

## Supramolecular Self-Assembling of $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$ [ $\text{R} = \text{EtOC}(\text{O})$ ] through Reciprocal Metal- $\eta^2$ -arene $\pi$ -Interactions and Non Classical C–H $\cdots$ O Bonding: Synthesis and X-ray Characterization of a Bis Diaryl Symmetric-substituted Triazenido Complex Polymer of Hg(II)

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1,3-bis(4-etoxicarbonilfenil)triazeno desprotonado reage com  $\text{Hg}(\text{CH}_3\text{COO})_2$  em tetraidrofurano para formar cristais amarelos de  $\{[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]_2\}_n$  [ $\text{R} = \text{EtOC}(\text{O})$ ]. Os tectons  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$  encontram-se ligados aos pares como dímeros centro simétricos por meio de interações  $\pi$  recíprocas do tipo metal- $\eta^2$ -areno. As unidades dímeras relacionadas entre si através de um plano de reflexão-translação diagonal  $n$ , são operadas ao longo da direção cristalográfica [101] originando cadeias através de ligações de hidrogênio não clássicas C–H $\cdots$ (O)COEt envolvendo o grupamento *orto* C–H do ligante piridina. Estas cadeias por sua vez, relacionam-se entre si por translação na cela elementar através de um segundo tipo de ligação de hidrogênio não-clássica, esta envolvendo átomos de hidrogênio e oxigênio de grupos etoxicarbonilfenil adjacentes na direção cristalográfica [100], resultando um arranjo cristalino supramolecular (2D) estendido paralelo ao plano cristalográfico (011).

Deprotonated 1,3-bis(4-ethoxycarbonylphenyl)triazene reacts with  $\text{Hg}(\text{CH}_3\text{COO})_2$  in tetrahydrofuran to give light-yellow crystals of  $\{[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]_2\}_n$  [ $\text{R} = \text{EtOC}(\text{O})$ ]. The  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$  tectons are linked to pairs as centrosymmetric dimers through reciprocal metal- $\eta^2$ -arene  $\pi$ -interactions. The dimeric units – related to each other by a  $n$ -glide plane – are linked into chains along to the crystallographic direction [101] through non classical C–H $\cdots$ (O)COEt (hydrogen) bonds involving the *ortho* C–H group of the pyridine ligand. These chains are related by translation in the unit cell along the direction [100] through another kind of non classical hydrogen bonding, this one involving hydrogen and oxygen atoms of adjacent ethoxycarbonylphenyl groups of the same plane, resulting an extended supramolecular bidimensional (2D) assembling parallel to the crystallographic plane (011).

**Keywords:** triazenes, triazenido-complexes, supramolecular assembling of Hg complex-tectons, Hg- $\eta^2$ -arene  $\pi$ -interactions

### Introduction

Nowadays it is well known that secondary bonds or interactions can play a significant role in the structural assembling of a wide variety of compounds. These interactions present  $\sigma$  or  $\pi$  character, and have not been recognized in earlier works, in spite of their real existence. Organotellurium compounds, for example, in addition to secondary Te $\cdots$ halogen bonds, show mostly intermolecular bonds of the type Te $\cdots$  $\pi$ -aryl.<sup>1,2</sup> Crystallographic aspects of this complex type have been described in the literature, and although intermolecular interactions exist in almost all

the reported cases, they have not been mentioned by the authors,<sup>3-6</sup> especially the hydrogen bonds and the metal $\cdots$  $\pi$ -aryl interactions. This could be explained by the fact that only in recent years the real chemical significance of these selective, directional and strongly attractive noncovalent interactions, which can induce the self-assembly of predictable supramolecular aggregates, has become evident. The molecules which play the role of building blocks in a self-assembled, ordered supramolecular structure are called *tectons*.<sup>7-9</sup> According to S. Simard and co-workers,<sup>8</sup> a tecton (from Greek, *tekton*, builder) is defined as “any molecule whose interactions are dominated by particular associative forces that induce the self-assembly of an organized network with specific architectural or functional

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features". Supramolecular synthesis would be the design and construction of multicomponent supermolecules or supramolecular arrays utilizing non-covalent bonding of tectons.<sup>9</sup> The supramolecular synthesis successfully exploits hydrogen-bonding and other types of non-covalent interaction, in building supramolecular systems.<sup>9-11</sup>

Recently we have shown<sup>12,13</sup> that triazenide complexes of Hg(II) are tectons with a remarkably good ability to self-assemble of different manners through metal- $\eta$ -arene  $\pi$ -interactions: the synthesis of  $\{\text{Hg}[\text{PhN}_3\text{C}_6\text{H}_4\text{N}_3(\text{H})\text{Ph}](\text{NO}_3)\}$ <sup>14</sup> – a rare Hg(II) complex containing two phenyltriazenide chains – was one of the first evidences that in this complex type besides Metal–N bonds also metal-arene  $\pi$ -interactions perform a significant role in the architecture (or self-assembling) of the crystal lattice, in as much as the mentioned organotellurium compounds.

