Supplementary Material

Coordination preferences of NNO and NNS Schiff base ligands with Co(III) complexes: Synthesis, characterization and DFT calculation

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Table S1. Selected bond lengths (Å) and angles (°) of complexes 1 and 2.

<table>
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<td>O1–C8</td>
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* Corresponding author.
E-mail address: bozidar@chem.bg.ac.rs (B. Čobeljić)
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<td>N8–Co1–N5</td>
<td>91.68(7)</td>
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Table S2. Comparison of Co-Nthiazole, Co-Nimine and Co-Sthiolate bond lengths (Å) in octahedral Co(III)-N₄S₂ complexes with thiosemicarbazone based ligands.

<table>
<thead>
<tr>
<th>Complexes</th>
<th>Co-Nthiazole mean values</th>
<th>Co-Nimine mean values</th>
<th>Co-Sthiolate mean values</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Co(L¹)₂]BF₄·H₂O (1)</td>
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<td>1.909(2) 1.908</td>
<td>2.2230(8) 2.2243</td>
<td>this work</td>
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<td>[Co(L¹)₂][Co(NCS)₄]·2H₂O CCDC 1854180</td>
<td>1.95(5) 1.960</td>
<td>1.903(5) 1.907</td>
<td>2.225(2) 2.222</td>
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<tr>
<td>[Co(L³)₂]BF₄·H₂O CCDC 1498846</td>
<td>1.945(2) 1.955</td>
<td>1.907(3) 1.905</td>
<td>2.228(1) 2.226</td>
<td>[2]</td>
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<td>[Co(L⁴)₂]BF₄·Et₂O CCDC 1498852</td>
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<td>1.933(2) 1.936</td>
<td>1.903(2) 1.9015</td>
<td>2.225(1) 2.229</td>
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<td>[Co(L⁵)₂][NO₃]·H₂O CCDC 759082</td>
<td>1.936(3) 1.933</td>
<td>1.897(3) 1.900</td>
<td>2.216(1) 2.223</td>
<td>[3]</td>
</tr>
</tbody>
</table>

Co-Nthiazoline

[HL¹] = (E)-2-(1(1hiazol-2-yl)ethylidene)hydrazine-1-carbothioamide;
[HL²] = condensation product of 2-thiazolecarboxaldehyde and 4-phenylthiosemicarbazide; [HL³] = condensation product of 4-methyl-2-thiazolecarboxaldehyde and 4-phenylthiosemicarbazide; [HL⁴] = 2-acetyl-2-thiazoline thiosemicarbazone.

**Table S3.** Comparison of Co-N$_{py}$, Co-N$_{imine}$, Co-N$_{azide}$ and Co-O$_{enolate}$ bond lengths (Å) in octahedral Co(III)N$_4$O$_2$–Co(III)N$_2$O(N$_3$)$_3$ complexes with hydrazone and azide ligands.

<table>
<thead>
<tr>
<th>Complexes</th>
<th>Co-N$_{py}$</th>
<th>Co-N$_{imine}$</th>
<th>Co-N$_{azide}$</th>
<th>Co-O$_{enolate}$</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Co(L$^3$)(N$_3$)$_3$] (2)</td>
<td>1.9189(16)</td>
<td>1.8516(15)</td>
<td>1.9704(18)</td>
<td>1.9272(13)</td>
<td>this work</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.9632(16)</td>
</tr>
<tr>
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<td></td>
<td>1.9615(17)</td>
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<td></td>
<td></td>
<td></td>
<td>1.9650</td>
</tr>
<tr>
<td>[Co(L$^6$)$_2$][Co(L$^5$)(N$_3$)$_3$]$^+\cdot$CH$_3$OH</td>
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<td>1.8606(12)</td>
<td>1.9573(15)</td>
<td>1.9235(13)</td>
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<tr>
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<td>1.8644(13)</td>
<td>1.9633(14)</td>
<td>1.9060(12)</td>
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<td>1.9162(14)</td>
<td>1.8482(14)</td>
<td>1.9685(14)</td>
<td>1.9110(12)</td>
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<td>mean value:</td>
<td>mean value:</td>
<td>mean value:</td>
<td>mean value:</td>
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<tr>
<td></td>
<td>1.9190</td>
<td>1.8577</td>
<td>1.9630</td>
<td>1.9135</td>
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<tr>
<td>[Co(L$^7$)$_2$][Co(L$^7$)(N$_3$)$_3$]</td>
<td>1.916(3)</td>
<td>1.860(3)</td>
<td>1.971(3)</td>
<td>1.922(2)</td>
<td>[2]</td>
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<tr>
<td>CCDC 894063</td>
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<td>1.861(3)</td>
<td>1.949(3)</td>
<td>1.896(2)</td>
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</tr>
<tr>
<td></td>
<td>1.917(3)</td>
<td>1.862(3)</td>
<td>1.956(3)</td>
<td>1.944(3)</td>
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<tr>
<td></td>
<td>mean value:</td>
<td>mean value:</td>
<td>mean value:</td>
<td>mean value:</td>
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<tr>
<td></td>
<td>1.914</td>
<td>1.861</td>
<td>1.959</td>
<td>1.921</td>
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</table>

