ESI

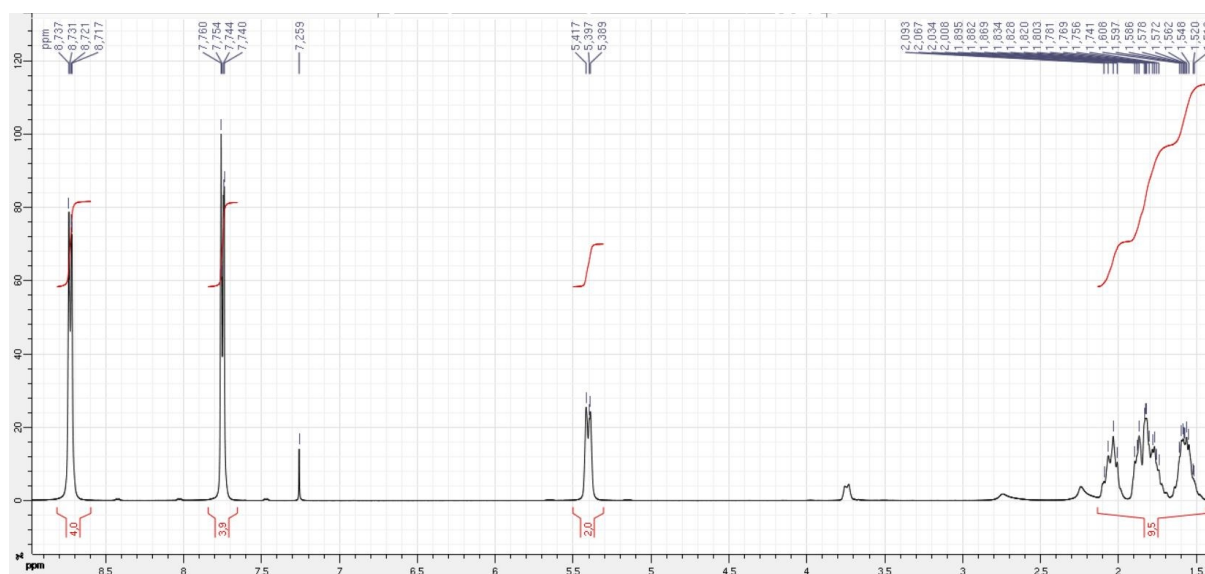## Crystals formation of 1D coordination polymers based on chiral, achiral and racemic 1,2 cyclohexane scaffold

Abdelaziz Jouaiti,[a*] Philippe Grosshans,[a] Nathalie Kyritsakas,[a] Sylvie Ferlay,[a*], Marc Henry,[b] Mir Wais Hosseini[a]
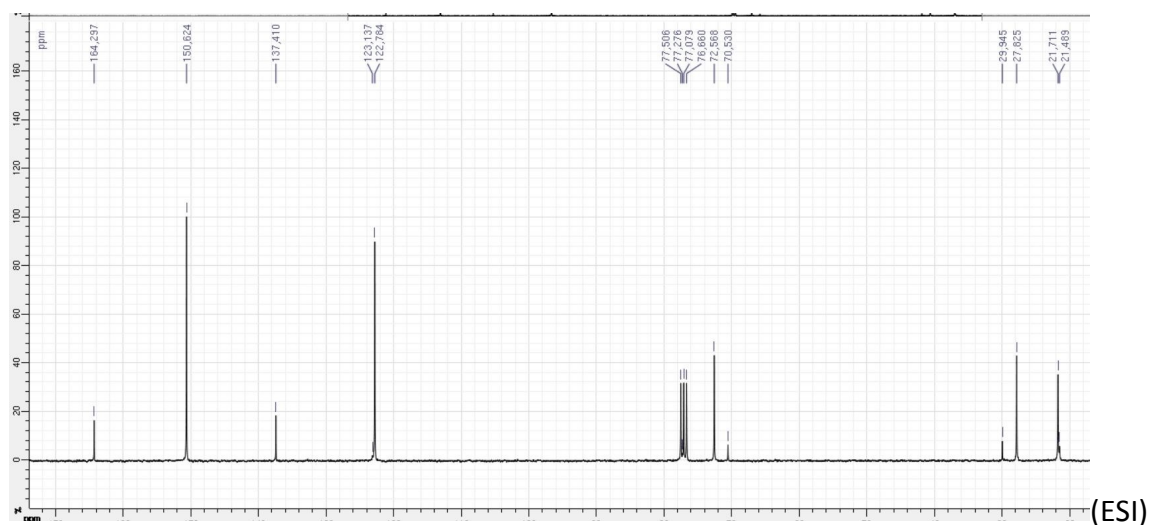
Characterization

