

Self-assembly of a new cobalt complex, $(C_6H_{14}N_2)_3[CoCl_4]Cl$: Synthesis, empirical and DFT calculations

Mariem Tahenti ^(a), Noureddine Issaoui ^{(b)*}, Thierry Roisnel ^(c), Houda Marouani ^(a),
Omar Al-Dossary ^d

^(a) University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Material Chemistry (LR13ES08), 7021 Bizerte, Tunisia

^(b) University of Monastir, Faculty of Sciences, Laboratory of Quantum and Statistical Physics (LR18ES18), Monastir 5079, Tunisia

^(c) Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France

^(d) Department of Physics and Astronomy, College of Science, King Saud University, PO Box 2455, Riyadh 11451, Saudi Arabia

*Corresponding author: issaoui_noureddine@yahoo.fr

Table captions

Table S1: Crystal data and structure parameters for $(C_6H_{14}N)_3[CoCl_4]Cl$.

Table S2: Enrichment ratio of different inter-contact and percentage of each atom on HS in $(C_6H_{14}N)_3[CoCl_4]Cl$.

Table S3: Global reactivity descriptors and calculated frontier molecular orbital parameters of $(C_6H_{14}N)_3[CoCl_4]Cl$ compound.

Figure captions

Fig. S1. 2D-FP of the main interactions in the crystal packing and % age of atoms present in $(C_6H_{14}N)_3[CoCl_4]Cl$.

Fig. S2. Percentage of atoms present in $(C_6H_{14}N)_3[CoCl_4]Cl$.

Fig. S3. Theoretical and experimental IR spectrum of $(C_6H_{14}N)_3[CoCl_4]Cl$.

Fig. S4. DTA and TG curves of $(C_6H_{14}N)_3[CoCl_4]Cl$.

Fig.S5. HOMO-LUMO orbital plots of $(C_6H_{14}N)_3[CoCl_4]Cl$ computed with B3LYP/6-311+G(d,p).

Table S1: Crystal data and structure parameters for $(C_6H_{14}N)_3[CoCl_4]Cl$.

CCDC	2102182
Temperature	150K
Empirical formula	$3(C_6H_{14}N) \cdot Cl_4Co \cdot Cl$
Formula weight (g mol ⁻¹)	536.72
Crystal system	Monoclinic
Space group	$P2_1/n$
a	15.2645 (12) Å
b	10.0843(7) Å
c	17.4450(13) Å
β	95.957(3) °
Z	4
V	2670.8 (3) Å ³
F(000)	1132
$\mu(Mo\ K\alpha)$	0.71073 Å
Index ranges	$-19 < h_{max} < 19, -13 < k_{max} < 13, -22 < l_{max} < 22$
Reflections collected	24384
Independent reflections	6103
Reflections with $I > 2\sigma(I)$	4718
R _{int}	0.037
Absorption correction: <i>multi-scan</i>	$T_{min} = 0.703, T_{max} = 0.813$
Refined parameters	271
R[F ² > 2σ(F ²)]	0.032
wR(F ²)	0.071
Goodness of fit	1.03
$\Delta\rho_{max} = 0.63\ e\ \text{\AA}^{-3}$	$\Delta\rho_{min} = -0.58\ e\ \text{\AA}^{-3}$

Table S2: Enrichment ratio of different inter-contact and percentage of each atom on HS in $(C_6H_{14}N)_3[CoCl_4]Cl$.

RE	H	Co	Cl
H	0.95	-	1.24
Co		-	-
Cl		-	-
%surface	79.45	0.25	19.8

Table S3: Global reactivity descriptors and calculated frontier molecular orbital parameters of $(C_6H_{14}N)_3[CoCl_4]Cl$ using DFT/LANL2DZ level.