**HL$^2$ = naziv liganda;**

**HL$^5$ = N^e-[1E]-1-pyridin-2-ylylidene]-2-furohydrazide; HL$^7$= methyl 2-pyridyl ketone semicarbazone.**

### Table S4. Hydrogen-bond parameters for complex 1.

<table>
<thead>
<tr>
<th>D–H···A</th>
<th>D–H (Å)</th>
<th>H···A (Å)</th>
<th>D···A (Å)</th>
<th>D–H···A (°)</th>
<th>Symm. operation on A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N4–H4NA···N7</td>
<td>0.86</td>
<td>2.59</td>
<td>3.446(4)</td>
<td>172</td>
<td>-1/2+x, y, 3/2-z</td>
</tr>
<tr>
<td>N8–H8NA···N3</td>
<td>0.86</td>
<td>2.28</td>
<td>3.109(4)</td>
<td>162</td>
<td>1/2+x, y, 3/2-z</td>
</tr>
<tr>
<td>N4–H4NB···S4</td>
<td>0.86</td>
<td>2.81</td>
<td>3.611(3)</td>
<td>155</td>
<td>1-x,1/2+y,3/2-z</td>
</tr>
<tr>
<td>O1W–H2W···F1</td>
<td>1.01(7)</td>
<td>1.74(8)</td>
<td>2.728(7)</td>
<td>167(8)</td>
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</tr>
<tr>
<td>O1W–H1W···N3</td>
<td>1.02(7)</td>
<td>2.01(8)</td>
<td>2.962(7)</td>
<td>155(9)</td>
<td></td>
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</table>

### Table S5. Intermolecular π···π interaction parameters for complex 1.

<table>
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<tr>
<th>Cg(I)\textsuperscript{a}</th>
<th>Cg(J)\textsuperscript{a}</th>
<th>Cg(I)···Cg(J)\textsuperscript{b} (Å)</th>
<th>(\alpha) (°)</th>
<th>(\beta) (°)</th>
<th>(\gamma) (°)</th>
<th>Slippage\textsuperscript{d} (Å)</th>
<th>Sym. code on (J)</th>
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</thead>
<tbody>
<tr>
<td>Cg(1)</td>
<td>Cg(1)</td>
<td>4.0189(16)</td>
<td>0.00(14)</td>
<td>25.9</td>
<td>25.9</td>
<td>1.755</td>
<td>1-x, 1-y, 2-z</td>
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<td>Cg(2)</td>
<td>Cg(2)</td>
<td>3.8200(16)</td>
<td>0.00(14)</td>
<td>23.9</td>
<td>23.9</td>
<td>1.550</td>
<td>1-x, 2-y, 2-z</td>
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</tbody>
</table>

\textsuperscript{a}Labels of aromatic rings: (1) = S(1),C(2),C(1),N(1),C(3); (2) = S(3),C(8),C(7),N(5),C(9).
\textsuperscript{b}Cg(I)···Cg(J) = Distance between ring centroids (Ang.).
\textsuperscript{c}\(\alpha\) = Dihedral angle between planes (I) and (J) (Deg).
\textsuperscript{d}\(\beta\) = Angle between Cg(I)–Cg(J) vector and normal to plane (I) (Deg).
\textsuperscript{e}\(\gamma\) = Angle between Cg(I) –Cg(J) vector and normal to plane (J) (Deg).
Slippage = Distance between Cg(J) and perpendicular projection of Cg(J) on ring (I) (Ang).
Table S6. Intermolecular $\pi\cdots\pi$ interaction parameters for complex 2.