Compound c, Bis-pyridin, 4,4'-[cis-1,2-cyclohexanediylbis(oxy)]

^{1}H-RMN (300 MHz, CDCl$_3$, 25 °C

^{13}C-RMN (125 MHz, CDCl$_3$, 25 °C)

(ESI)

Analysis Info

Analysis Name	F04730SK.d			Acquisition Date	9/3/2019 10:35:42 AM	
Method	Tune_pos_Standard.m			Operator	BDAL@DE	
Sample Name	AJ Cis			Instrument	micrOTOF II	

Acquisition Parameter

Source Type	ESI	Capillary	4500 V	Nebulizer	0.3 Bar	Set Hexapole RF	55.0 Vpp
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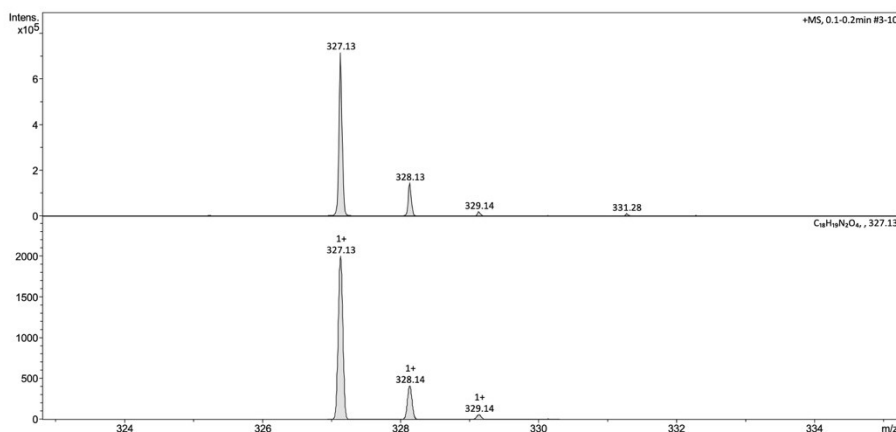
PACHA: General considerations

The PACHA formalism is a very useful method for probing intermolecular interaction energies in a perfectly non-empirical way that do not follow the usual decomposition of the total energy into coulombic, polarization, dispersion, repulsive, H-bonding terms. The crucial physical reason for not relying on such a partition of the total energy in PACHA is that all these terms depend on the same electromagnetic interaction involving electrons and protons.

However, for such an approach to be reliable, three requirements should imperatively be met:

i) The partial charges distributions should be self-consistent and should not involve empirical scalings. With PACHA this requirement is met using an electronegativity equalization principle coupled to the universal Allen's scale and to atomic radii computed using relativistic wavefunctions solutions of the Dirac equations.

ii) The SE (Self-Energy)-term should be at least one order of magnitude large than the F-term meaning that the method is not well-suited for completely apolar compounds. In practice this requirement is met as soon as it exists one oxygen or nitrogen atom in the investigated compound. This means that crystalline elements and pure hydrocarbons characterized by a null or rather small electronegativity differences between constituting atoms are not well-handled by PACHA and should be treated by other methods.

iii) Compounds displaying an energy difference between the ground state and the first excited electronic state less than 1 eV (semi-conductors, semi-metals, metals, radicals, etc...) should be considered with extreme care as in this case the adiabatic approximation may not apply. For such compounds, a full quantum-mechanical treatment becomes mandatory.

One of the big advantage of the PACHA approach is that hydrogen-bonded systems may be easily and rigorously treated on the same theoretical ground as non hydrogen-bonded systems. This is crucial as in most other methods, hydrogen bonding is usually considered as a very difficult problem needing ad hoc potentials. In PACHA, hydrogen bonding is automatically included as a consequence of the validity of the Hellman-Feynman theorem and is just a particular case of the universal electromagnetic interaction that is easily handled by the SE (Self-Energy) term.

