

Supplementary Information

1. Displacement Ellipsoid Plots

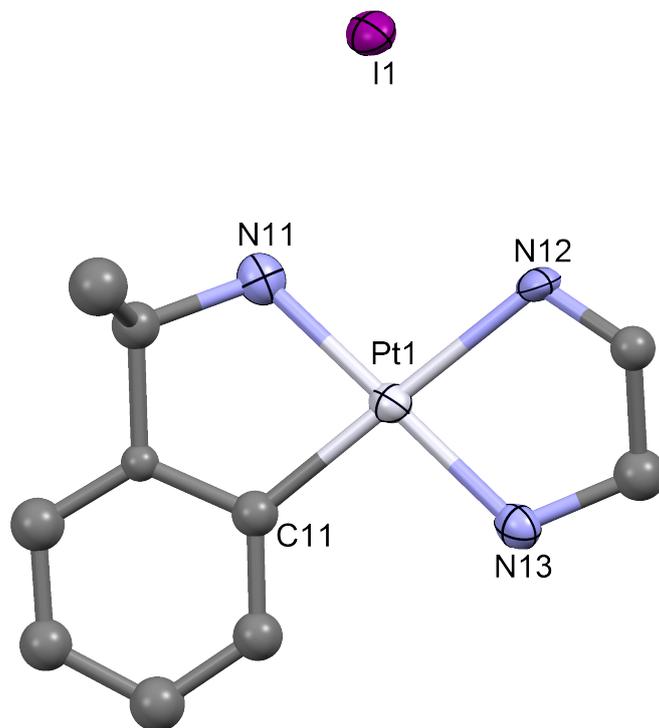


Figure S1. Displacement ellipsoid plot of molecule 1. Hydrogen atoms are omitted for clarity.

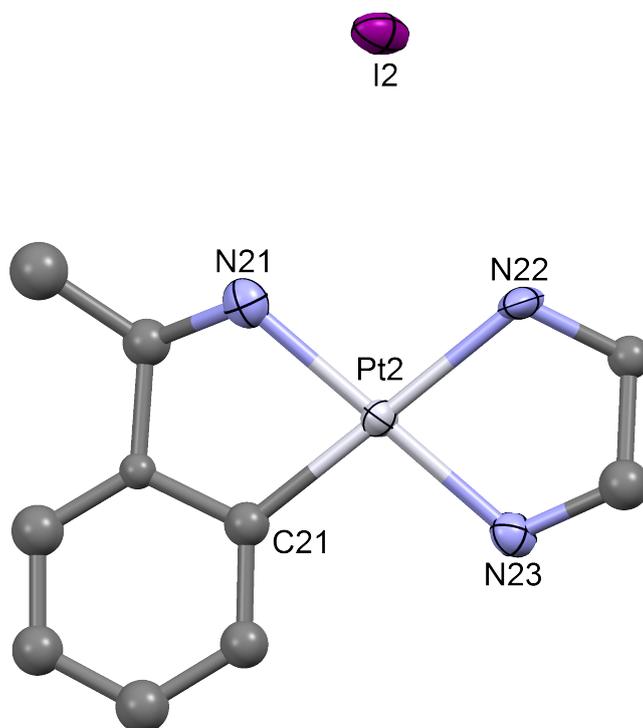


Figure S2. Displacement ellipsoid plot of molecule 2. Hydrogen atoms are omitted for clarity.

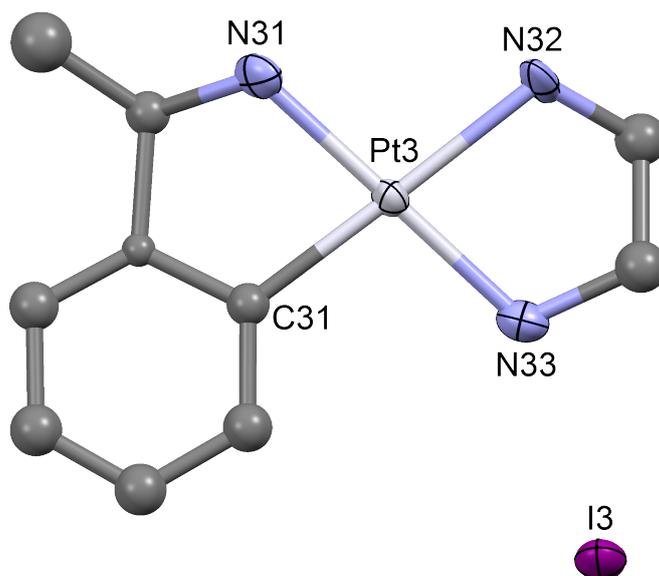


Figure S3. Displacement ellipsoid plot of molecule 3. Hydrogen atoms are omitted for clarity.

