	0.0181 (10)	0.0162 (9)	0.0186 (9)	0.0031 (8)	0.0061 (7)	0.0054 (7)
C8B	0.0155 (9)	0.0190 (9)	0.0173 (9)	0.0074 (8)	0.0042 (7)	0.0009 (7)
C11A	0.0192 (10)	0.0253 (11)	0.0157 (9)	0.0092 (9)	0.0072 (8)	0.0036 (8)
C9B	0.0164 (9)	0.0274 (11)	0.0152 (9)	0.0108 (8)	0.0039 (7)	−0.0006 (8)
C5B	0.0251 (11)	0.0189 (10)	0.0126 (8)	0.0102 (8)	0.0035 (7)	0.0032 (7)
C13B	0.0212 (10)	0.0206 (10)	0.0164 (9)	0.0094 (8)	0.0037 (8)	0.0008 (7)
C10A	0.0203 (10)	0.0234 (10)	0.0160 (9)	0.0094 (8)	0.0063 (8)	0.0001 (8)
C9A	0.0148 (9)	0.0174 (9)	0.0163 (9)	0.0061 (7)	0.0041 (7)	−0.0003 (7)
C5A	0.0182 (9)	0.0139 (8)	0.0155 (8)	0.0041 (7)	0.0046 (7)	0.0020 (7)
C7A	0.0147 (8)	0.0147 (8)	0.0134 (8)	0.0057 (7)	0.0030 (7)	0.0017 (6)
C14A	0.0188 (10)	0.0172 (9)	0.0190 (9)	−0.0003 (8)	0.0057 (8)	0.0004 (7)
C3B	0.0201 (10)	0.0153 (9)	0.0190 (9)	0.0093 (8)	0.0039 (8)	0.0008 (7)
C10B	0.0219 (11)	0.0342 (13)	0.0184 (10)	0.0142 (10)	0.0050 (8)	−0.0025 (9)
C12B	0.0284 (12)	0.0239 (11)	0.0252 (11)	0.0160 (10)	0.0053 (9)	0.0003 (9)
C14B	0.0340 (14)	0.0258 (12)	0.0226 (11)	0.0139 (11)	0.0030 (10)	0.0071 (9)
C11B	0.0278 (12)	0.0309 (13)	0.0236 (11)	0.0174 (11)	0.0040 (9)	−0.0028 (9)

Geometric parameters (Å, º)

I1—Cd1	2.7202 (2)	C12A—H12A	0.9500
I2—Cd1	2.7104 (2)	C12A—C11A	1.387 (3)
Cd1—O1A	2.2157 (15)	C4B—H4B	0.9500
Cd1—O1B	2.2312 (15)	C4B—C5B	1.374 (3)
O1A—C1A	1.306 (3)	C4B—C3B	1.397 (3)
O1B—C1B	1.299 (3)	C8A—C9A	1.395 (3)
O2A—C13A	1.359 (3)	C4A—H4A	0.9500
O2A—C14A	1.439 (3)	C4A—C5A	1.373 (3)
O2B—C13B	1.361 (3)	C8B—C9B	1.395 (3)

O2B—C14B	1.440 (3)	C8B—C13B	1.404 (3)
N1A—H1A	0.8800	C11A—H11A	0.9500
N1A—C8A	1.415 (3)	C11A—C10A	1.389 (3)
N1A—C7A	1.306 (3)	C9B—H9B	0.9500
N1B—H1B	0.8800	C9B—C10B	1.398 (3)
N1B—C7B	1.305 (3)	C5B—H5B	0.9500
N1B—C8B	1.426 (3)	C13B—C12B	1.393 (3)
C1B—C6B	1.435 (3)	C10A—H10A	0.9500
C1B—C2B	1.421 (3)	C10A—C9A	1.395 (3)
C6B—C7B	1.416 (3)	C9A—H9A	0.9500
C6B—C5B	1.411 (3)	C5A—H5A	0.9500
C3A—H3A	0.9500	C7A—H7A	0.9500
C3A—C2A	1.380 (3)	C14A—H14A	0.9800
C3A—C4A	1.405 (3)	C14A—H14B	0.9800
C1A—C2A	1.418 (3)	C14A—H14C	0.9800
C1A—C6A	1.436 (3)	C3B—H3B	0.9500
C2A—H2A	0.9500	C10B—H10B	0.9500
C7B—H7B	0.9500	C10B—C11B	1.385 (4)
C2B—H2B	0.9500	C12B—H12B	0.9500
C2B—C3B	1.379 (3)	C12B—C11B	1.393 (4)
C6A—C5A	1.418 (3)	C14B—H14D	0.9800
C6A—C7A	1.417 (3)	C14B—H14E	0.9800
C13A—C12A	1.396 (3)	C14B—H14F	0.9800
C13A—C8A	1.409 (3)	C11B—H11B	0.9500

I2—Cd1—I1	130.043 (8)	C5A—C4A—C3A	119.2 (2)
O1A—Cd1—I1	103.73 (4)	C5A—C4A—H4A	120.4
O1A—Cd1—I2	104.76 (4)	C9B—C8B—N1B	122.4 (2)
O1A—Cd1—O1B	111.56 (6)	C9B—C8B—C13B	120.6 (2)
O1B—Cd1—I1	102.91 (4)	C13B—C8B—N1B	116.9 (2)
O1B—Cd1—I2	103.54 (4)	C12A—C11A—H11A	119.5
C1A—O1A—Cd1	124.04 (13)	C12A—C11A—C10A	121.0 (2)
C1B—O1B—Cd1	125.04 (13)	C10A—C11A—H11A	119.5
C13A—O2A—C14A	116.36 (17)	C8B—C9B—H9B	120.4
C13B—O2B—C14B	117.4 (2)	C8B—C9B—C10B	119.2 (2)
C8A—N1A—H1A	117.1	C10B—C9B—H9B	120.4
C7A—N1A—H1A	117.1	C6B—C5B—H5B	119.6
C7A—N1A—C8A	125.77 (18)	C4B—C5B—C6B	120.7 (2)
C7B—N1B—H1B	117.3	C4B—C5B—H5B	119.6
C7B—N1B—C8B	125.34 (19)	O2B—C13B—C8B	115.4 (2)
C8B—N1B—H1B	117.3	O2B—C13B—C12B	125.1 (2)
O1B—C1B—C6B	120.25 (19)	C12B—C13B—C8B	119.6 (2)
O1B—C1B—C2B	122.92 (19)	C11A—C10A—H10A	120.0
C2B—C1B—C6B	116.83 (19)	C11A—C10A—C9A	120.0 (2)
C7B—C6B—C1B	121.86 (19)	C9A—C10A—H10A	120.0
C5B—C6B—C1B	120.45 (19)	C8A—C9A—C10A	119.6 (2)
C5B—C6B—C7B	117.66 (19)	C8A—C9A—H9A	120.2
C2A—C3A—H3A	119.3	C10A—C9A—H9A	120.2