Aiming at the study of new self-assembling possibilities of systems involving symmetrical substituted triazenide chains and Hg(II), we report here on the successful achievement of a new sort of Hg- $\eta$ -arene dimerization by blocking one of the axial positions of the Hg(II) ion with pyridine, as well as the broadening of the supramolecular lattice through additional, non classical hydrogen bonding. Detailed analytical structural data, with emphasis on X-ray diffractometry of mono crystals will be also presented and discussed.

## Experimental

A single crystal fixed on a glass fiber was used for the X-ray data collection. Data were collected with a Bruker APEX II CCD area-detector diffractometer and graphite-monochromatized Mo- $K_\alpha$  radiation. The data reduction and the absorption correction were performed using *SAINTE*<sup>15</sup> and *SADABS*<sup>16</sup> programs, respectively. The structure of  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$  [ $\text{R} = \text{EtOC}(\text{O})$ ] was solved by direct methods<sup>17</sup> and refined on  $F^2$  with anisotropic temperature parameters for all non H atoms.<sup>18</sup> H atoms of the phenyl, methylene, and methyl groups were positioned geometrically ( $\text{C}-\text{H} = 0.93 \text{ \AA}$  for  $\text{Csp}^2$ ,  $0.96 \text{ \AA}$  ( $\text{CH}_3$ ) and  $0.97 \text{ \AA}$  ( $\text{CH}_2$ ) for  $\text{Csp}^3$  atoms) and treated as riding on their respective C atoms, with  $U_{\text{iso}}(\text{H})$  values set at  $1.2U_{\text{eq}}(\text{Csp}^2)$  and  $1.5U_{\text{eq}}(\text{Csp}^3)$ . The crystallographic parameters and details of data collection and refinement are given in Table 1.

*Preparation of  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]_2$  [ $\text{R} = \text{EtOC}(\text{O})$ ] bis{bis[1,3-bis(4-ethoxycarbonyl phenyl)triazenide]pyridinyl-mercury(II)}*

All manipulations were carried out under nitrogen by use of standard Schlenk techniques.

**Table 1.** Crystal and structure refinement data for  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$  [ $\text{R} = \text{EtOC}(\text{O})$ ]

Empirical formula	$\text{C}_{41}\text{H}_{41}\text{HgN}_7\text{O}_8$
Formula weight	960.40
T/(K)	293(2)
Radiation, $\lambda$ ( $\text{\AA}$ )	0.71073
Crystal system, space group	monoclinic, $2_1/n$
Unit cell dimensions, $a, b, c$ ( $\text{\AA}$ )	$a = 13.4624(2)$ $b = 11.4138(2)$ $c = 26.9974(5)$ $\beta = 97.6850(10)$
Volume/( $\text{\AA}^3$ )	4111.08(12)
Z, Calculated Density/( $\text{g cm}^{-3}$ )	4, 1.552
Absorption coefficient/( $\text{mm}^{-1}$ )	3.804
$F(000)$	1920
Crystal size (mm)	$0.32 \times 0.23 \times 0.21$
Theta range/( $^\circ$ )	$1.52 - 25.50^\circ$ .
Index ranges	$-16 \leq h \leq 16, -13 \leq k \leq 13, -32 \leq l \leq 32$
Reflections collected	45404
Independent reflections	7656 [ $R_{\text{int}} = 0.0255$ ]
Completeness to theta max.	100.0 %
Max. and min. transmission	0.5022 and 0.3757
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	7656 / 0 / 514
Goodness-of-fit on $F^2$	1.216
Final indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0260, wR_2 = 0.0896$
indices (all data)	$R_1 = 0.0382, wR_2 = 0.1260$
Largest diff. peak and hole/( $\text{e.\AA}^{-3}$ )	$1.04^*$ and $-1.67^*$

\*Highest peak:  $1.04 (\text{e.\AA}^{-3})$  at  $0.0604 \ 0.9309 \ 0.1310 [1.60 \text{ \AA} \text{ from H}(72\text{A})]$ ; \*Deepest hole:  $-1.67 (\text{e.\AA}^{-3})$  at  $0.8771 \ 0.3772 \ 0.0154 [1.20 \text{ \AA} \text{ from Hg}(1)]$ .