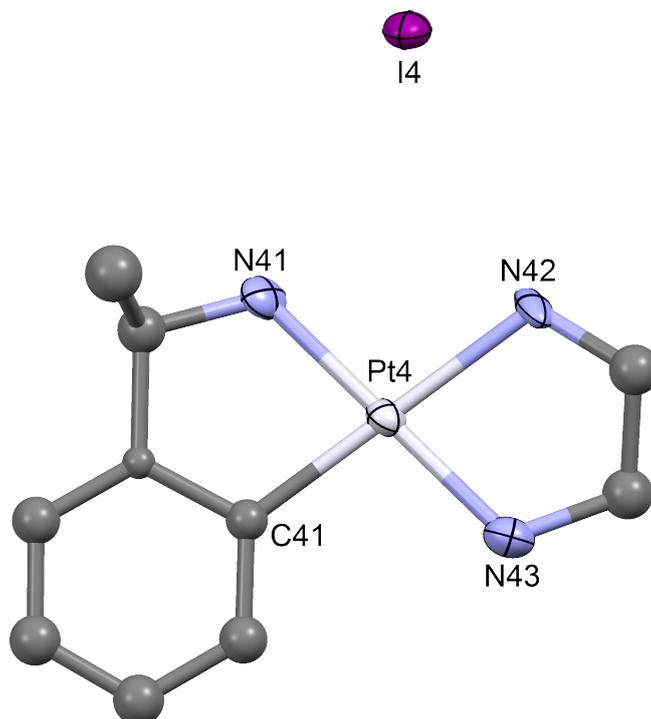


Figure S4. Displacement ellipsoid plot of molecule 4. Hydrogen atoms are omitted for clarity.

2. Short Contacts

Table S1. Hydrogen-bond geometry in Å and °.

D-H...A	D-H	H...A	D...A	D-H...A
N(11)-H(11A)...I(1)	0.99	2.75	3.720(14)	165
N(12)-H(12A)...I(2) ⁱ	0.99	2.81	3.677(13)	147
N(12)-H(12B)...I(1)	0.99	2.74	3.677(15)	159
N(13)-H(13A)...I(4) ⁱⁱ	0.99	2.74	3.720(12)	172
N(13)-H(13B)...I(1) ⁱⁱⁱ	0.99	2.75	3.633(15)	149
N(21)-H(21B)...I(2)	0.99	2.65	3.626(14)	169
N(22)-H(22A)...I(2)	0.99	2.80	3.720(15)	154
N(22)-H(22B)...I(1) ^{iv}	0.99	2.91	3.729(13)	141
N(23)-H(23A)...I(2) ^v	0.99	2.69	3.574(15)	148
N(23)-H(23B)...I(3) ^v	0.99	2.79	3.747(12)	162
N(31)-H(31B)...I(3) ^v	0.99	2.69	3.665(14)	169
N(32)-H(32A)...I(3) ^v	0.99	2.80	3.713(16)	153
N(32)-H(32B)...I(4) ^{vi}	0.99	2.85	3.738(13)	149
N(33)-H(33A)...I(3)	0.99	2.68	3.564(15)	148
N(33)-H(33B)...I(2)	0.99	2.76	3.662(12)	151
N(41)-H(41A)...I(4)	0.99	2.75	3.706(14)	162
N(42)-H(42A)...I(3) ⁱ	0.99	2.82	3.706(13)	149
N(42)-H(42B)...I(4)	0.99	2.72	3.636(16)	154
N(43)-H(43A)...I(1) ^{vii}	0.99	2.80	3.685(12)	149
N(43)-H(43B)...I(4) ^v	0.99	2.74	3.611(15)	147

Symmetry codes: (i) $x, 1 + y, z$; (ii) $1 + x, y, -1 + z$; (iii) $-1 + x, y, z$; (iv) $x, -1 + y, z$; (v) $1 + x, y, z$; (vi) $1 + x, -1 + y, z$; (vii) $-1 + x, y, 1 + z$.

Table S2. Short hydrogen contacts in Å.