C2A—C3A—C4A	121.4 (2)	C6A—C5A—H5A	119.6
C4A—C3A—H3A	119.3	C4A—C5A—C6A	120.9 (2)
O1A—C1A—C2A	122.80 (19)	C4A—C5A—H5A	119.6
O1A—C1A—C6A	120.39 (18)	N1A—C7A—C6A	124.70 (19)
C2A—C1A—C6A	116.81 (19)	N1A—C7A—H7A	117.7
C3A—C2A—C1A	121.3 (2)	C6A—C7A—H7A	117.7
C3A—C2A—H2A	119.3	O2A—C14A—H14A	109.5
C1A—C2A—H2A	119.3	O2A—C14A—H14B	109.5
N1B—C7B—C6B	124.4 (2)	O2A—C14A—H14C	109.5
N1B—C7B—H7B	117.8	H14A—C14A—H14B	109.5
C6B—C7B—H7B	117.8	H14A—C14A—H14C	109.5
C1B—C2B—H2B	119.5	H14B—C14A—H14C	109.5
C3B—C2B—C1B	121.10 (19)	C2B—C3B—C4B	121.4 (2)
C3B—C2B—H2B	119.5	C2B—C3B—H3B	119.3
C5A—C6A—C1A	120.41 (18)	C4B—C3B—H3B	119.3
C7A—C6A—C1A	122.09 (19)	C9B—C10B—H10B	119.9
C7A—C6A—C5A	117.49 (18)	C11B—C10B—C9B	120.1 (2)
O2A—C13A—C12A	125.0 (2)	C11B—C10B—H10B	119.9
O2A—C13A—C8A	115.48 (18)	C13B—C12B—H12B	120.2
C12A—C13A—C8A	119.57 (19)	C11B—C12B—C13B	119.6 (2)
C13A—C12A—H12A	120.2	C11B—C12B—H12B	120.2
C11A—C12A—C13A	119.6 (2)	O2B—C14B—H14D	109.5
C11A—C12A—H12A	120.2	O2B—C14B—H14E	109.5
C5B—C4B—H4B	120.2	O2B—C14B—H14F	109.5
C5B—C4B—C3B	119.5 (2)	H14D—C14B—H14E	109.5
C3B—C4B—H4B	120.2	H14D—C14B—H14F	109.5
C13A—C8A—N1A	116.80 (18)	H14E—C14B—H14F	109.5
C9A—C8A—N1A	122.9 (2)	C10B—C11B—C12B	120.9 (2)
C9A—C8A—C13A	120.26 (19)	C10B—C11B—H11B	119.6
C3A—C4A—H4A	120.4	C12B—C11B—H11B	119.6

Cd1—O1A—C1A—C2A	−10.7 (3)	C2B—C1B—C6B—C7B	177.5 (2)
Cd1—O1A—C1A—C6A	169.28 (14)	C2B—C1B—C6B—C5B	−0.5 (3)
Cd1—O1B—C1B—C6B	168.58 (15)	C6A—C1A—C2A—C3A	0.4 (3)
Cd1—O1B—C1B—C2B	−11.4 (3)	C13A—C12A—C11A—C10A	−0.4 (4)
O1A—C1A—C2A—C3A	−179.6 (2)	C13A—C8A—C9A—C10A	−1.0 (3)
O1A—C1A—C6A—C5A	179.2 (2)	C12A—C13A—C8A—N1A	−179.4 (2)
O1A—C1A—C6A—C7A	−2.2 (3)	C12A—C13A—C8A—C9A	1.5 (3)
O1B—C1B—C6B—C7B	−2.5 (3)	C12A—C11A—C10A—C9A	0.9 (4)
O1B—C1B—C6B—C5B	179.5 (2)	C8A—N1A—C7A—C6A	179.9 (2)
O1B—C1B—C2B—C3B	180.0 (2)	C8A—C13A—C12A—C11A	−0.9 (3)
O2A—C13A—C12A—C11A	179.0 (2)	C4A—C3A—C2A—C1A	0.6 (3)
O2A—C13A—C8A—N1A	0.7 (3)	C8B—N1B—C7B—C6B	−179.5 (2)
O2A—C13A—C8A—C9A	−178.4 (2)	C8B—C9B—C10B—C11B	0.7 (4)
O2B—C13B—C12B—C11B	−180.0 (3)	C8B—C13B—C12B—C11B	−0.5 (4)
N1A—C8A—C9A—C10A	−180.0 (2)	C11A—C10A—C9A—C8A	−0.2 (4)
N1B—C8B—C9B—C10B	179.5 (2)	C9B—C8B—C13B—O2B	−179.4 (2)
N1B—C8B—C13B—O2B	−0.1 (3)	C9B—C8B—C13B—C12B	1.1 (4)

N1B—C8B—C13B—C12B	−179.6 (2)	C9B—C10B—C11B—C12B	−0.1 (4)
C1B—C6B—C7B—N1B	1.0 (4)	C5B—C6B—C7B—N1B	179.0 (2)
C1B—C6B—C5B—C4B	0.2 (4)	C5B—C4B—C3B—C2B	−1.2 (4)
C1B—C2B—C3B—C4B	0.8 (4)	C13B—C8B—C9B—C10B	−1.2 (4)
C6B—C1B—C2B—C3B	0.0 (3)	C13B—C12B—C11B—C10B	0.0 (4)
C3A—C4A—C5A—C6A	0.9 (3)	C5A—C6A—C7A—N1A	179.7 (2)
C1A—C6A—C5A—C4A	0.2 (3)	C7A—N1A—C8A—C13A	174.5 (2)
C1A—C6A—C7A—N1A	1.2 (3)	C7A—N1A—C8A—C9A	−6.4 (3)
C2A—C3A—C4A—C5A	−1.2 (4)	C7A—C6A—C5A—C4A	−178.4 (2)
C2A—C1A—C6A—C5A	−0.8 (3)	C14A—O2A—C13A—C12A	−7.9 (3)
C2A—C1A—C6A—C7A	177.7 (2)	C14A—O2A—C13A—C8A	172.1 (2)
C7B—N1B—C8B—C9B	−8.5 (4)	C3B—C4B—C5B—C6B	0.6 (4)
C7B—N1B—C8B—C13B	172.3 (2)	C14B—O2B—C13B—C8B	178.0 (2)
C7B—C6B—C5B—C4B	−177.9 (2)	C14B—O2B—C13B—C12B	−2.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O1*A*	0.88	1.98	2.660 (2)	134
N1*B*—H1*B*···O1*B*	0.88	1.96	2.641 (2)	134
C7*B*—H7*B*···I1^{i}	0.95	3.06	3.979 (2)	164

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.

Dichloridobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-κ*O*)mercury(II) (Compound_5)

Crystal data

[$HgCl_2(C_{28}H_{26}N_2O_4)$]	Z = 2
M_r = 726.00	F(000) = 708
Triclinic, $P\overline{1}$	D_x = 1.818 Mg m^{-3}
a = 9.2456 (4) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
b = 10.1510 (4) Å	Cell parameters from 9113 reflections
c = 15.8499 (6) Å	θ = 2.2–28.3°
α = 96.5447 (15)°	μ = 6.04 mm^{-1}
β = 99.7441 (15)°	T = 100 K
γ = 112.6735 (14)°	Block, yellow
V = 1326.25 (9) Å^3	0.17 × 0.14 × 0.08 mm

Data collection

Bruker APEXII area detector diffractometer	T_{min} = 0.630, T_{max} = 0.746
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C	22779 measured reflections
Graphite monochromator	22779 independent reflections
Detector resolution: 7.9 pixels mm^{-1}	21098 reflections with $I > 2\sigma(I)$
ω and φ scans	R_{int} = 0.012
Absorption correction: multi-scan (TWINABS; Bruker, 2012)	θ_{max} = 28.4°, θ_{min} = 2.2°
	h = −12→12
	k = −13→13
	l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.052$
$S = 1.03$
22779 reflections
337 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2 + 0.8324P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.29$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