Table 1 gives the atomic parameterization that have been used in this paper. As packing energies are very sensitive to H-atom positions in PACHA, coordinates for H-atoms derived from X-ray structures cannot be used owing to the large errors made on these atomic positions. In order to avoid introducing unphysical values, all C-H bond lengths have been fixed at the standard value of 108 pm allowing performing reliable comparisons between crystal structures derived from single-crystal X-ray diffraction.

Element	H	C	N	O	Cl	Hg
van der Waals radius /pm	120	170	155	152	175	155
Electronegativity /eV	13.61	15.05	18.13	21.36	16.97	10438
Atomic radius /pm	53.0	62.0	52.1	45.0	72.4	112.6

Table 1: Standard sets of van der Waals radii [1] used for the computation of packing coefficients, with associated atomic electronegativities [2] and radii [3] used for partial charges evaluation in PACHA.

The PACHA algorithm, based on charge partial calculations, has been described in previous publications, (M. Henry, *ChemPhysChem*, **2002**, 3, 561-569. M. Henry, *ChemPhysChem*, **2002**, 3, 607-616.). Moreover, it is the only algorithm able to interpret 183W NMR chemical shifts with the computed partial charges distribution [*N. J. Chem*, **2017**, 41, 6112-6119].
The algorithm has been applied with success in a wide range of compounds containing metals:
Ferey et al. J. Am. Chem. Soc. 2003, 125, 1912-1922
Steed et al. J. Am. Chem. Soc. 2005, 127, 11063-11074
Souillard et al. J. Col. Inter. Sc, 2006, 307, 175-182
Steed et al. Chem. Eur. J. 2011, 17, 10259-10271
Steed et al. Cryst. Gr.&Des. 2012, 12, 1395-1401

Calculations

Calculation of Packing Energy (PE)

[1] A. Bondi, *J. Phys. Chem.,* 1964, **68**, 441-451.
[2] J. B. Mann, T. L. Meek and L. C. Allen*, J. Am. Chem. Soc.*, 2000, **122**, 2780.
[3] J. T. Waber and D. T. Cromer, *J. Chem. Phys*., 1965, **42**, 4116.

In the crystalline state, the Packing Energy may depend on the different crystallographic directions. In this case, we propose to introduce three structure descriptors, reflecting the anisotropy of the molecular packing. The basic idea is to use three partial space-group symmetries (packing sub-groups) creating large voids in the structure that lead to a strong reduction of the Packing Energy. The three Partial Packing Energy (PPE), reflecting the packing anisotropy, are assumed to be in the order $PPE_1 < PPE_2 < PPE_3$, one may define the isotropic *Partial Packing Energy* <PE>:

$$<PE> = (PPE_1 + PPE_2 + PPE_3)/3$$

And the *Packing Energy span* ΔPE:
$$\Delta PE = PPE_1 - PPE_3$$
And the *Packing Energy skew* ηPE:
$$\eta PE = 3(PPE_2 - <PE>)/\Delta PE$$
(with $\eta = 0$ in the case of spherical symmetry when $\Delta = 0$).

$-1 < \eta PE < +1$ (tri-axial ellispoid) is measuring the deviation from pure axial symmetry characterized by $\eta PE = +1$ (oblate ellipsoid) and $\eta PE = -1$ (prolate ellipsoid).

Calculation of Cooperativity Index (CI)

A last structure descriptor would then be the CI *cooperativity index*:
$$CI = 3<PE> - PE$$
reflecting the cooperativity (CI < 0) or anti-cooperativity (CI > 0) of the stacking of the layers generated by each sub-group.
On purely intuitive grounds, one may expect low packing anisotropies for achiral space-goups and large packing anisotropies for chiral space-groups.