To a solution prepared by dissolving 0.06g (0.15 mmol) of 1,3-bis(4-ethoxycarbonylphenyl)triazene in 20 mL of a mixture of tetrahydrofuran / methanol (1:3), three drops of a saturated solution of potassium methanolate were added under stirring turning the color orange. A solution of 0.023 g (0.07 mmol) of  $\text{Hg}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$  in 10 mL of absolute methanol was added which caused a light-yellow precipitate. After 2 h stirring the yellow solid was separated by filtration, dried at room temperature and dissolved in 10 mL of a tetrahydrofuran / pyridine mixture 3:1. The slow evaporation of the solvent within a week leads to the formation of prismatic crystals suitable for X-ray analysis.

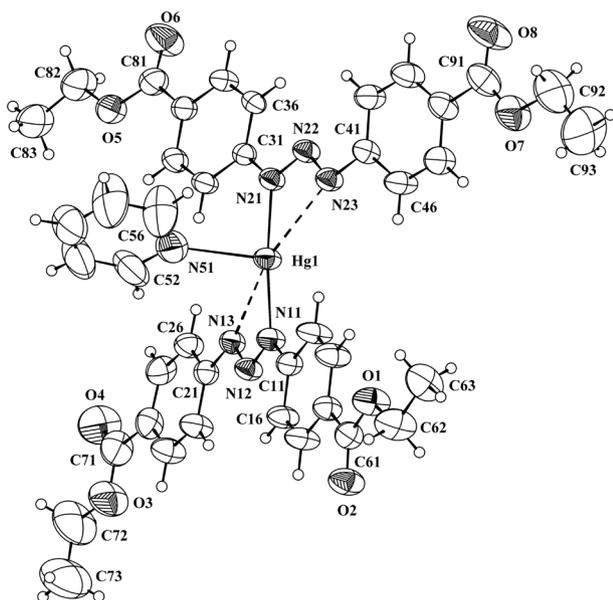
Properties: prismatic light-yellow crystalline substance.  $\text{C}_{41}\text{H}_{41}\text{HgN}_7\text{O}_8$  (960.40). Yield: 0.118g (0.123 mmol), 70% based on  $\text{Hg}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ . Melting point: 258-260  $^\circ\text{C}$ . C, H, N-analysis: calcd. C 51.27, H 4.30, N 10.21; found C 51.19, H 4.33, N 10.26.

IR (CsI) *free ligand* 1,3-bis(4-ethoxycarbonylphenyl) triazene:  $\nu_{\text{max}}/\text{cm}^{-1}$  2978 [m,  $\nu(\text{C}-\text{H})$ ] 3228 [s,  $\nu_{\text{as}}(\text{N}-\text{H})$ ], 1717 [vs,  $\nu(\text{C}=\text{O})$ ], 1609 [vs,  $\nu(\text{C}=\text{C})$ ], 1412 [s,  $\nu(\text{N}=\text{N})$ ], 1201 [s,  $\nu_{\text{s}}(\text{N}-\text{N})$ ], 853 [m,  $\nu(\text{C}-\text{N})$ ].

[Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py]<sub>2</sub> [R = C<sub>2</sub>H<sub>5</sub>OC(O)]: the N–H band is absent.  $\nu_{\max}$ /cm<sup>-1</sup> 2982 [m,  $\nu$ (C–H)], 1717 [vs,  $\nu$ (C=O)], 1599 [vs,  $\nu$ (C=C)], 1275 [vs,  $\nu_{\text{as}}$ (NNN)], a mean value with respect to the N–N absorptions in the free ligand (average bond order), 863 [s,  $\nu$ (C–N)]. Far infrared, FIR (CsI):  $\nu_{\max}$ /cm<sup>-1</sup> 591 [s,  $\nu$ (Hg–N)].

## Results and Discussion

Crystal data and experimental conditions are given in Table 1. Selected bond distances and angles of the title complex are listed in Table 2. Figure 1 shows the molecular structure of the tecton [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py] [R = EtOC(O)] in a thermal ellipsoid representation<sup>19</sup>. Figure 2 shows a section of the polymeric bidimensional lattice, linked through reciprocal secondary metal– $\eta^2$ ,  $\beta$ -arene  $\pi$ -interactions and C–H $\cdots$ O bonding (dashed lines).