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. The structure was solved as a rotational twin. Rotated from first domain by 179.9 degrees about reciprocal axis -0.001 1.000 -0.999 and real axis 0.345 1.000 -0.274. Twin law to convert hkl from first to this domain (SHELXL TWIN matrix): -1.000 -0.001 0.001 0.541 0.570 -0.431 -0.543 -1.570 -0.570.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.30358 (2)	0.41553 (2)	0.70492 (2)	0.01398 (4)
Cl2	0.06386 (10)	0.43743 (9)	0.64325 (5)	0.02133 (17)
Cl1	0.58885 (10)	0.51131 (10)	0.73464 (5)	0.02286 (18)
O2A	0.5129 (3)	0.2848 (2)	0.49846 (15)	0.0175 (5)
O1B	0.2698 (3)	0.3921 (2)	0.84731 (14)	0.0150 (4)
O1A	0.2471 (3)	0.1792 (2)	0.63192 (14)	0.0147 (4)
O2B	0.1477 (3)	0.6740 (3)	0.87712 (15)	0.0214 (5)
N1A	0.2871 (3)	0.0338 (3)	0.49857 (16)	0.0123 (5)
H1A	0.3172	0.1153	0.5364	0.015*
N1B	0.2302 (3)	0.5248 (3)	0.98489 (17)	0.0135 (5)
H1B	0.2219	0.5096	0.9281	0.016*
C6A	0.0819 (4)	−0.0724 (3)	0.57465 (19)	0.0119 (6)
C8A	0.3768 (3)	0.0384 (3)	0.43409 (19)	0.0130 (6)
C2A	0.0318 (4)	0.0563 (3)	0.69823 (19)	0.0146 (6)
H2A	0.0564	0.1423	0.7392	0.018*
C7A	0.1641 (4)	−0.0786 (3)	0.50788 (19)	0.0126 (6)
H7A	0.1287	−0.1683	0.4681	0.015*
C9A	0.3520 (4)	−0.0831 (4)	0.3737 (2)	0.0161 (6)
H9A	0.2712	−0.1757	0.3741	0.019*
C1A	0.1262 (3)	0.0614 (3)	0.63542 (19)	0.0122 (6)
C13A	0.4973 (4)	0.1755 (3)	0.43428 (19)	0.0140 (6)
C12A	0.5898 (4)	0.1900 (4)	0.3723 (2)	0.0175 (6)
H12A	0.6704	0.2823	0.3713	0.021*
C6B	0.3353 (4)	0.3439 (3)	0.98874 (19)	0.0128 (6)
C4A	−0.1357 (4)	−0.2007 (3)	0.6417 (2)	0.0158 (6)
H4A	−0.2226	−0.2875	0.6448	0.019*
C5A	−0.0490 (4)	−0.2005 (3)	0.5798 (2)	0.0148 (6)

H5A	−0.0771	−0.2881	0.5394	0.018*
C2B	0.3820 (4)	0.2177 (3)	0.8629 (2)	0.0153 (6)
H2B	0.3789	0.1999	0.8023	0.018*
C10A	0.4462 (4)	−0.0686 (4)	0.3128 (2)	0.0195 (7)
H10A	0.4308	−0.1516	0.2719	0.023*
C7B	0.2878 (4)	0.4476 (3)	1.0288 (2)	0.0150 (6)
H7B	0.2982	0.4616	1.0902	0.018*
C11A	0.5626 (4)	0.0670 (4)	0.3116 (2)	0.0199 (7)
H11A	0.6247	0.0763	0.2688	0.024*
C1B	0.3269 (3)	0.3208 (3)	0.89657 (19)	0.0126 (6)
C3A	−0.0941 (4)	−0.0702 (4)	0.7008 (2)	0.0150 (6)
H3A	−0.1548	−0.0699	0.7435	0.018*
C8B	0.1798 (4)	0.6305 (3)	1.0193 (2)	0.0156 (6)
C9B	0.1697 (4)	0.6556 (4)	1.1058 (2)	0.0194 (7)
H9B	0.1983	0.6011	1.1452	0.023*
C3B	0.4400 (4)	0.1430 (4)	0.9168 (2)	0.0186 (7)
H3B	0.4768	0.0752	0.8925	0.022*
C5B	0.3953 (4)	0.2647 (3)	1.0420 (2)	0.0174 (6)
H5B	0.4005	0.2810	1.1029	0.021*
C13B	0.1358 (4)	0.7097 (4)	0.9603 (2)	0.0176 (6)
C4B	0.4460 (4)	0.1646 (4)	1.0069 (2)	0.0204 (7)
H4B	0.4846	0.1108	1.0428	0.024*
C10B	0.1178 (4)	0.7604 (4)	1.1341 (2)	0.0246 (8)
H10B	0.1101	0.7776	1.1930	0.029*
C14A	0.6461 (4)	0.4226 (4)	0.5090 (2)	0.0246 (8)
H14A	0.6325	0.4646	0.4570	0.037*
H14B	0.7465	0.4090	0.5165	0.037*
H14C	0.6505	0.4885	0.5605	0.037*
C12B	0.0854 (4)	0.8158 (4)	0.9899 (2)	0.0228 (7)
H12B	0.0568	0.8710	0.9510	0.027*
C11B	0.0772 (4)	0.8402 (4)	1.0765 (3)	0.0254 (8)
H11B	0.0432	0.9128	1.0966	0.030*
C14B	0.0805 (5)	0.7343 (4)	0.8123 (2)	0.0246 (7)
H14D	0.0861	0.6931	0.7546	0.037*
H14E	0.1414	0.8403	0.8245	0.037*
H14F	−0.0323	0.7110	0.8134	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01692 (6)	0.01312 (6)	0.01094 (6)	0.00545 (5)	0.00344 (4)	0.00119 (4)
Cl2	0.0208 (4)	0.0204 (4)	0.0215 (4)	0.0104 (3)	0.0002 (3)	−0.0001 (3)
Cl1	0.0166 (4)	0.0301 (4)	0.0151 (4)	0.0023 (3)	0.0043 (3)	0.0045 (3)
O2A	0.0194 (12)	0.0133 (11)	0.0176 (11)	0.0030 (9)	0.0098 (9)	−0.0001 (9)
O1B	0.0189 (11)	0.0184 (11)	0.0122 (10)	0.0115 (9)	0.0051 (8)	0.0041 (8)
O1A	0.0141 (10)	0.0109 (10)	0.0167 (11)	0.0028 (8)	0.0056 (8)	−0.0009 (8)
O2B	0.0288 (13)	0.0255 (13)	0.0175 (12)	0.0180 (11)	0.0066 (10)	0.0067 (10)
N1A	0.0127 (12)	0.0130 (12)	0.0108 (12)	0.0058 (10)	0.0030 (9)	−0.0007 (9)