Calculations for 1a-HgCl$_2$, 1b-HgCl$_2$, 1c-HgCl$_2$ and 1a$_{0.5}$1b$_{0.5}$-HgCl$_2$

Table 1 shows the results obtained by applying the PACHA approach to **1a-HgCl$_2$, 1b-HgCl$_2$, 1c-HgCl$_2$** and **1a$_{0.5}$1b$_{0.5}$-HgCl$_2$**. The evaluation of *PE* is performed step by step: the Self-Energies (*SE* in $kJ \cdot mol^{-1}$) for mercury dichloride $HgCl_2$, the free ligand and a molecular chain generated by complexation between $HgCl_2$ and the ligands. Then «*Net*» corresponds to the self-energy of the fully interacting chains in $kJ \cdot mol^{-1}$, from which a Packing Energy may be evaluated as

$$PE = (Net - Chain*4)$$

For the solvated network (**1a$_{0.5}$1b$_{0.5}$-HgCl$_2$**) this Packing Energy corresponds to Packing = [Net - (Chain+CHCl$_3$)*4] with CHCl$_3$ = -6 $kJ \cdot mol^{-1}$.

Then, the average Hg-N bond energy ($kJ \cdot mol^{-1}$) has been evaluated according to:
$$Hg-N = (Chain - HgCl_2 - ligand)/2.$$

Crystal	Group	HgCl$_2$	Ligand	Chain	Net	PE	CI	Hg-N
1a-HgCl$_2$	P2$_1$2$_1$2$_1$	-150(2)	-299(2)	-536(2)	-2267(9)	-123(9)	-2(2)	-43(2)

Crystal	Group	HgCl$_2$	Ligand	Chain	Net	PE	CI	Hg-N
1b-HgCl$_2$	P2$_1$2$_1$2$_1$	-150(2)	-299(2)	-535(2)	-2264(9)	-124(9)	-2(2)	-43(2)
1c-HgCl$_2$	P2$_1$2$_1$2	-151/-152(2)	-309(2)	-534(2)	-2314(9)	-178(9)	-33(2)	-37(2)
1a$_{0.5}$1b$_{0.5}$-HgCl$_2$.	P2$_1$/n	-150(2)	-295(2)	-532(2)	-2368(9)	-214(9)	-3(2)	-44(2)

Table 2: Calculation performed for 1a-HgCl$_2$, 1b-HgCl$_2$, 1c-HgCl$_2$ and 1a$_{0.5}$1b$_{0.5}$-HgCl$_2$ using the PACHA approach.

As mentioned above, the three different PPE (Partial Packing Energies) have to be evaluated considering the symmetry associated with different space groups of the coordination networks and their associated sub-space groups.

1a-HgCl$_2$ or 1b-HgCl$_2$ (Space group P2$_1$2$_1$2$_1$)

These compounds crystallise in the P2$_1$2$_1$2$_1$ space-group, the choice of subgroups is obvious (P2$_1$.1.1, P1.2$_1$.1 and P1.1.2$_1$) as this group contains only twofold screw axes that all act as packing operators. The three partial packing energies (PPE) have been calculated as :

$$PPE1 = SE (P1.2_1.1)/2 - SE = -23(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1b-HgCl}_2$$
$$\text{and} = -22(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1a-HgCl}_2$$
$$PPE2 = SE (P1.1.2_1)/2 - SE = -7(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1b-HgCl}_2$$
$$\text{and} = -7(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1a-HgCl}_2$$
$$PPE3 = SE (P2_1.1.1)/2 - SE = -2(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1b-HgCl}_2$$
$$\text{and} = -2(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1a-HgCl}_2$$

$$<PE> = -11 \text{ kJ·mol}^{-1}, \Delta PE = -21(9) \text{ kJ·mol}^{-1} \text{ and } \eta PE = -0,57$$

The Cooperativity Index (CI) reflecting the cooperativity between the chains is:

$$CI = 3<PE> - PE/4 = 31 - 33 = -2(2) \text{ kJ·mol}^{-1} \text{ for } \textbf{1a-HgCl}_2 \text{ or } \textbf{1b-HgCl}_2$$

1c-HgCl$_2$ (Space group P2$_1$2$_1$2)

This compound crystallizes in the P2$_1$2$_1$2 space-group, the twofold axis acts as an intramolecular symmetry operator that has no effect on the packing efficiency. In order to be able to discuss the packing anisotropy in this compound, we have considered a supercell of the P2$_1$2$_1$2 space-group, obtained by doubling the *c*-parameter leading to a new space group displaying 8 symmetry operators instead of 4:

#1 = x,y,z -> 1
#2 = x,y,1/2+z -> 1(0,0,1/2)
#3 = -x,-y,z -> 2 0,0,z
#4 = 1/2-x,1/2+y,-z -> 2(0,1/2,0) 1/4,y,0
#5 = -x,-y,1/2+z -> 2(0,0,1/2) 0,0,z
#6 = 1/2-x,1/2+y,1/2-z -> 2(0,1/2,0) 1/4,y,1/4
#7 = 1/2+x,1/2-y,-z -> 2(1/2,0,0) x,1/4,0
#8 = 1/2+x,1/2-y,1/2-z -> 2(1/2,0,0) x,1/4,1/4

It is then possible to generate three packing sub-groups: P112$_1$(2) by choosing operators #(1,2,3,5), P2$_1$2$_1$2 (screw axes at z = 0) using operators #(1,3,4,7) and P'2$_1$2$_1$2

(screw axes at z = 1/4) using operators #(1,3,6,8). The three partial packing energies (PPE) have been then calculated as:

$$PPE1 = SE\ [P1.1.2(2_1)]/4 - SE = -30(2)\ kJ \cdot mol^{-1}$$
$$PPE2 = SE\ (P'2_1.2_1.2)/4 - SE = -25(2)\ kJ \cdot mol^{-1}$$
$$PPE3 = SE\ (P2_1.2_1.2)/4 - SE = -24(2)\ kJ \cdot mol^{-1}$$

$$<PE> = -26\ kJ \cdot mol^{-1},\ \Delta PE_{SR} = -6(2)\ kJ \cdot mol^{-1}\ and\ \eta PE = -0,5.$$

The computed Cooperativity Index CI is then:

$$CI = 3<PE> - PE/4 = 45 - 78 = -33(2)\ kJ \cdot mol^{-1}$$

$1a_{0.5}1b_{0.5}$-$HgCl_2$ (Space group $P2_1/n$)

In this case, the choice of subgroups is obvious ($P2_1$, P-1and Pn) since all symmetry operators are used for packing molecular chains. The three partial packing energies (PPE) have been calculated as :

$$PPE1 = SE(P2_1)/4 - SE = -23(2)\ kJ \cdot mol^{-1}$$
$$PPE2 = SE(P-1)/4 - SE = -10(2)\ kJ \cdot mol^{-1}$$
$$PPE3 = SE(Pn)/4 - SE = -2(2)\ kJ \cdot mol^{-1}$$

$$<PE> = -12\ kJ \cdot mol^{-1},\ \Delta PE = -21(2)\ kJ \cdot mol^{-1}\ and\ \eta PE = -0,29$$

The computed Cooperativity Index CI is then:

$$CI = 3<PE> - PE/4 = 33 - 36 = -3(2)\ kJ \cdot mol^{-1}$$

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100.554(10)   90.00000 P121/n1
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 2 Cl1 0.0679(2) 1.35829(18) 0.83369(14) z-1 c41 @17 :4a
 3 Cl2 0.1655(2) 1.4184(2) 0.57762(14) z-1 c41 @17 :4a
 4 N1 0.3151(6) 1.2492(6) 0.7427(5) c5 @7 :4a
 5 C1 0.3653(8) 1.2192(7) 0.6797(5) c2 @6 :4a
 6 H1 0.32984 1.24772 0.61799 z1 c89 @1 :4a
 7 C2 0.4601(7) 1.1537(7) 0.6895(5) c2 @6 :4a
 8 H2 0.49764 1.13072 0.63649 z1 c89 @1 :4a
 9 C3 0.5064(7) 1.1177(6) 0.7683(5) c2 @6 :4a
10 C4 0.4547(8) 1.1479(7) 0.8345(5) c2 @6 :4a
11 H4 0.48734 1.11992 0.89683 z1 c89 @1 :4a
12 C5 0.3610(8) 1.2143(7) 0.8185(5) c2 @6 :4a
13 H5 0.32217 1.23974 0.87028 z1 c89 @1 :4a
14 C6 0.6123(8) 1.0487(7) 0.7779(5) c2 @6 :4a
15 O1 0.6742(5) 1.0473(4) 0.7255(3) z-2 c84 @8 :4a
16 O2 0.6280(5) 0.9915(4) 0.8474(3) z-2 c84 @8 :4a
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19 C8 0.7099(8) 0.8372(7) 0.9195(5) z0 c2 @6 :4a
20 H8 0.68991 0.87091 0.97590 z1 c89 @1 :4a
21 C9 0.8158(8) 0.7649(7) 0.9395(6) z-2 c2 @6 :4a
22 H9A 0.80162 0.70831 0.98584 z1 c89 @1 :4a
23 H9B 0.82585 0.72242 0.88403 z1 c89 @1 :4a
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29 H11B 1.02149 0.95371 0.93350 z1 c89 @1 :4a
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_EBND
¬ß
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Partial Charge Distribution Evaluation -> e1450
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[H19 C19 N2 O4 Cl5 Hg ]*4 = 2868.96 amu