Parameters (eV)	
E_{HOMO}	-6.027913632
E_{LUMO}	-3.459138592
$\Delta E = E_{LUMO} - E_{HOMO}$	2.56877504
E_{HOMO-1}	-6.276627656
E_{LUMO+1}	0.568178208
$\Delta E = E_{LUMO+1} - E_{HOMO-1}$	6.844805864
Chemical potential (μ)	-4.743526112
Softness (ζ)	0.389290609
Ionization energy (I)	6.027913632
Electron affinity (A)	3.459138592
Electronegativity (χ)	4.788526112
Chemical hardness (η)	1.28438752
Electrophilicity index (ω)	8.759443557

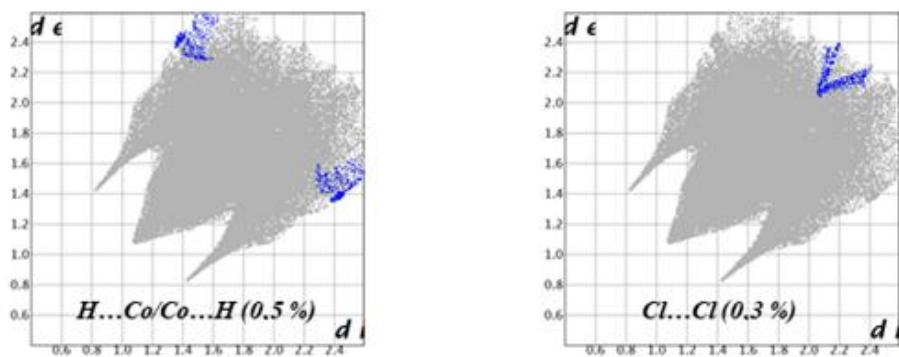
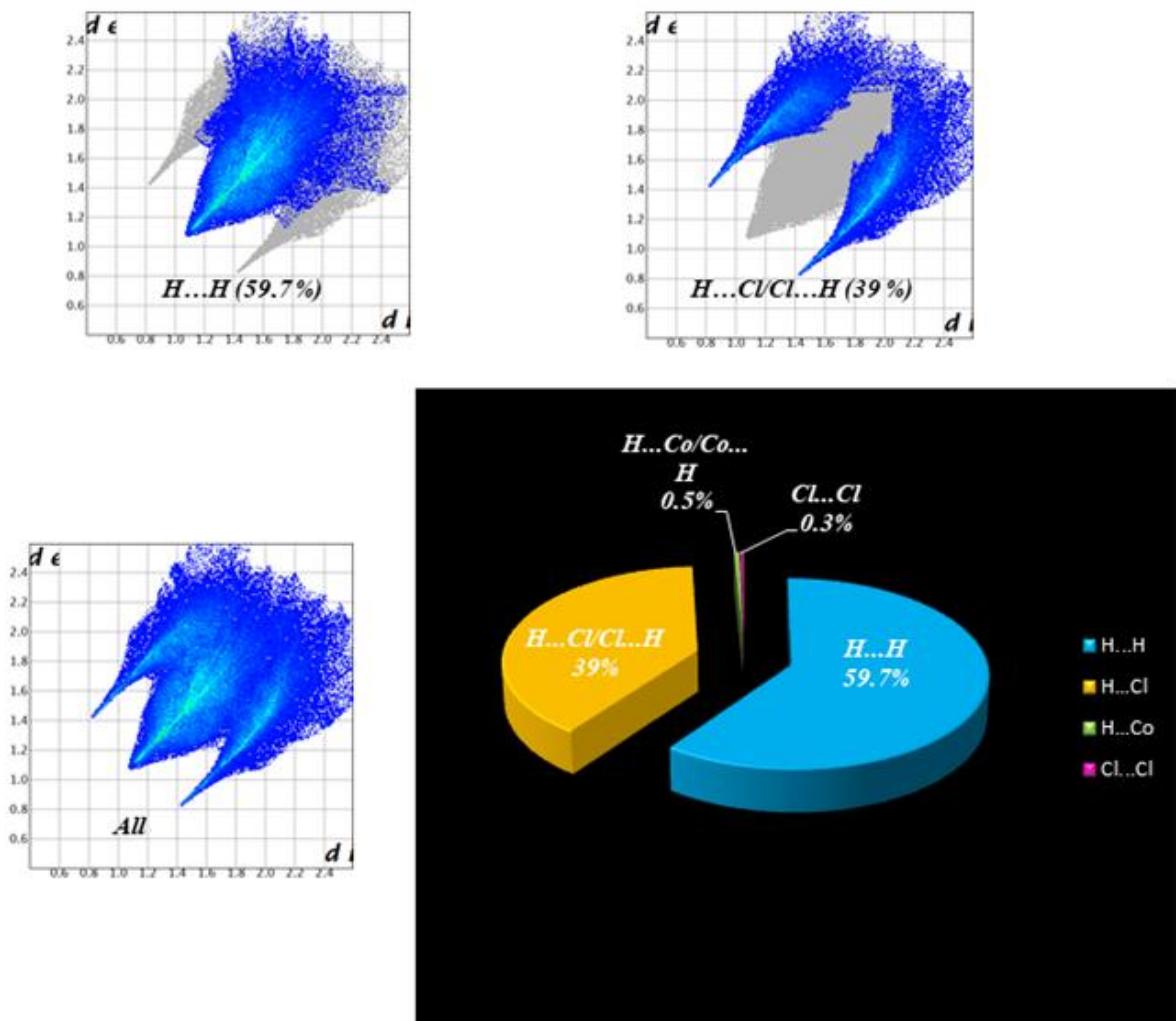