**Figure 1.** Molecular structure with atom-labeling scheme of the tecton [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py] [R = EtOC(O)]. Displacement ellipsoids at the 50% level. Dashed lines represent secondary interactions.

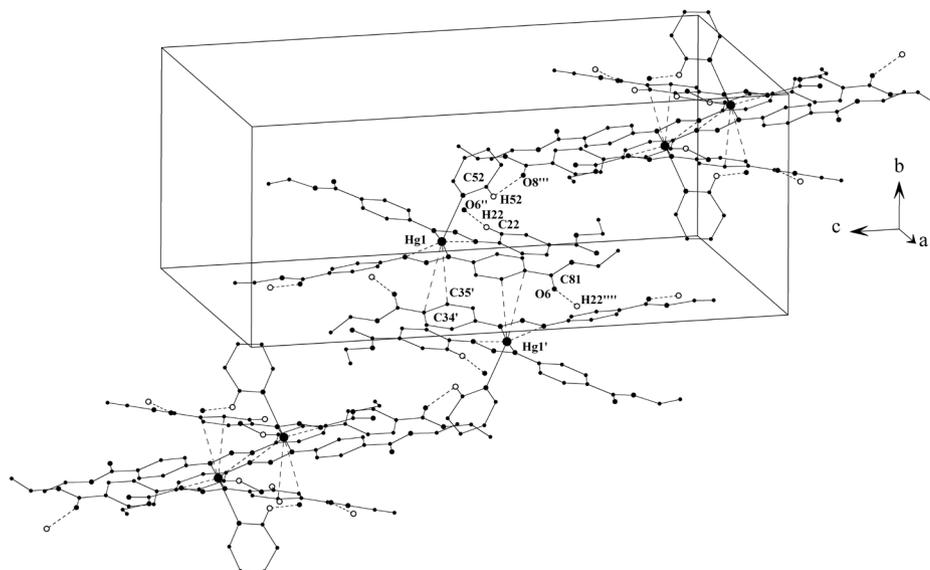
In a single tecton [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py] [R = EtOC(O)] the Hg(II) centre is planar coordinated by two triazenide ions through two primary, identical Hg–N bonds [Hg–N(11) = Hg–N(21) = 2.100(4) Å] and two secondary ones [Hg $\cdots$ N(13) = 2.718(3), Hg $\cdots$ N(23) = 2.753(4) Å]. The square pyramidal configuration of [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py] is achieved with a neutral pyridine ligand in the apical position [Hg–N(51) = 2.581(5) Å]. The Hg(II) ion is 0.258(2) Å out of the plane settled by the four coordinating nitrogen atoms. The pyridine ring attains with this plane an angle of 75.2(2)°. This appreciable deviation of the ideal interplanar angle (90°) can be viewed

as a consequence of the non classical C–H $\cdots$ (O)COEt (hydrogen) bonding involving the *ortho* C–H group of the pyridine ring [C(52) $\cdots$ O(8)'' = 3.130(8) Å, C(52)–H(52) = 0.93 Å, H(52) $\cdots$ O(8)''' = 2.53 Å, C(52)–H(52) $\cdots$ O8''' = 123°, symmetry code (''') –1/2+x, 1/2–y, –1/2+z]. The tectons [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py] [R = EtOC(O)] are linked to pairs as centrosymmetric dimers through reciprocal Hg–arene secondary interactions (see discussion later). The tectonic dimers, related by a *n*-glide plane, are linked into chains along to the crystallographic direction [101] through the intermolecular above mentioned C–H $\cdots$ (O)COEt bonding involving the *ortho* C–H group of the pyridine ring. On the other hand, these chains are related by translation in the unit cell along the direction [100] through another kind of non classical hydrogen bonding, involving hydrogen and oxygen atoms of adjacent ethoxycarbonylphenyl groups of the same plane [C(22) $\cdots$ O(6)'' = 3.384(6) Å, C(22)–H(22) = 0.93 Å, C(22)–H(22) $\cdots$ O6'' = 150°, symmetry code (') –1+x, y, z]. Thus an extended, supramolecular bidimensional (2D) assembling of the dimeric tectons through secondary interactions results parallel to the (011) plane, as indicated in Figure 2.