Madelung summation details
Ewald parameter for 1/R summation was K = 0.129 √Ö-1 (accuracy = 4e-
010)
Reciprocal space exploration: -2 <= (h, k, l) <= 2
min = 8.89860 eV < mean = 16.42282 eV < max = 125.45198 eV
Madelung constant A = 147.9474020/4 = 36.9868505 (dmin = 0.94945 √Ö)
Orbital compression factor was OCF = 82.00%
Total electrostatic balance = -2243.8149 eV = -216495.2 kJ.mol-1

***Atomic electronegativies (eV) and radii (pm) ***
Hg(    10.438,       112.6)
Cl(    16.970,        72.4)
N (    18.130,        52.1)
C (    15.050,        62.0)
H (    13.610,        53.0)
O (    21.360,        45.0)

Level of significance for Madelung elements eps = 5.292126e-009
Convergence criterion |Ax - b|/|b| < eps
Estimated error on charges after 24 iterations = 2.058074e-010

*** PACHA signature ***
Mean electronegativity <EN> = 15.0369 eV
Partial electrostatic balance: <EB> = -24.5298 eV = -2366.8 kJ.mol-1
Reduced electrostatic balance: <EB/4> = -6.1324 eV = -591.7 kJ.mol-1
Global ionicity: <GI> = 10.4557 %
#n              Label(¬±ox)[CN]        Charge ¬±q
#33                O3(-2)[ 2] =         -0.27664 -> 10.12 V
#35                O4(-2)[ 1] =         -0.27600 -> 10.03 V
#16                O2(-2)[ 2] =         -0.27297 -> 9.65 V
#15                O1(-2)[ 1] =         -0.26867 -> 9.10 V
#2                Cl1(-1)[ 1] =         -0.23061 -> 10.61 V
#3                Cl2(-1)[ 1] =         -0.22614 -> 10.26 V
#4                 N1(-2)[ 2] =         -0.20969 -> 10.81 V
#41                N2(-2)[ 2] =         -0.20772 -> 10.59 V
#50               Cl5(-1)[ 1] =         -0.13267 -> 2.82 V
#48               Cl3(-1)[ 1] =         -0.12359 -> 2.10 V
#49               Cl4(-1)[ 1] =         -0.11652 -> 1.54 V
#27               C11(-2)[ 4] =         -0.07887 -> 7.28 V
#21                C9(-2)[ 4] =         -0.07799 -> 7.19 V
#24               C10(-2)[ 4] =         -0.07759 -> 7.16 V
#30               C12(-2)[ 4] =         -0.07714 -> 7.11 V
#44               C18(-1)[ 3] =         -0.04063 -> 3.72 V
#7                 C2(-1)[ 3] =         -0.03912 -> 3.58 V
#10                C4(-1)[ 3] =         -0.03712 -> 3.40 V
#37               C15(-1)[ 3] =         -0.03289 -> 3.00 V
#9                 C3(+0)[ 3] =         +0.00235 -> -0.27 V
#36               C14(+0)[ 3] =         +0.00441 -> -0.46 V
#5                 C1(+0)[ 3] =         +0.00717 -> -0.72 V
#42               C17(+0)[ 3] =         +0.00908 -> -0.90 V
#12                C5(+0)[ 3] =         +0.01174 -> -1.14 V
#39               C16(+0)[ 3] =         +0.01623 -> -1.56 V
#19                C8(+0)[ 4] =         +0.03405 -> -3.22 V
```