Fig. S1

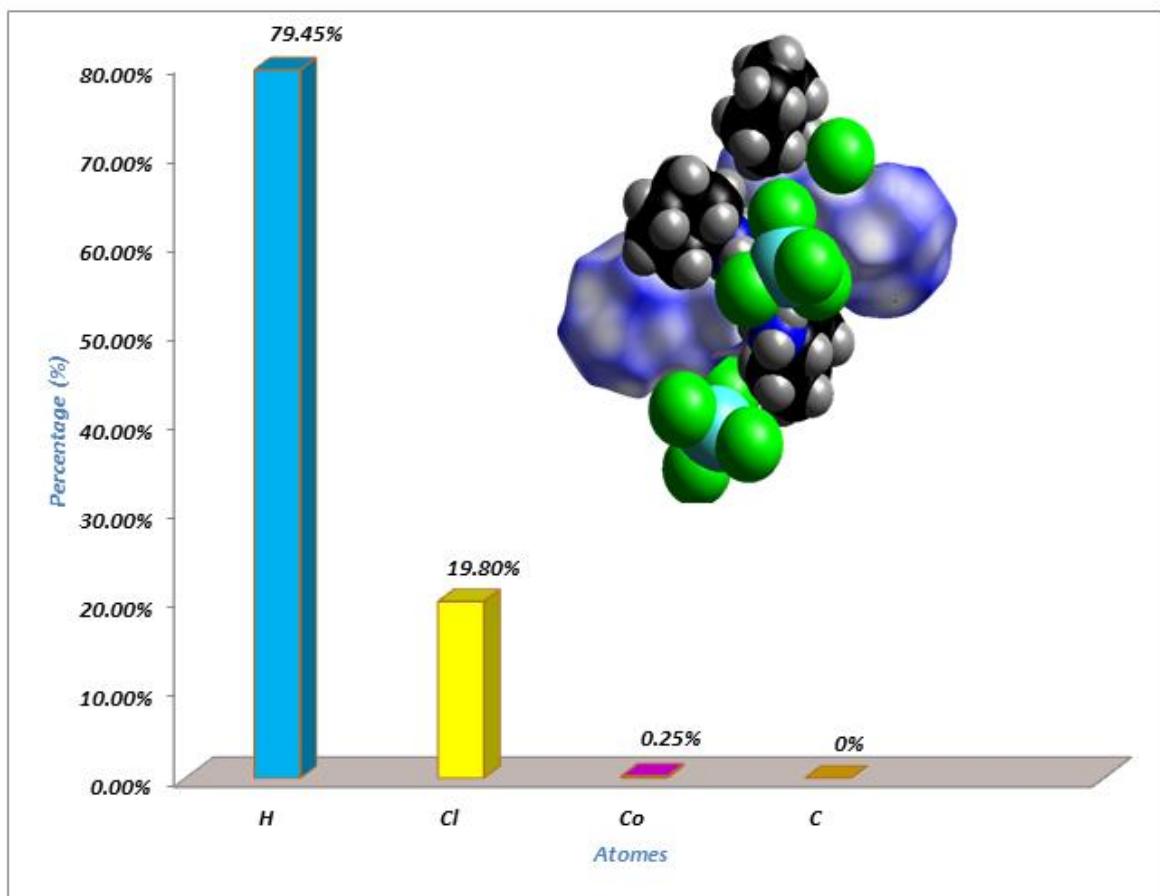


Fig. S2. Percentage of atoms present in $(\text{C}_6\text{H}_{14}\text{N})_3[\text{CoCl}_4]\text{Cl}$.