The  $\eta^2, \eta^2$  bonding phenyl rings are oriented parallel to the main molecular plane and coordinate the Hg atom in a  $\pi$  type of bonding. Two carbon atoms of the phenyl rings have remarkably short distances to the Hg(II) ion: these shorter secondary interactions are of 3.226(5) [Hg(1) $\cdots$ C(35)'] and 3.619(4) Å [Hg(1) $\cdots$ C(34)'], symmetry code (') 1–x, –y, 1–z. The distance of the  $\pi$ -interaction from Hg(1) to the midpoint of the C(34)′–C(35)′ bond is 3.54 Å, somewhat larger than the distance from the metallic ion to the midpoint of the C(31)′–C(36)′ bond [3.38 Å, symmetry code (') x, y–1, z] in {Hg[PhN<sub>3</sub>C<sub>6</sub>H<sub>4</sub>N<sub>3</sub>(H)Ph](NO<sub>3</sub>)},<sup>14</sup> but very close to the midpoint distance C(34)′–C(35)′ [3.51 Å, symmetry code (') –x+1, –y, –z] in the complex [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R')<sub>2</sub>Py]<sub>2</sub> (R = NO<sub>2</sub>, R' = F).<sup>13</sup>

The C–Hg–C angles of the metal–arene  $\pi$  interactions of the title compound {[Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py]<sub>2</sub>]<sub>n</sub> are 22.5(1)° [C(34)′ $\cdots$ Hg(1) $\cdots$ C(35)′], 62.6(3)° [Hg(1) $\cdots$ C(34)′–C(35)′] and 94.9(3)° [C(34)′–C(35)′ $\cdots$ Hg(1)], with one exception, fairly different of the angles found in [Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R')<sub>2</sub>Py]<sub>2</sub> (R = NO<sub>2</sub>, R' = F), 22.5(1)° (C34′ $\cdots$ Hg $\cdots$ C35′), 74.3(3)° (Hg $\cdots$ C34′–C35′) and 83.3(3)° (C34′–C35′ $\cdots$ Hg).<sup>13</sup>

The asymmetry of the Hg $\cdots$ C  $\pi$  contacts in {[Hg<sup>II</sup>(RC<sub>6</sub>H<sub>4</sub>NNNC<sub>6</sub>H<sub>4</sub>R)<sub>2</sub>Py]<sub>2</sub>]<sub>n</sub> [R = EtOC(O)] – like the early mentioned examples – allows to exclude the possibility of occurrence of intermolecular interactions of the type Hg $\cdots$  $\eta^6$ -arene. In conclusion we have observed a second kind of non classical intermolecular C–H $\cdots$ O bonds involving hydrogen and oxygen atoms of adjacent



**Figure 2.** Section of the supramolecular, bidimensional (2D) assembling of  $\{[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]_n\}$  [ $\text{R} = \text{EtOC}(\text{O})$ ], showing three dimeric moieties. Intermolecular, centrosymmetric  $\text{Hg}-\eta^2, \eta^2$ -arene  $\pi$ -interactions (along the  $b$  axis) and non-classical  $\text{C}-\text{H}\cdots\text{O}$  bonding in dashed lines. Symmetry transformations used to generate equivalent atoms: (')  $1-x, -y, 1-z$ ; (')  $-1+x, y, z$ ; (')  $-1/2+x, 1/2-y, -1/2+z$ ; (')  $-1/2+x, 1/2-y, -1/2+z$ .

**Table 2.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for  $[\text{Hg}^{\text{II}}(\text{RC}_6\text{H}_4\text{NNNC}_6\text{H}_4\text{R})_2\text{Py}]$  [ $\text{R} = \text{EtOC}(\text{O})$ ]