<table>
<thead>
<tr>
<th>Cg(I)$^a$</th>
<th>Cg(J)$^a$</th>
<th>Cg(I)--Cg(J)$^b$ (Å)</th>
<th>$\alpha^c$ (°)</th>
<th>$\beta^d$ (°)</th>
<th>$\gamma^e$ (°)</th>
<th>Slippage$^f$ (Å)</th>
<th>Sym. code on (J)</th>
</tr>
</thead>
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<tr>
<td>Cg(1)</td>
<td>Cg(1)</td>
<td>3.4540(13)</td>
<td>0.03(11)</td>
<td>24.3</td>
<td>24.3</td>
<td>1.419</td>
<td>1-x, 1-y, 1-z</td>
</tr>
<tr>
<td>Cg(2)</td>
<td>Cg(2)</td>
<td>3.9788(14)</td>
<td>0.00</td>
<td>28.5</td>
<td>28.5</td>
<td>1.901</td>
<td>-x, 1-y, -z</td>
</tr>
</tbody>
</table>

$^a$Labels of aromatic rings: (1) = N(1),C(1),C(2),C(3),C(4),C(5); (2) = N(4),C(10),C(11),C(12),C(13),C(14).
$^b$Cg(I)--Cg(J) = Distance between ring centroids (Ang.).
$^c\alpha$ = Dihedral angle between planes (I) and (J) (Deg).
$^d\beta$ = Angle between Cg(I)--Cg(J) vector and normal to plane (I) (Deg).
$^e\gamma$ = Angle between Cg(I) --Cg(J) vector and normal to plane (J) (Deg).
Slippage = Distance between Cg(J) and perpendicular projection of Cg(J) on ring (I) (Ang).

Table S7. Hydrogen-bond parameters for complex 2.

<table>
<thead>
<tr>
<th>D–H···A</th>
<th>D–H (Å)</th>
<th>H···A (Å)</th>
<th>D···A (Å)</th>
<th>D–H···A (°)</th>
<th>Symm. operation on A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1–H1···N7</td>
<td>0.95</td>
<td>2.53</td>
<td>3.341(3)</td>
<td>143</td>
<td>1+x, y, z</td>
</tr>
<tr>
<td>C7–H7B···N11</td>
<td>0.98</td>
<td>2.48</td>
<td>3.445(3)</td>
<td>167</td>
<td>1-x, -y, 1-z</td>
</tr>
<tr>
<td>C9–H9A···N10</td>
<td>0.99</td>
<td>2.54</td>
<td>3.379(3)</td>
<td>142</td>
<td>x, -1+y, z</td>
</tr>
<tr>
<td>C10–H10···N10</td>
<td>0.95</td>
<td>2.51</td>
<td>3.339(3)</td>
<td>145</td>
<td>x, -1+y, z</td>
</tr>
<tr>
<td>C12–H12···O1</td>
<td>0.95</td>
<td>2.52</td>
<td>3.272(3)</td>
<td>136</td>
<td>-x, 1-y, -z</td>
</tr>
<tr>
<td>C14–H14···N8</td>
<td>0.95</td>
<td>2.30</td>
<td>3.230(3)</td>
<td>167</td>
<td>-1+x, y, z</td>
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<tr>
<td>Intra C7–H7C···N3</td>
<td>0.98</td>
<td>2.56</td>
<td>2.935(2)</td>
<td>103</td>
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</table>
**Fig. S1.** (a) Crystal packing of 1 showing self-assembled complex cations within a layer parallel with the (001) lattice plane by means of intermolecular N–H···N and N–H···S hydrogen bonds and (b) Intermolecular π···π interactions between thiazole rings.
Fig. S2. Crystal packing of 2 showing 2D assembly parallel with the (10-1) lattice plane generated by intermolecular π⋯π interactions and C–H⋯N hydrogen bonds.
### Cartesian coordinates of all optimized structures

All structures from Table 2 in the main text, optimized at BP86-D3BJ/Def2-TZVP-PCM(H2O) level of theory:

<table>
<thead>
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<th>39</th>
<th>[Co(L\textsubscript{1})\textsubscript{2}]\textsuperscript{+}</th>
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<td>1.319338 9.758729 4.392051</td>
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<td>-0.188263 7.168252 5.530595</td>
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</tr>
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<td>3.347693  8.525118  5.732125</td>
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43

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