N1B	0.0153 (12)	0.0159 (13)	0.0112 (12)	0.0085 (10)	0.0043 (10)	0.0006 (10)
C6A	0.0123 (14)	0.0123 (14)	0.0111 (13)	0.0053 (11)	0.0025 (11)	0.0015 (11)
C8A	0.0107 (13)	0.0192 (15)	0.0110 (13)	0.0080 (12)	0.0034 (11)	0.0028 (11)
C2A	0.0149 (14)	0.0160 (15)	0.0126 (14)	0.0065 (12)	0.0037 (11)	0.0004 (11)
C7A	0.0140 (14)	0.0118 (14)	0.0117 (13)	0.0062 (11)	0.0016 (11)	0.0001 (11)
C9A	0.0129 (14)	0.0191 (15)	0.0148 (14)	0.0066 (12)	0.0021 (11)	−0.0004 (12)
C1A	0.0116 (13)	0.0135 (14)	0.0121 (13)	0.0060 (11)	0.0020 (11)	0.0025 (11)
C13A	0.0142 (14)	0.0169 (15)	0.0121 (14)	0.0083 (12)	0.0022 (11)	0.0013 (11)
C12A	0.0153 (15)	0.0217 (16)	0.0173 (15)	0.0082 (13)	0.0061 (12)	0.0051 (12)
C6B	0.0116 (13)	0.0147 (14)	0.0131 (14)	0.0056 (11)	0.0048 (11)	0.0038 (11)
C4A	0.0138 (14)	0.0146 (15)	0.0170 (15)	0.0034 (12)	0.0042 (12)	0.0043 (12)
C5A	0.0142 (14)	0.0118 (14)	0.0155 (15)	0.0035 (12)	0.0021 (12)	0.0004 (11)
C2B	0.0167 (15)	0.0161 (15)	0.0131 (14)	0.0068 (12)	0.0052 (12)	0.0008 (11)
C10A	0.0192 (16)	0.0261 (17)	0.0136 (15)	0.0118 (14)	0.0034 (12)	−0.0027 (13)
C7B	0.0146 (14)	0.0182 (15)	0.0106 (13)	0.0055 (12)	0.0032 (11)	0.0010 (11)
C11A	0.0186 (16)	0.0299 (19)	0.0145 (15)	0.0130 (14)	0.0063 (12)	0.0029 (13)
C1B	0.0110 (13)	0.0127 (14)	0.0134 (14)	0.0041 (11)	0.0035 (11)	0.0020 (11)
C3A	0.0152 (15)	0.0194 (16)	0.0124 (14)	0.0081 (13)	0.0046 (12)	0.0045 (12)
C8B	0.0133 (14)	0.0163 (15)	0.0172 (15)	0.0075 (12)	0.0032 (12)	−0.0011 (12)
C9B	0.0155 (15)	0.0248 (17)	0.0165 (15)	0.0098 (13)	0.0018 (12)	−0.0033 (13)
C3B	0.0209 (16)	0.0155 (15)	0.0212 (17)	0.0100 (13)	0.0051 (13)	0.0016 (13)
C5B	0.0194 (16)	0.0177 (15)	0.0138 (15)	0.0061 (13)	0.0036 (12)	0.0043 (12)
C13B	0.0144 (15)	0.0178 (16)	0.0204 (16)	0.0070 (13)	0.0045 (12)	0.0012 (12)
C4B	0.0248 (17)	0.0180 (16)	0.0218 (16)	0.0120 (14)	0.0037 (13)	0.0085 (13)
C10B	0.0193 (17)	0.0309 (19)	0.0206 (17)	0.0121 (15)	0.0022 (13)	−0.0087 (14)
C14A	0.0262 (18)	0.0151 (16)	0.0260 (18)	−0.0002 (14)	0.0126 (15)	0.0010 (13)
C12B	0.0191 (17)	0.0186 (17)	0.0302 (19)	0.0097 (14)	0.0031 (14)	0.0003 (14)
C11B	0.0204 (17)	0.0234 (18)	0.0296 (19)	0.0108 (15)	0.0028 (14)	−0.0073 (15)
C14B	0.0303 (19)	0.0247 (18)	0.0235 (18)	0.0152 (15)	0.0054 (14)	0.0105 (14)

Geometric parameters (Å, º)

Hg1—Cl2	2.3693 (8)	C4A—H4A	0.9500
Hg1—Cl1	2.3709 (8)	C4A—C5A	1.369 (4)
Hg1—O1B	2.356 (2)	C4A—C3A	1.407 (4)
Hg1—O1A	2.359 (2)	C5A—H5A	0.9500
O2A—C13A	1.363 (4)	C2B—H2B	0.9500
O2A—C14A	1.432 (4)	C2B—C1B	1.421 (4)
O1B—C1B	1.302 (4)	C2B—C3B	1.377 (4)
O1A—C1A	1.299 (4)	C10A—H10A	0.9500
O2B—C13B	1.361 (4)	C10A—C11A	1.387 (5)
O2B—C14B	1.427 (4)	C7B—H7B	0.9500
N1A—H1A	0.8800	C11A—H11A	0.9500
N1A—C8A	1.415 (4)	C3A—H3A	0.9500
N1A—C7A	1.308 (4)	C8B—C9B	1.391 (4)
N1B—H1B	0.8800	C8B—C13B	1.406 (5)
N1B—C7B	1.305 (4)	C9B—H9B	0.9500
N1B—C8B	1.416 (4)	C9B—C10B	1.387 (5)

C6A—C7A	1.413 (4)	C3B—H3B	0.9500
C6A—C1A	1.442 (4)	C3B—C4B	1.409 (5)
C6A—C5A	1.417 (4)	C5B—H5B	0.9500
C8A—C9A	1.389 (4)	C5B—C4B	1.374 (5)
C8A—C13A	1.407 (4)	C13B—C12B	1.394 (4)
C2A—H2A	0.9500	C4B—H4B	0.9500
C2A—C1A	1.424 (4)	C10B—H10B	0.9500
C2A—C3A	1.372 (4)	C10B—C11B	1.385 (6)
C7A—H7A	0.9500	C14A—H14A	0.9800
C9A—H9A	0.9500	C14A—H14B	0.9800
C9A—C10A	1.389 (4)	C14A—H14C	0.9800
C13A—C12A	1.393 (4)	C12B—H12B	0.9500
C12A—H12A	0.9500	C12B—C11B	1.386 (5)
C12A—C11A	1.397 (5)	C11B—H11B	0.9500
C6B—C7B	1.415 (4)	C14B—H14D	0.9800
C6B—C1B	1.437 (4)	C14B—H14E	0.9800
C6B—C5B	1.417 (4)	C14B—H14F	0.9800

Cl2—Hg1—Cl1	148.23 (3)	C11A—C10A—C9A	120.1 (3)
O1B—Hg1—Cl2	100.65 (6)	C11A—C10A—H10A	119.9
O1B—Hg1—Cl1	98.78 (6)	N1B—C7B—C6B	122.7 (3)
O1B—Hg1—O1A	105.56 (7)	N1B—C7B—H7B	118.6
O1A—Hg1—Cl2	100.40 (6)	C6B—C7B—H7B	118.6
O1A—Hg1—Cl1	98.27 (6)	C12A—C11A—H11A	119.5
C13A—O2A—C14A	117.3 (3)	C10A—C11A—C12A	120.9 (3)
C1B—O1B—Hg1	125.42 (19)	C10A—C11A—H11A	119.5
C1A—O1A—Hg1	124.97 (19)	O1B—C1B—C6B	120.3 (3)
C13B—O2B—C14B	117.0 (3)	O1B—C1B—C2B	122.5 (3)
C8A—N1A—H1A	116.5	C2B—C1B—C6B	117.1 (3)
C7A—N1A—H1A	116.5	C2A—C3A—C4A	121.7 (3)
C7A—N1A—C8A	126.9 (3)	C2A—C3A—H3A	119.2
C7B—N1B—H1B	116.7	C4A—C3A—H3A	119.2
C7B—N1B—C8B	126.6 (3)	C9B—C8B—N1B	123.3 (3)
C8B—N1B—H1B	116.7	C9B—C8B—C13B	120.3 (3)
C7A—C6A—C1A	121.4 (3)	C13B—C8B—N1B	116.3 (3)
C7A—C6A—C5A	118.5 (3)	C8B—C9B—H9B	120.2
C5A—C6A—C1A	120.1 (3)	C10B—C9B—C8B	119.7 (3)
C9A—C8A—N1A	123.5 (3)	C10B—C9B—H9B	120.2
C9A—C8A—C13A	120.4 (3)	C2B—C3B—H3B	119.1
C13A—C8A—N1A	116.1 (3)	C2B—C3B—C4B	121.7 (3)
C1A—C2A—H2A	119.3	C4B—C3B—H3B	119.1
C3A—C2A—H2A	119.3	C6B—C5B—H5B	119.5
C3A—C2A—C1A	121.3 (3)	C4B—C5B—C6B	120.9 (3)
N1A—C7A—C6A	122.8 (3)	C4B—C5B—H5B	119.5
N1A—C7A—H7A	118.6	O2B—C13B—C8B	115.2 (3)
C6A—C7A—H7A	118.6	O2B—C13B—C12B	125.5 (3)
C8A—C9A—H9A	120.2	C12B—C13B—C8B	119.3 (3)
C10A—C9A—C8A	119.6 (3)	C3B—C4B—H4B	120.5