Bond angles			
$\text{C}(22)\cdots\text{O}(6)''$	3.383(6)	$\text{N}(13)-\text{N}(12)-\text{N}(11)$	111.8(4)
$\text{C}(52)\cdots\text{O}(8)'''$	3.130(8)	$\text{N}(12)-\text{N}(13)\cdots\text{Hg}(1)$	84.0(2)
$\text{C}(81)-\text{O}(5)$	1.340(6)	$\text{C}(21)-\text{N}(13)\cdots\text{Hg}(1)$	161.6(3)
$\text{C}(81)-\text{O}(6)$	1.196(6)	$\text{N}(22)-\text{N}(21)-\text{Hg}(1)$	115.3(3)
$\text{C}(81)\cdots\text{H}(22)''''$	3.68	$\text{C}(31)-\text{N}(21)-\text{Hg}(1)$	127.0(3)
$\text{C}(82)-\text{O}(5)$	1.461(6)	$\text{N}(23)-\text{N}(22)-\text{N}(21)$	110.6(4)
$\text{N}(11)-\text{N}(12)$	1.310(5)	$\text{N}(22)-\text{N}(23)\cdots\text{Hg}(1)$	84.0(3)
$\text{N}(11)-\text{Hg}(1)$	2.100(4)	$\text{C}(41)-\text{N}(23)\cdots\text{Hg}(1)$	162.1(3)
$\text{N}(12)-\text{N}(13)$	1.280(5)	$\text{C}(56)-\text{N}(51)-\text{Hg}(1)$	120.8(5)
$\text{N}(13)\cdots\text{Hg}(1)$	2.718(3)	$\text{C}(52)-\text{N}(51)-\text{Hg}(1)$	122.4(5)
$\text{N}(21)-\text{N}(22)$	1.314(6)	$\text{N}(11)-\text{Hg}(1)-\text{N}(21)$	173.8(1)
$\text{N}(21)-\text{Hg}(1)$	2.100(4)	$\text{N}(11)-\text{Hg}(1)-\text{N}(51)$	95.1(2)
$\text{N}(22)-\text{N}(23)$	1.286(6)	$\text{N}(21)-\text{Hg}(1)-\text{N}(51)$	91.0(2)
$\text{N}(23)\cdots\text{Hg}(1)$	2.753(4)	$\text{N}(21)-\text{Hg}(1)\cdots\text{N}(13)$	129.1(1)
$\text{N}(51)-\text{Hg}(1)$	2.581(5)	$\text{N}(11)-\text{Hg}(1)\cdots\text{N}(23)$	127.6(1)
$\text{Hg}(1)\cdots\text{C}(34)'$	3.619(4)	$\text{N}(51)-\text{Hg}(1)\cdots\text{N}(23)$	109.5(2)
$\text{Hg}(1)\cdots\text{C}(35)'$	3.226(5)	$\text{N}(13)\cdots\text{Hg}(1)\cdots\text{N}(23)$	163.0(1)
		$\text{N}(11)-\text{Hg}(1)\cdots\text{C}(35)'$	90.0(1)
		$\text{N}(21)-\text{Hg}(1)\cdots\text{C}(35)'$	84.3(1)
		$\text{N}(51)-\text{Hg}(1)\cdots\text{C}(35)'$	151.4(2)
$\text{C}(23)-\text{C}(22)\cdots\text{O}(6)''$	98.5(3)	$\text{N}(13)\cdots\text{Hg}(1)\cdots\text{C}(35)'$	74.3(1)
$\text{C}(21)-\text{C}(22)\cdots\text{O}(6)''$	142.0(3)	$\text{N}(23)\cdots\text{Hg}(1)\cdots\text{C}(35)'$	89.0(1)
$\text{N}(51)-\text{C}(52)\cdots\text{O}(8)'''$	149.5(6)	$\text{N}(11)-\text{Hg}(1)\cdots\text{C}(34)'$	98.1(1)
$\text{C}(53)-\text{C}(52)-\text{O}(8)'''$	78.7(5)	$\text{N}(21)-\text{Hg}(1)\cdots\text{C}(34)'$	75.7(1)
$\text{N}(51)-\text{C}(52)-\text{H}(52)$	117	$\text{N}(51)-\text{Hg}(1)\cdots\text{C}(34)'$	165.0(2)
$\text{O}(5)-\text{C}(81)\cdots\text{H}(22)''''$	109	$\text{N}(13)\cdots\text{Hg}(1)\cdots\text{C}(34)'$	95.5(1)
$\text{N}(12)-\text{N}(11)-\text{Hg}(1)$	113.2(3)	$\text{N}(23)\cdots\text{Hg}(1)\cdots\text{C}(34)'$	67.5(1)
$\text{C}(11)-\text{N}(11)-\text{Hg}(1)$	128.9(3)	$\text{C}(35)'\cdots\text{Hg}(1)\cdots\text{C}(34)'$	22.5(1)

Symmetry transformations used to generate equivalent atoms: (')  $1-x, -y, 1-z$ ; (')  $-1+x, y, z$ ; (')  $-1/2+x, 1/2-y, -1/2+z$ ; (')  $1+x, y, z$ .

ethoxycarbonylphenyl groups on the same plane, which had not been noted in the earlier reported self-assembling patterns.

## Supplementary Material

Crystallographic data for the structural analyses have been deposited with the Cambridge Crystallographic Data Centre CCDC 291877. Further details of the crystal structures investigations are available free of charge via [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html) (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)).

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