Anion Receptor Coordination Tripods Capped by [9]aneS₃

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Supplementary Information

(a)

(b)

Figure S1 Chemical shift changes of (a) amine N-H and (b) pyridyl C-H protons of 2 with a variety of anions.
**Figure S2** Chemical shift changes of pyridyl CH resonances of 3 with a variety of anions.

**Figure S3** Chemical shift changes of amine NH resonances of 4 with a variety of anions.
Figure S4. Chemical shift changes of urea NH resonance of 5 at ca. 8.5 ppm with a variety of anions.
Figure S5 UV/Visible absorbance profiles of 4 as the PF$_6$ salt (black), and with addition of 500 equivalents of chloride (green), acetate (blue) and bromide (red) at a concentration of 4 x 10$^{-6}$ mol dm$^{-3}$ in 30% DMSO in CHCl$_3$. Anions are added as TBA salts.
NMR spectroscopic Titration data

Ru 3APy with acetate

concentration of Guest

chemical shifts for nucleus NH

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 4.5273E-3)

Compound 1 with acetate
Ru 3APy with bromide

concentration of Guest

chemical shifts for nucleus NH

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 1.6513E-2)

Compound 1 with bromide
Ru 3APy with chloride

concentration of Guest

chemical shifts for nucleus NHα

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 1.3702E-3)

Compound 1 with chloride
Compound 1 with fluoride
Project title

concentration of Guest
6.8 7.2 7.6

chemical shifts for nucleus NH

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 6.8871E-3)

Compound 2 with acetate
Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Project title

concentration of Guest
6.75
6.85
6.95
7.05

chemical shifts for nucleus NH

% formation relative to Host
unweighted error in chemical shift. (unweighted rms = 6.2982E-3)

Compound 2 with bromide
Compound 2 with chloride
Compound 2 with nitrate
3 Acetate

concentration of Guest

chemical shifts for nucleus CH

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 2.6442E-3)

Compound 3 with acetate
3 Bromide

concentration of Guest

chemical shifts for nucleus CH

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 2.5021E-3)

Compound 3 with Bromide
Compound 3 with chloride

unweighted error in chemical shift. (unweighted rms = 5.1617E-3)
Chemical shifts for nucleus CH

Concentration of Guest

% formation relative to Host

Unweighted error in chemical shift. (Unweighted rms = 1.1650E-3)

Compound 3 with nitrate
Ru-pyrene dilution

concentration of Host

chemical shifts for nucleus NHa

unweighted error in chemical shift. (unweighted rms = 2.0564E-3)

% formation relative to Host

Self-association of compound 4
Compound 4 with acetate
Compound 4 with chloride
[(9-anthracene-3S)-Ru(PyNHPyrene)3 with bromide

<table>
<thead>
<tr>
<th>Guest Concentration</th>
<th>Chemical Shift for Nucleus NH</th>
<th>% Formation Relative to Host</th>
<th>Unweighted Error in Chemical Shift</th>
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<tbody>
<tr>
<td>0.000</td>
<td>6.85</td>
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<td>-0.002</td>
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<td>0.010</td>
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<td>10</td>
<td>0.000</td>
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<tr>
<td>0.030</td>
<td>7.00</td>
<td>30</td>
<td>0.002</td>
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</tbody>
</table>

**Compound 4 with bromide**
(9ane-S3)Ru(PyNHPyrene)3 with chloride

<table>
<thead>
<tr>
<th>Concentration of Guest</th>
<th>% Formation Relative to Host</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0</td>
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<tr>
<td>0.010</td>
<td>10</td>
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<tr>
<td>0.020</td>
<td>20</td>
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<tr>
<td>0.030</td>
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</tbody>
</table>

Chemical shifts for nucleus NHa

Unweighted error in chemical shift. (unweighted rms = 2.6903E-3)

Compound 4 with chloride
((9ane-S3)Ru(PyNHPyrene)3 with nitrate

Chemical shifts for nucleus NH

Concentration of Guest

% formation relative to Host

Unweighted error in chemical shift. (unweighted rms = 2.3480E-3)

Compound 4 with nitrate
Ru-TUP with acetate

concentration of Guest

chemical shifts for nucleus NH-a

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 1.8945E-2)

Compound 5 with acetate
Ru-TUP with bromide

concentration of Guest

9.0
9.2
9.4
9.6

chemical shifts for nucleus NHα

% formation relative to Host

unweighted error in chemical shift. (unweighted rms = 5.4588E-3)

Compound 5 with bromide
Ru-TUP with chloride

concentration of Guest

chemical shifts for nucleus NHa

unweighted error in chemical shift. (unweighted rms = 1.6142E-2)

Compound 5 with chloride
Ru-TUP with nitrate

chemical shifts for nucleus NHa

unweighted error in chemical shift. (unweighted rms = 8.2676E-3)

Compound 5 with nitrate