C10A—C9A—H9A	120.2	C5B—C4B—C3B	119.0 (3)
O1A—C1A—C6A	120.6 (3)	C5B—C4B—H4B	120.5
O1A—C1A—C2A	122.8 (3)	C9B—C10B—H10B	120.0
C2A—C1A—C6A	116.7 (3)	C11B—C10B—C9B	120.0 (3)
O2A—C13A—C8A	114.7 (3)	C11B—C10B—H10B	120.0
O2A—C13A—C12A	125.5 (3)	O2A—C14A—H14A	109.5
C12A—C13A—C8A	119.8 (3)	O2A—C14A—H14B	109.5
C13A—C12A—H12A	120.4	O2A—C14A—H14C	109.5
C13A—C12A—C11A	119.1 (3)	H14A—C14A—H14B	109.5
C11A—C12A—H12A	120.4	H14A—C14A—H14C	109.5
C7B—C6B—C1B	121.3 (3)	H14B—C14A—H14C	109.5
C7B—C6B—C5B	118.4 (3)	C13B—C12B—H12B	120.2
C5B—C6B—C1B	120.3 (3)	C11B—C12B—C13B	119.6 (3)
C5A—C4A—H4A	120.5	C11B—C12B—H12B	120.2
C5A—C4A—C3A	119.0 (3)	C10B—C11B—C12B	121.0 (3)
C3A—C4A—H4A	120.5	C10B—C11B—H11B	119.5
C6A—C5A—H5A	119.4	C12B—C11B—H11B	119.5
C4A—C5A—C6A	121.3 (3)	O2B—C14B—H14D	109.5
C4A—C5A—H5A	119.4	O2B—C14B—H14E	109.5
C1B—C2B—H2B	119.5	O2B—C14B—H14F	109.5
C3B—C2B—H2B	119.5	H14D—C14B—H14E	109.5
C3B—C2B—C1B	120.9 (3)	H14D—C14B—H14F	109.5
C9A—C10A—H10A	119.9	H14E—C14B—H14F	109.5

Hg1—O1B—C1B—C6B	164.0 (2)	C5A—C6A—C1A—C2A	−0.5 (4)
Hg1—O1B—C1B—C2B	−16.4 (4)	C5A—C4A—C3A—C2A	−0.6 (5)
Hg1—O1A—C1A—C6A	166.7 (2)	C2B—C3B—C4B—C5B	−1.1 (5)
Hg1—O1A—C1A—C2A	−13.6 (4)	C7B—N1B—C8B—C9B	−7.0 (5)
O2A—C13A—C12A—C11A	178.4 (3)	C7B—N1B—C8B—C13B	174.3 (3)
O2B—C13B—C12B—C11B	179.3 (3)	C7B—C6B—C1B—O1B	−2.3 (4)
N1A—C8A—C9A—C10A	−179.8 (3)	C7B—C6B—C1B—C2B	178.0 (3)
N1A—C8A—C13A—O2A	1.4 (4)	C7B—C6B—C5B—C4B	−178.8 (3)
N1A—C8A—C13A—C12A	−179.2 (3)	C1B—C6B—C7B—N1B	1.9 (5)
N1B—C8B—C9B—C10B	−179.4 (3)	C1B—C6B—C5B—C4B	−0.1 (5)
N1B—C8B—C13B—O2B	−0.1 (4)	C1B—C2B—C3B—C4B	0.5 (5)
N1B—C8B—C13B—C12B	−179.8 (3)	C3A—C2A—C1A—O1A	−179.3 (3)
C8A—N1A—C7A—C6A	−179.9 (3)	C3A—C2A—C1A—C6A	0.5 (4)
C8A—C9A—C10A—C11A	−0.9 (5)	C3A—C4A—C5A—C6A	0.5 (5)
C8A—C13A—C12A—C11A	−0.9 (5)	C8B—N1B—C7B—C6B	180.0 (3)
C7A—N1A—C8A—C9A	−4.8 (5)	C8B—C9B—C10B—C11B	−0.4 (5)
C7A—N1A—C8A—C13A	175.9 (3)	C8B—C13B—C12B—C11B	−0.9 (5)
C7A—C6A—C1A—O1A	−2.3 (4)	C9B—C8B—C13B—O2B	−178.8 (3)
C7A—C6A—C1A—C2A	178.0 (3)	C9B—C8B—C13B—C12B	1.4 (5)
C7A—C6A—C5A—C4A	−178.5 (3)	C9B—C10B—C11B—C12B	0.9 (6)
C9A—C8A—C13A—O2A	−177.9 (3)	C3B—C2B—C1B—O1B	−179.3 (3)
C9A—C8A—C13A—C12A	1.5 (5)	C3B—C2B—C1B—C6B	0.4 (4)
C9A—C10A—C11A—C12A	1.4 (5)	C5B—C6B—C7B—N1B	−179.5 (3)
C1A—C6A—C7A—N1A	2.1 (5)	C5B—C6B—C1B—O1B	179.1 (3)

C1A—C6A—C5A—C4A	0.0 (5)	C5B—C6B—C1B—C2B	−0.5 (4)
C1A—C2A—C3A—C4A	0.1 (5)	C13B—C8B—C9B—C10B	−0.8 (5)
C13A—C8A—C9A—C10A	−0.6 (5)	C13B—C12B—C11B—C10B	−0.2 (5)
C13A—C12A—C11A—C10A	−0.5 (5)	C14A—O2A—C13A—C8A	172.4 (3)
C6B—C5B—C4B—C3B	1.0 (5)	C14A—O2A—C13A—C12A	−6.9 (5)
C5A—C6A—C7A—N1A	−179.4 (3)	C14B—O2B—C13B—C8B	170.3 (3)
C5A—C6A—C1A—O1A	179.2 (3)	C14B—O2B—C13B—C12B	−9.9 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O1*A*	0.88	1.89	2.599 (3)	137
N1*B*—H1*B*···O1*B*	0.88	1.87	2.585 (3)	137
C7*A*—H7*A*···Cl2^{i}	0.95	2.80	3.719 (3)	163
C7*B*—H7*B*···Cl1^{ii}	0.95	2.74	3.656 (3)	163

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

Diiodidobis(2-{(*E*)-[(2-methoxyphenyl)azaniumylidene]methyl}phenolato-*κO*)mercury(II) (Compound_6)

Crystal data

$[HgI_2(C_{28}H_{26}N_2O_4)]$
M_r = 908.90
Triclinic, $P\overline{1}$
a = 9.2783 (14) Å
b = 10.0060 (15) Å
c = 16.695 (3) Å
α = 98.777 (1)°
β = 100.296 (1)°
γ = 109.396 (1)°
V = 1400.4 (4) Å^3
Z = 2
F(000) = 852
D_x = 2.155 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9897 reflections
θ = 4.4–54.9°
μ = 7.74 mm^{-1}
T = 100 K
Block, orange
0.38 × 0.19 × 0.13 mm