```
#17              C7(+0)[ 4] =          +0.03724 -> -3.51 V
#46             C19(+2)[ 4] =          +0.04594 -> -4.32 V
#43             H17(+1)[ 1] =          +0.04824 -> 0.47 V
#29            H11B(+1)[ 1] =          +0.05259 -> -0.01 V
#25            H10A(+1)[ 1] =          +0.06018 -> -0.83 V
#6               H1(+1)[ 1] =          +0.06416 -> -1.26 V
#28            H11A(+1)[ 1] =          +0.07129 -> -2.04 V
#26            H10B(+1)[ 1] =          +0.07391 -> -2.32 V
#13              H5(+1)[ 1] =          +0.07639 -> -2.59 V
#40             H16(+1)[ 1] =          +0.07745 -> -2.71 V
#31            H12A(+1)[ 1] =          +0.08153 -> -3.15 V
#45             H18(+1)[ 1] =          +0.08274 -> -3.28 V
#8               H2(+1)[ 1] =          +0.08727 -> -3.78 V
#20              H8(+1)[ 1] =          +0.09116 -> -4.20 V
#32            H12B(+1)[ 1] =          +0.09166 -> -4.25 V
#23             H9B(+1)[ 1] =          +0.09455 -> -4.57 V
#18              H7(+1)[ 1] =          +0.09487 -> -4.60 V
#22             H9A(+1)[ 1] =          +0.09519 -> -4.64 V
#11              H4(+1)[ 1] =          +0.10145 -> -5.32 V
#47             H19(+1)[ 1] =          +0.10193 -> -5.37 V
#38             H15(+1)[ 1] =          +0.10367 -> -5.56 V
#34             C13(+3)[ 3] =          +0.17673 -> -16.47 V
#14              C6(+3)[ 3] =          +0.17725 -> -16.52 V
#1               Hg(+2)[ 2] =          +0.73017 -> -18.95 V

Total sum for Charge = 0.0

Statistical report:
<Atom>[num] = mean ¬± 3√óstdev (stdev) <avdev>
<q(H)> = 0.08159 (0.01663) <0.01354>
<q(C)> = 0.00320 (0.07363) <0.05135>
<q(N)> = -0.20870 (0.00139) <0.00098>
<q(O)> = -0.27357 (0.00364) <0.00275>
<q(Cl)> = -0.16590 (0.05734) <0.04998>
<q(Hg)> = 0.73017 (0.00000) <0.00000>

Statistical report:
<Atom>[num] = mean ¬± 3√óstdev (stdev) <avdev>
<q(black)> = 0.00320 (0.07363) <0.05135>
<q(royal_blue)> = -0.20870 (0.00139) <0.00098>
<q(green)> = -0.16590 (0.05734) <0.04998>
<q(red)> = -0.27357 (0.00364) <0.00275>
<q(silver)> = 0.08159 (0.01663) <0.01354>
<q(wood)> = 0.73017 (0.00000) <0.00000>




#1               Hg(+2)[ 2] =          +0.73
#2              Cl1(-1)[ 1] =          -0.23
#3              Cl2(-1)[ 1] =          -0.23
#4               N1(-2)[ 2] =          -0.21
#5               C1(+0)[ 3] =          +0.01
#6               H1(+1)[ 1] =          +0.06
#7               C2(-1)[ 3] =          -0.04
#8               H2(+1)[ 1] =          +0.09
#9               C3(+0)[ 3] =          +0.00
#10              C4(-1)[ 3] =          -0.04
#11              H4(+1)[ 1] =          +0.10
```

```
#12              C5(+0)[ 3] =              +0.01
#13              H5(+1)[ 1] =              +0.08
#14              C6(+3)[ 3] =              +0.18
#15              O1(-2)[ 1] =              -0.27
#16              O2(-2)[ 2] =              -0.27
#17              C7(+0)[ 4] =              +0.04
#18              H7(+1)[ 1] =              +0.09
#19              C8(+0)[ 4] =              +0.03
#20              H8(+1)[ 1] =              +0.09
#21              C9(-2)[ 4] =              -0.08
#22             H9A(+1)[ 1] =              +0.10
#23             H9B(+1)[ 1] =              +0.09
#24             C10(-2)[ 4] =              -0.08
#25            H10A(+1)[ 1] =              +0.06
#26            H10B(+1)[ 1] =              +0.07
#27             C11(-2)[ 4] =              -0.08
#28            H11A(+1)[ 1] =              +0.07
#29            H11B(+1)[ 1] =              +0.05
#30             C12(-2)[ 4] =              -0.08
#31            H12A(+1)[ 1] =              +0.08
#32            H12B(+1)[ 1] =              +0.09
#33              O3(-2)[ 2] =              -0.28
#34             C13(+3)[ 3] =              +0.18
#35              O4(-2)[ 1] =              -0.28
#36             C14(+0)[ 3] =              +0.00
#37             C15(-1)[ 3] =              -0.03
#38             H15(+1)[ 1] =              +0.10
#39             C16(+0)[ 3] =              +0.02
#40             H16(+1)[ 1] =              +0.08
#41              N2(-2)[ 2] =              -0.21
#42             C17(+0)[ 3] =              +0.01
#43             H17(+1)[ 1] =              +0.05
#44             C18(-1)[ 3] =              -0.04
#45             H18(+1)[ 1] =              +0.08
#46             C19(+2)[ 4] =              +0.05
#47             H19(+1)[ 1] =              +0.10
#48             Cl3(-1)[ 1] =              -0.12
#49             Cl4(-1)[ 1] =              -0.12
#50             Cl5(-1)[ 1] =              -0.13