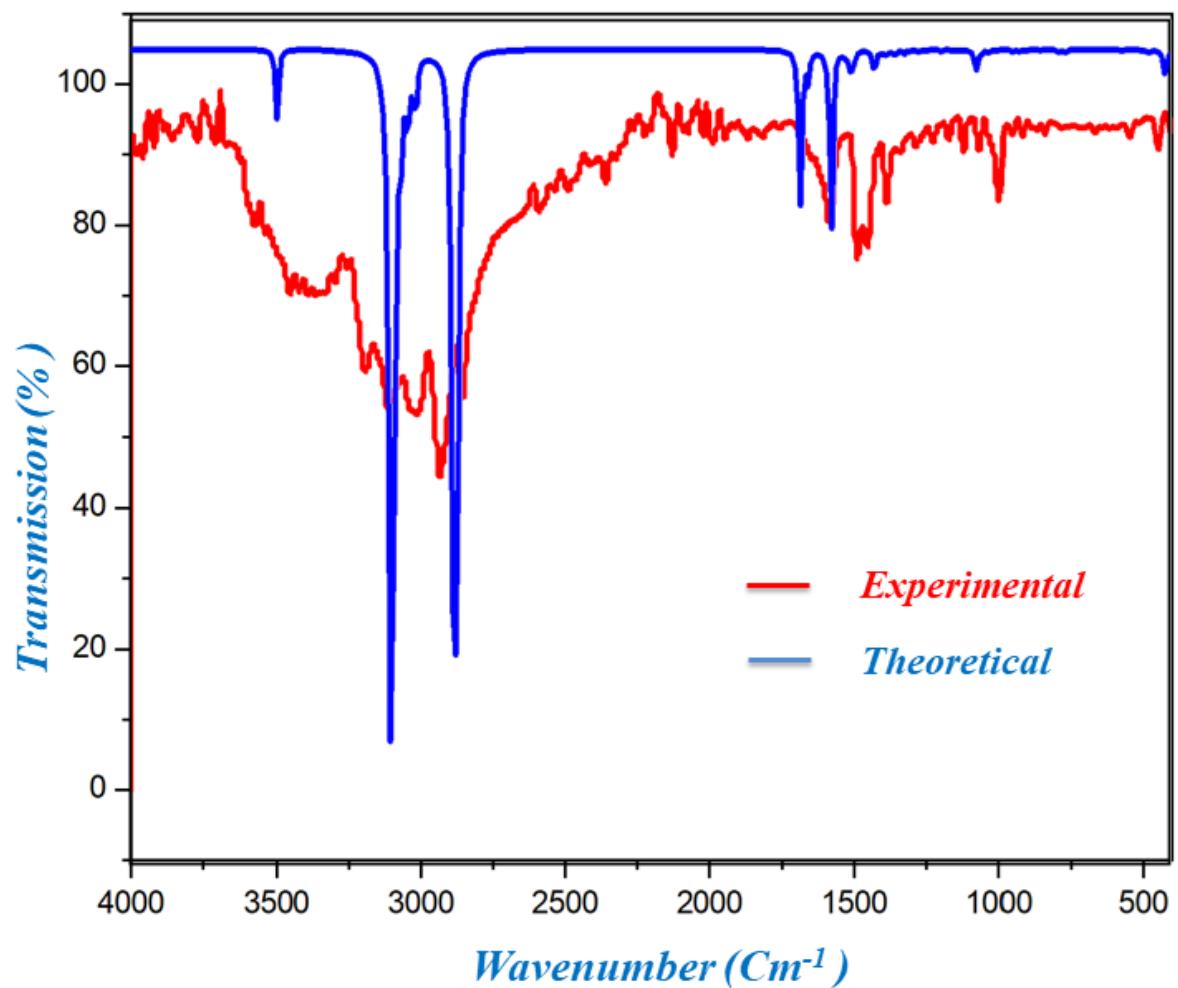


Fig. S3. Theoretical and experimental IR spectrum of $(\text{C}_6\text{H}_{14}\text{N})_3[\text{CoCl}_4]\text{Cl}$.