Data collection

Bruker APEXII area detector diffractometer
Radiation source: standard sealed X-ray tube, Siemens, KFF Mo 2K -90 C
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and *φ* scans
Absorption correction: multi-scan (TWINABS; Bruker, 2012)
T_{min} = 0.441, T_{max} = 0.746
11185 measured reflections
11185 independent reflections
10132 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −12→12
k = −12→12
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.112
S = 1.08
11185 reflections
337 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0782P)^2 + 0.6965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.78 e Å^{-3}

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. The structure was solved as a rotational twin. Rotated from first domain by 149.8 degrees about reciprocal axis 1.000 0.235 0.787 and real axis 1.000 0.533 0.319. Twin law to convert hkl from first to this domain (SHELXL TWIN matrix) 0.534 0.949 0.308, 0.116 -0.693 0.359, 1.269 -0.145 -0.569.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.6673 (8)	0.6731 (7)	0.1093 (4)	0.0127 (13)
C1B	0.8585 (8)	0.9260 (7)	0.3661 (4)	0.0125 (13)
C2A	0.6036 (9)	0.7737 (8)	0.1421 (4)	0.0174 (14)
H2A	0.6028	0.7890	0.1996	0.021*
C2B	0.9490 (8)	0.9298 (8)	0.3052 (4)	0.0149 (13)
H2B	0.9249	0.8450	0.2630	0.018*
C3A	0.5431 (8)	0.8495 (8)	0.0928 (4)	0.0169 (15)
H3A	0.5022	0.9168	0.1171	0.020*
C3B	1.0718 (8)	1.0564 (8)	0.3071 (4)	0.0152 (14)
H3B	1.1330	1.0555	0.2672	0.018*
C4A	0.5396 (9)	0.8304 (8)	0.0060 (5)	0.0190 (16)
H4A	0.4963	0.8832	−0.0274	0.023*
C4B	1.1086 (9)	1.1864 (8)	0.3666 (5)	0.0171 (16)
H4B	1.1906	1.2730	0.3654	0.020*
C5A	0.5999 (9)	0.7349 (8)	−0.0278 (4)	0.0180 (15)
H5A	0.5998	0.7224	−0.0854	0.022*
C5B	1.0261 (8)	1.1863 (7)	0.4251 (4)	0.0142 (14)
H5B	1.0525	1.2735	0.4659	0.017*
C6A	0.6634 (8)	0.6528 (8)	0.0212 (4)	0.0143 (14)
C6B	0.9001 (8)	1.0591 (7)	0.4277 (4)	0.0135 (13)
C7A	0.7163 (8)	0.5513 (7)	−0.0189 (4)	0.0134 (13)
H7A	0.7096	0.5419	−0.0770	0.016*
C7B	0.8215 (8)	1.0664 (7)	0.4921 (4)	0.0124 (13)
H7B	0.8552	1.1565	0.5315	0.015*
C8A	0.8298 (8)	0.3650 (8)	−0.0185 (4)	0.0156 (14)
C8B	0.6225 (8)	0.9598 (8)	0.5647 (4)	0.0129 (13)
C9A	0.8442 (8)	0.3500 (8)	−0.1012 (4)	0.0165 (14)
H9A	0.8185	0.4122	−0.1340	0.020*
C9B	0.6492 (8)	1.0855 (8)	0.6224 (4)	0.0165 (14)
H9B	0.7256	1.1750	0.6203	0.020*
C10A	0.8962 (9)	0.2439 (9)	−0.1351 (5)	0.0247 (17)
H10A	0.9060	0.2333	−0.1912	0.030*
C10B	0.5643 (9)	1.0816 (8)	0.6839 (4)	0.0179 (15)
H10B	0.5808	1.1681	0.7230	0.022*
C11A	0.9336 (10)	0.1536 (9)	−0.0865 (5)	0.0259 (18)
H11A	0.9694	0.0815	−0.1099	0.031*

C11B	0.4558 (9)	0.9494 (8)	0.6866 (4)	0.0179 (15)
H11B	0.4002	0.9453	0.7293	0.022*
C12A	0.9197 (9)	0.1665 (9)	−0.0045 (5)	0.0225 (16)
H12A	0.9452	0.1034	0.0278	0.027*
C12B	0.4262 (9)	0.8216 (8)	0.6279 (5)	0.0183 (15)
H12B	0.3498	0.7323	0.6303	0.022*
C13A	0.8680 (8)	0.2727 (8)	0.0302 (5)	0.0156 (14)
C13B	0.5088 (8)	0.8260 (8)	0.5663 (4)	0.0150 (14)
C14A	0.8940 (10)	0.2095 (8)	0.1624 (5)	0.0227 (17)
H14A	0.8269	0.1069	0.1389	0.034*
H14B	0.8797	0.2400	0.2182	0.034*
H14C	1.0046	0.2219	0.1667	0.034*
C14B	0.3629 (9)	0.5751 (8)	0.5007 (5)	0.0227 (16)
H14D	0.2643	0.5922	0.4983	0.034*
H14E	0.3874	0.5375	0.5502	0.034*
H14F	0.3513	0.5040	0.4503	0.034*
Hg1	0.69274 (3)	0.57222 (3)	0.28950 (2)	0.01351 (9)
I1	0.38080 (6)	0.46487 (6)	0.26379 (3)	0.01957 (13)
I2	0.95749 (6)	0.53212 (5)	0.34679 (3)	0.01950 (13)
N1A	0.7749 (7)	0.4679 (6)	0.0195 (4)	0.0150 (12)
H1A	0.7800	0.4773	0.0734	0.018*
N1B	0.7048 (7)	0.9565 (6)	0.5009 (4)	0.0136 (11)
H1B	0.6748	0.8735	0.4641	0.016*
O1A	0.7251 (6)	0.5993 (5)	0.1535 (3)	0.0156 (10)
O1B	0.7437 (6)	0.8100 (5)	0.3671 (3)	0.0162 (10)
O2A	0.8515 (7)	0.2962 (6)	0.1094 (3)	0.0223 (12)
O2B	0.4891 (6)	0.7101 (5)	0.5057 (3)	0.0186 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.008 (3)	0.012 (3)	0.018 (3)	0.004 (3)	0.002 (3)	0.004 (3)
C1B	0.012 (3)	0.012 (3)	0.017 (3)	0.006 (3)	0.005 (3)	0.007 (3)
C2A	0.019 (4)	0.018 (3)	0.016 (3)	0.009 (3)	0.005 (3)	0.000 (3)
C2B	0.017 (3)	0.017 (3)	0.014 (3)	0.010 (3)	0.006 (3)	0.003 (3)
C3A	0.015 (3)	0.012 (3)	0.018 (3)	0.005 (3)	−0.001 (3)	−0.007 (3)
C3B	0.012 (3)	0.022 (4)	0.013 (3)	0.007 (3)	0.005 (3)	0.005 (3)
C4A	0.017 (4)	0.012 (3)	0.022 (4)	0.003 (3)	0.000 (3)	0.001 (3)
C4B	0.019 (4)	0.017 (4)	0.021 (4)	0.008 (3)	0.012 (3)	0.012 (3)
C5A	0.024 (4)	0.016 (3)	0.014 (3)	0.007 (3)	0.006 (3)	0.004 (3)
C5B	0.017 (3)	0.010 (3)	0.011 (3)	0.003 (3)	0.001 (3)	0.000 (3)
C6A	0.016 (3)	0.014 (3)	0.013 (3)	0.006 (3)	0.001 (3)	0.005 (3)
C6B	0.015 (3)	0.012 (3)	0.010 (3)	0.004 (3)	−0.002 (3)	0.001 (2)
C7A	0.013 (3)	0.013 (3)	0.013 (3)	0.001 (3)	0.006 (3)	0.002 (3)
C7B	0.009 (3)	0.009 (3)	0.015 (3)	0.001 (3)	−0.001 (3)	0.001 (3)
C8A	0.018 (4)	0.016 (3)	0.014 (3)	0.008 (3)	0.005 (3)	0.000 (3)
C8B	0.011 (3)	0.015 (3)	0.015 (3)	0.007 (3)	0.005 (3)	0.004 (3)
C9A	0.010 (3)	0.023 (4)	0.015 (3)	0.006 (3)	0.001 (3)	0.003 (3)