Total sum for Charge = 0.0

Steric Energy Evaluation
After summing over 3x3x3 cells
Distance threshold for bonded atoms was 4.596 √Ö
Total steric energy = 10099.7 kJ.mol-1
Bonded steric energy = 9991.6 kJ.mol-1
Steric energy = 108.1 kJ.mol-1

Bond Valence Sum Evaluation
#1 Hg(+2) [2] = 1.57 -> Cl2 Cl1
#2 Cl1(-1) [1] = 0.78 -> Hg
#3 Cl2(-1) [1] = 0.79 -> Hg
#4 N1(-2) [2] = 2.80 -> C1 C5
#5 C1(+0) [3] = 3.51 -> H1 N1 C2
#6 H1(+1) [1] = 1.06 -> C1
#7 C2(-1) [3] = 3.13 -> H2 C1 C3
#8 H2(+1) [1] = 1.06 -> C2
```

```
#9  C3(+0)  [3]  = 2.78 -> C2 C4 C6
#10 C4(-1)  [3]  = 3.12 -> H4 C5 C3
#11 H4(+1)  [1]  = 1.06 -> C4
#12 C5(+0)  [3]  = 3.51 -> H5 N1 C4
#13 H5(+1)  [1]  = 1.06 -> C5
#14 C6(+3)  [3]  = 3.63 -> O1 O2 C3
#15 O1(-2)  [1]  = 1.70 -> C6
#16 O2(-2)  [2]  = 1.97 -> C6 C7
#17 C7(+0)  [4]  = 3.32 -> H7 O2 C8 C12
#18 H7(+1)  [1]  = 1.06 -> C7
#19 C8(+0)  [4]  = 3.26 -> H8 O3 C7 C9
#20 H8(+1)  [1]  = 1.06 -> C8
#21 C9(-2)  [4]  = 3.50 -> H9B H9A C10 C8
#22 H9A(+1) [1]  = 1.06 -> C9
#23 H9B(+1) [1]  = 1.06 -> C9
#24 C10(-2) [4]  = 3.55 -> H10B H10A C11 C9
#25 H10A(+1) [1] = 1.06 -> C10
#26 H10B(+1) [1] = 1.06 -> C10
#27 C11(-2) [4]  = 3.51 -> H11B H11A C10 C12
#28 H11A(+1) [1] = 1.06 -> C11
#29 H11B(+1) [1] = 1.06 -> C11
#30 C12(-2) [4]  = 3.51 -> H12B H12A C7 C11
#31 H12A(+1) [1] = 1.06 -> C12
#32 H12B(+1) [1] = 1.06 -> C12
#33 O3(-2)  [2]  = 1.95 -> C13 C8
#34 C13(+3) [3]  = 3.65 -> O4 O3 C14
#35 O4(-2)  [1]  = 1.72 -> C13
#36 C14(+0) [3]  = 2.87 -> C15 C18 C13
#37 C15(-1) [3]  = 3.17 -> H15 C14 C16
#38 H15(+1) [1]  = 1.06 -> C15
#39 C16(+0) [3]  = 3.57 -> H16 N2 C15
#40 H16(+1) [1]  = 1.06 -> C16
#41 N2(-2)  [2]  = 2.79 -> C16 C1
```