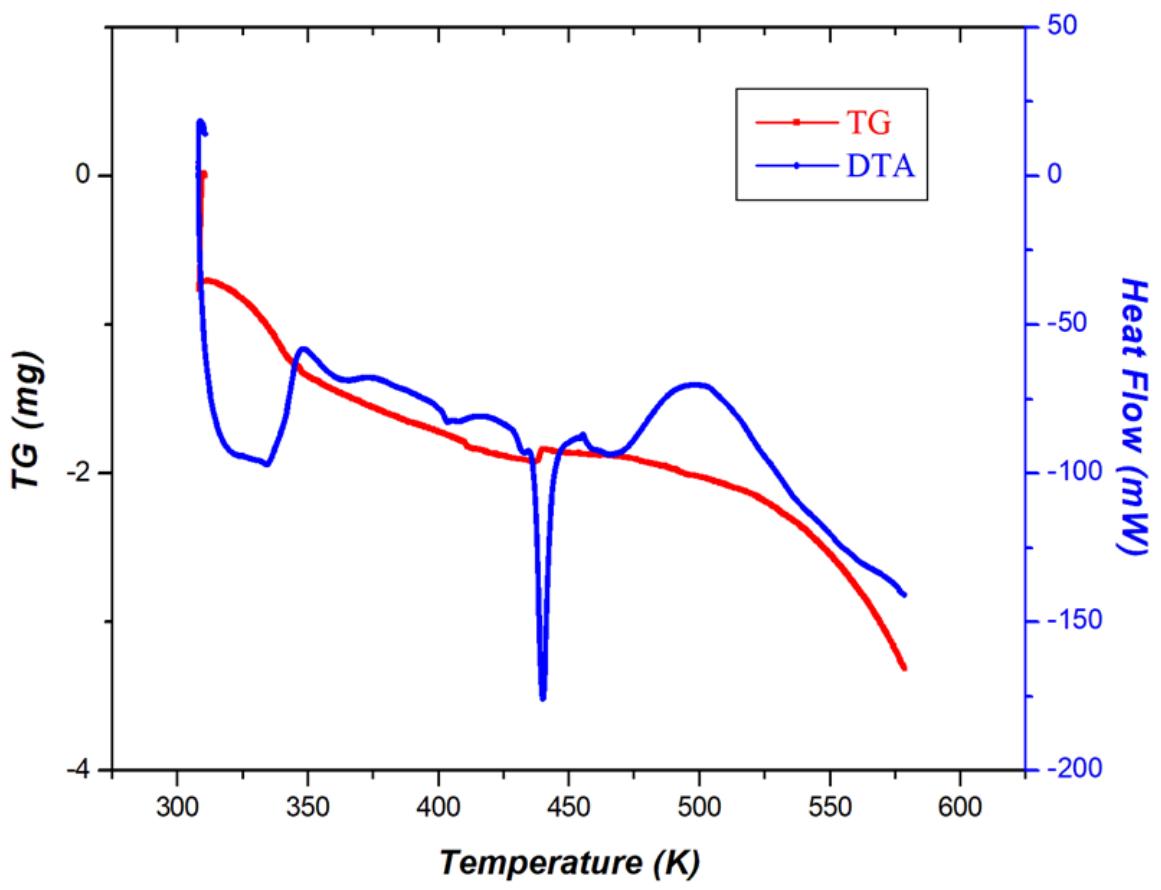


Fig. S4