C9B	0.014 (3)	0.019 (4)	0.015 (3)	0.005 (3)	0.004 (3)	0.002 (3)
C10A	0.014 (4)	0.035 (5)	0.017 (4)	0.009 (3)	−0.003 (3)	−0.009 (3)
C10B	0.017 (4)	0.019 (4)	0.017 (3)	0.010 (3)	0.003 (3)	−0.004 (3)
C11A	0.026 (4)	0.025 (4)	0.028 (4)	0.019 (4)	0.001 (3)	−0.003 (3)
C11B	0.016 (4)	0.021 (4)	0.017 (3)	0.008 (3)	0.004 (3)	0.003 (3)
C12A	0.023 (4)	0.022 (4)	0.024 (4)	0.013 (3)	0.002 (3)	0.002 (3)
C12B	0.016 (4)	0.028 (4)	0.014 (3)	0.009 (3)	0.007 (3)	0.008 (3)
C13A	0.013 (3)	0.014 (3)	0.023 (4)	0.011 (3)	0.002 (3)	0.003 (3)
C13B	0.016 (3)	0.018 (3)	0.010 (3)	0.008 (3)	0.000 (3)	0.001 (3)
C14A	0.030 (4)	0.022 (4)	0.020 (4)	0.014 (3)	0.002 (3)	0.009 (3)
C14B	0.024 (4)	0.016 (4)	0.023 (4)	0.000 (3)	0.008 (3)	0.003 (3)
Hg1	0.01544 (14)	0.01255 (14)	0.01221 (14)	0.00467 (11)	0.00395 (9)	0.00241 (10)
I1	0.0150 (2)	0.0260 (3)	0.0142 (2)	0.0019 (2)	0.00385 (18)	0.0070 (2)
I2	0.0182 (3)	0.0166 (2)	0.0215 (3)	0.0077 (2)	0.00010 (19)	0.00114 (19)
N1A	0.017 (3)	0.013 (3)	0.016 (3)	0.007 (3)	0.005 (2)	0.004 (2)
N1B	0.016 (3)	0.013 (3)	0.013 (3)	0.009 (2)	0.004 (2)	−0.002 (2)
O1A	0.019 (3)	0.017 (3)	0.015 (2)	0.010 (2)	0.006 (2)	0.004 (2)
O1B	0.017 (3)	0.011 (2)	0.021 (3)	0.005 (2)	0.010 (2)	0.002 (2)
O2A	0.032 (3)	0.023 (3)	0.017 (3)	0.015 (2)	0.007 (2)	0.009 (2)
O2B	0.021 (3)	0.016 (2)	0.017 (3)	0.004 (2)	0.008 (2)	0.001 (2)

Geometric parameters (Å, º)

C1A—C2A	1.417 (10)	C8B—N1B	1.418 (9)
C1A—C6A	1.446 (9)	C9A—H9A	0.9500
C1A—O1A	1.290 (8)	C9A—C10A	1.391 (11)
C1B—C2B	1.427 (9)	C9B—H9B	0.9500
C1B—C6B	1.442 (9)	C9B—C10B	1.398 (10)
C1B—O1B	1.294 (8)	C10A—H10A	0.9500
C2A—H2A	0.9500	C10A—C11A	1.388 (12)
C2A—C3A	1.370 (10)	C10B—H10B	0.9500
C2B—H2B	0.9500	C10B—C11B	1.384 (10)
C2B—C3B	1.385 (10)	C11A—H11A	0.9500
C3A—H3A	0.9500	C11A—C12A	1.390 (12)
C3A—C4A	1.426 (11)	C11B—H11B	0.9500
C3B—H3B	0.9500	C11B—C12B	1.400 (11)
C3B—C4B	1.409 (11)	C12A—H12A	0.9500
C4A—H4A	0.9500	C12A—C13A	1.395 (10)
C4A—C5A	1.359 (11)	C12B—H12B	0.9500
C4B—H4B	0.9500	C12B—C13B	1.386 (10)
C4B—C5B	1.343 (10)	C13A—O2A	1.352 (9)
C5A—H5A	0.9500	C13B—O2B	1.355 (8)
C5A—C6A	1.430 (9)	C14A—H14A	0.9800
C5B—H5B	0.9500	C14A—H14B	0.9800
C5B—C6B	1.427 (9)	C14A—H14C	0.9800
C6A—C7A	1.401 (10)	C14A—O2A	1.424 (8)
C6B—C7B	1.408 (10)	C14B—H14D	0.9800
C7A—H7A	0.9500	C14B—H14E	0.9800

C7A—N1A	1.320 (9)	C14B—H14F	0.9800
C7B—H7B	0.9500	C14B—O2B	1.443 (8)
C7B—N1B	1.312 (9)	Hg1—I1	2.6580 (7)
C8A—C9A	1.400 (10)	Hg1—I2	2.6536 (7)
C8A—C13A	1.408 (10)	Hg1—O1A	2.387 (5)
C8A—N1A	1.410 (9)	Hg1—O1B	2.378 (5)
C8B—C9B	1.382 (10)	N1A—H1A	0.8800
C8B—C13B	1.411 (10)	N1B—H1B	0.8800
C2A—C1A—C6A	116.8 (6)	C10B—C9B—H9B	119.8
O1A—C1A—C2A	123.4 (6)	C9A—C10A—H10A	120.2
O1A—C1A—C6A	119.8 (6)	C11A—C10A—C9A	119.5 (7)
C2B—C1B—C6B	116.9 (6)	C11A—C10A—H10A	120.2
O1B—C1B—C2B	122.7 (6)	C9B—C10B—H10B	120.6
O1B—C1B—C6B	120.5 (6)	C11B—C10B—C9B	118.7 (7)
C1A—C2A—H2A	119.3	C11B—C10B—H10B	120.6
C3A—C2A—C1A	121.5 (7)	C10A—C11A—H11A	119.3
C3A—C2A—H2A	119.3	C10A—C11A—C12A	121.4 (7)
C1B—C2B—H2B	119.7	C12A—C11A—H11A	119.3
C3B—C2B—C1B	120.5 (7)	C10B—C11B—H11B	119.3
C3B—C2B—H2B	119.7	C10B—C11B—C12B	121.5 (7)
C2A—C3A—H3A	119.1	C12B—C11B—H11B	119.3
C2A—C3A—C4A	121.9 (7)	C11A—C12A—H12A	120.2
C4A—C3A—H3A	119.1	C11A—C12A—C13A	119.5 (7)
C2B—C3B—H3B	119.1	C13A—C12A—H12A	120.2
C2B—C3B—C4B	121.8 (7)	C11B—C12B—H12B	120.1
C4B—C3B—H3B	119.1	C13B—C12B—C11B	119.7 (7)
C3A—C4A—H4A	120.8	C13B—C12B—H12B	120.1
C5A—C4A—C3A	118.4 (7)	C12A—C13A—C8A	119.6 (7)
C5A—C4A—H4A	120.8	O2A—C13A—C8A	115.7 (6)
C3B—C4B—H4B	120.5	O2A—C13A—C12A	124.7 (7)
C5B—C4B—C3B	119.1 (7)	C12B—C13B—C8B	118.9 (7)
C5B—C4B—H4B	120.5	O2B—C13B—C8B	116.1 (6)
C4A—C5A—H5A	119.2	O2B—C13B—C12B	125.0 (7)
C4A—C5A—C6A	121.6 (7)	H14A—C14A—H14B	109.5
C6A—C5A—H5A	119.2	H14A—C14A—H14C	109.5
C4B—C5B—H5B	119.0	H14B—C14A—H14C	109.5
C4B—C5B—C6B	122.0 (7)	O2A—C14A—H14A	109.5
C6B—C5B—H5B	119.0	O2A—C14A—H14B	109.5
C5A—C6A—C1A	119.8 (6)	O2A—C14A—H14C	109.5
C7A—C6A—C1A	121.8 (6)	H14D—C14B—H14E	109.5
C7A—C6A—C5A	118.4 (6)	H14D—C14B—H14F	109.5
C5B—C6B—C1B	119.7 (6)	H14E—C14B—H14F	109.5
C7B—C6B—C1B	121.6 (6)	O2B—C14B—H14D	109.5
C7B—C6B—C5B	118.7 (6)	O2B—C14B—H14E	109.5
C6A—C7A—H7A	118.1	O2B—C14B—H14F	109.5
N1A—C7A—C6A	123.8 (6)	I2—Hg1—I1	145.097 (18)
N1A—C7A—H7A	118.1	O1A—Hg1—I1	102.05 (12)

C6B—C7B—H7B	118.0	O1A—Hg1—I2	98.69 (12)
N1B—C7B—C6B	124.1 (6)	O1B—Hg1—I1	98.64 (12)
N1B—C7B—H7B	118.0	O1B—Hg1—I2	102.36 (13)
C9A—C8A—C13A	120.0 (7)	O1B—Hg1—O1A	105.74 (16)
C9A—C8A—N1A	123.2 (6)	C7A—N1A—C8A	125.4 (6)
C13A—C8A—N1A	116.8 (6)	C7A—N1A—H1A	117.3
C9B—C8B—C13B	120.7 (6)	C8A—N1A—H1A	117.3
C9B—C8B—N1B	123.1 (6)	C7B—N1B—C8B	125.7 (6)
C13B—C8B—N1B	116.2 (6)	C7B—N1B—H1B	117.2
C8A—C9A—H9A	120.0	C8B—N1B—H1B	117.2
C10A—C9A—C8A	120.0 (7)	C1A—O1A—Hg1	125.7 (4)
C10A—C9A—H9A	120.0	C1B—O1B—Hg1	124.7 (4)
C8B—C9B—H9B	119.8	C13A—O2A—C14A	118.1 (6)
C8B—C9B—C10B	120.4 (7)	C13B—O2B—C14B	117.2 (6)

C1A—C2A—C3A—C4A	0.6 (11)	C9A—C8A—C13A—O2A	179.5 (6)
C1A—C6A—C7A—N1A	−0.8 (11)	C9A—C8A—N1A—C7A	7.1 (11)
C1B—C2B—C3B—C4B	−2.3 (10)	C9A—C10A—C11A—C12A	0.2 (12)
C1B—C6B—C7B—N1B	−1.2 (10)	C9B—C8B—C13B—C12B	−1.3 (10)
C2A—C1A—C6A—C5A	1.2 (10)	C9B—C8B—C13B—O2B	178.4 (6)
C2A—C1A—C6A—C7A	−177.0 (6)	C9B—C8B—N1B—C7B	5.1 (10)
C2A—C1A—O1A—Hg1	13.7 (9)	C9B—C10B—C11B—C12B	−2.1 (11)
C2A—C3A—C4A—C5A	−0.6 (11)	C10A—C11A—C12A—C13A	−0.4 (12)
C2B—C1B—C6B—C5B	0.4 (9)	C10B—C11B—C12B—C13B	1.2 (11)
C2B—C1B—C6B—C7B	−178.1 (6)	C11A—C12A—C13A—C8A	0.3 (11)
C2B—C1B—O1B—Hg1	13.4 (9)	C11A—C12A—C13A—O2A	−179.3 (7)
C2B—C3B—C4B—C5B	2.6 (11)	C11B—C12B—C13B—C8B	0.5 (10)
C3A—C4A—C5A—C6A	1.0 (11)	C11B—C12B—C13B—O2B	−179.2 (7)
C3B—C4B—C5B—C6B	−1.4 (11)	C12A—C13A—O2A—C14A	1.9 (11)
C4A—C5A—C6A—C1A	−1.3 (11)	C12B—C13B—O2B—C14B	5.8 (10)
C4A—C5A—C6A—C7A	176.9 (7)	C13A—C8A—C9A—C10A	0.0 (11)
C4B—C5B—C6B—C1B	−0.1 (10)	C13A—C8A—N1A—C7A	−171.6 (7)
C4B—C5B—C6B—C7B	178.5 (7)	C13B—C8B—C9B—C10B	0.4 (11)
C5A—C6A—C7A—N1A	−179.0 (7)	C13B—C8B—N1B—C7B	−175.2 (6)
C5B—C6B—C7B—N1B	−179.7 (6)	N1A—C8A—C9A—C10A	−178.6 (7)
C6A—C1A—C2A—C3A	−0.8 (10)	N1A—C8A—C13A—C12A	178.6 (7)
C6A—C1A—O1A—Hg1	−165.2 (5)	N1A—C8A—C13A—O2A	−1.8 (9)
C6A—C7A—N1A—C8A	−179.7 (6)	N1B—C8B—C9B—C10B	−179.9 (6)
C6B—C1B—C2B—C3B	0.8 (10)	N1B—C8B—C13B—C12B	179.0 (6)
C6B—C1B—O1B—Hg1	−166.9 (5)	N1B—C8B—C13B—O2B	−1.3 (9)
C6B—C7B—N1B—C8B	−179.7 (6)	O1A—C1A—C2A—C3A	−179.8 (7)
C8A—C9A—C10A—C11A	−0.1 (11)	O1A—C1A—C6A—C5A	−179.8 (6)
C8A—C13A—O2A—C14A	−177.7 (6)	O1A—C1A—C6A—C7A	2.1 (10)
C8B—C9B—C10B—C11B	1.3 (11)	O1B—C1B—C2B—C3B	−179.4 (6)
C8B—C13B—O2B—C14B	−174.0 (6)	O1B—C1B—C6B—C5B	−179.4 (6)
C9A—C8A—C13A—C12A	−0.1 (10)	O1B—C1B—C6B—C7B	2.1 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O1*A*	0.88	1.92	2.611 (8)	134
N1*B*—H1*B*···O1*B*	0.88	1.94	2.629 (7)	134

Dihedral angles (°) between the two least-squares planes of the aromatic rings of ligand L

Plane A consists of atoms C1–C6 and plane B consists of atoms C8–C13.

Structure	Ligand A	Ligand B
1	4.34	10.68
2	8.76	5.17
3	4.10	7.07
4	5.86	8.20
5	3.62	5.23
6	8.83	5.31