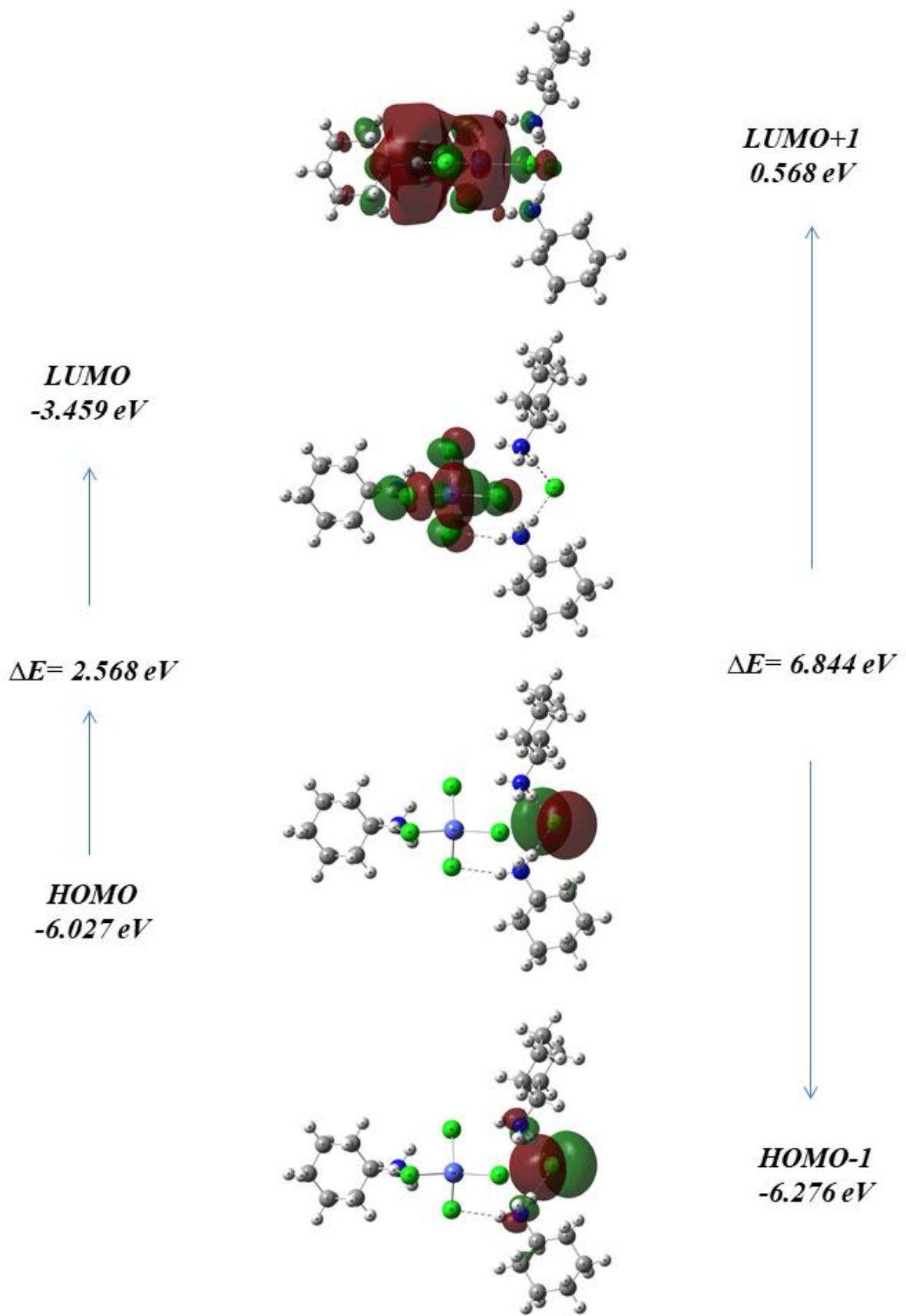


Fig. S5