D-H...π-System	D-H	H...π
N(11)-H(11A)... π (C21-C26)	0.99	2.21
N(21)-H(21A)... π (C11-C16)	0.99	2.30
N(31)-H(31A)... π (C41-C46)	0.99	2.27
N(41)-H(41B)... π (C31-C36)	0.99	2.21

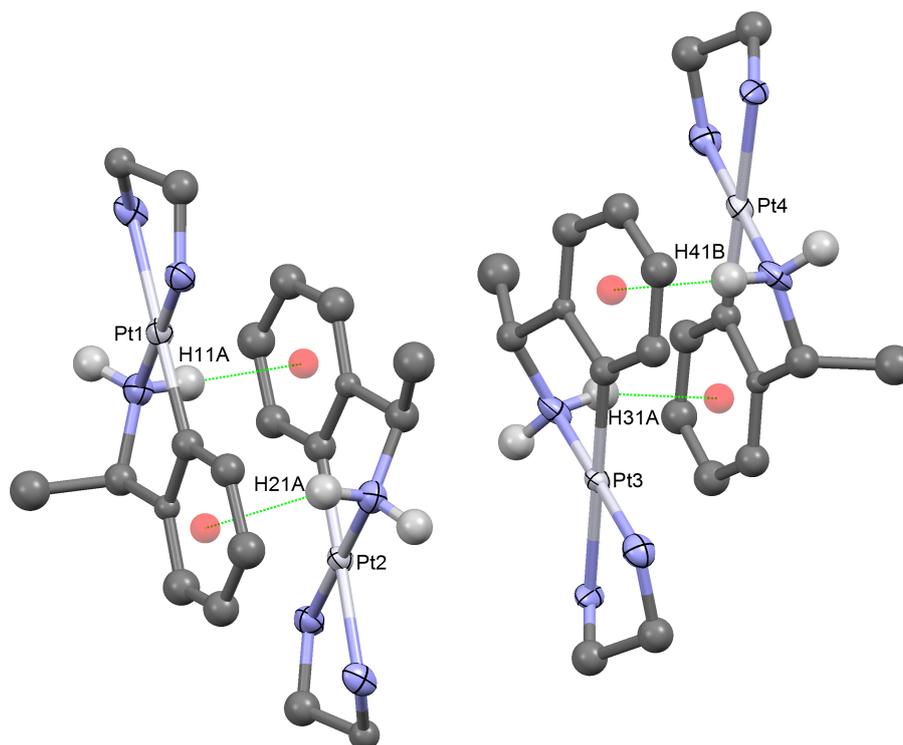


Figure S5. T stacking of cations. Most hydrogen atoms are omitted for clarity.

3. NMR-Spectroscopy

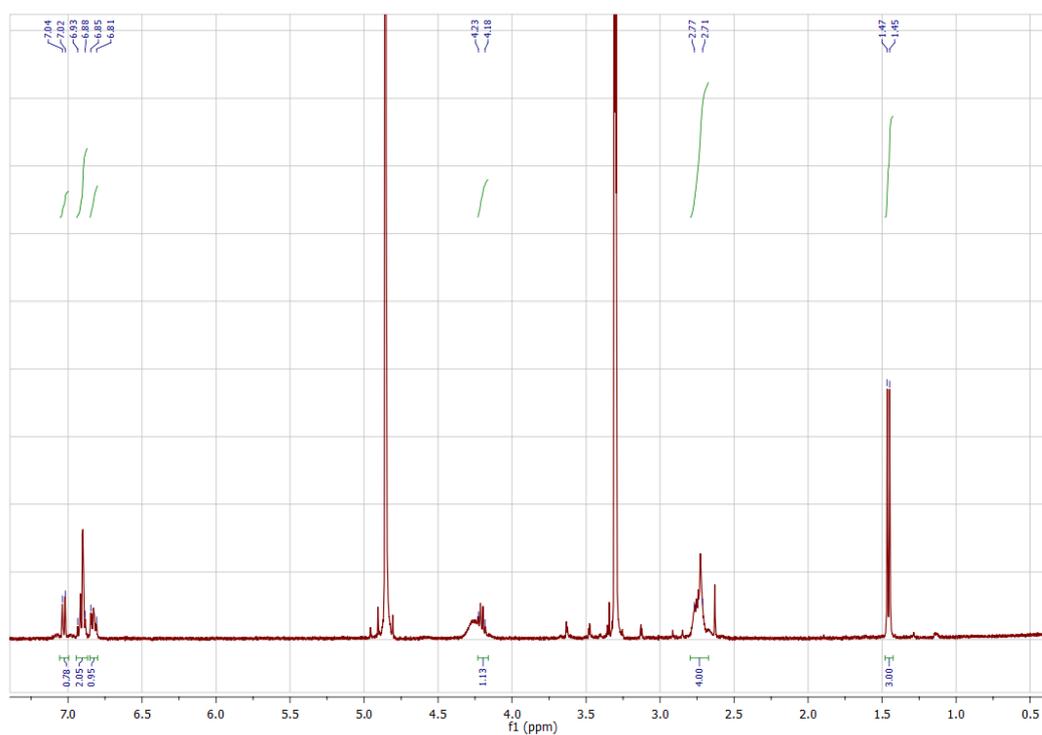


Figure S6. $^1\text{H-NMR}$ of 1, measured in CD_3OH .

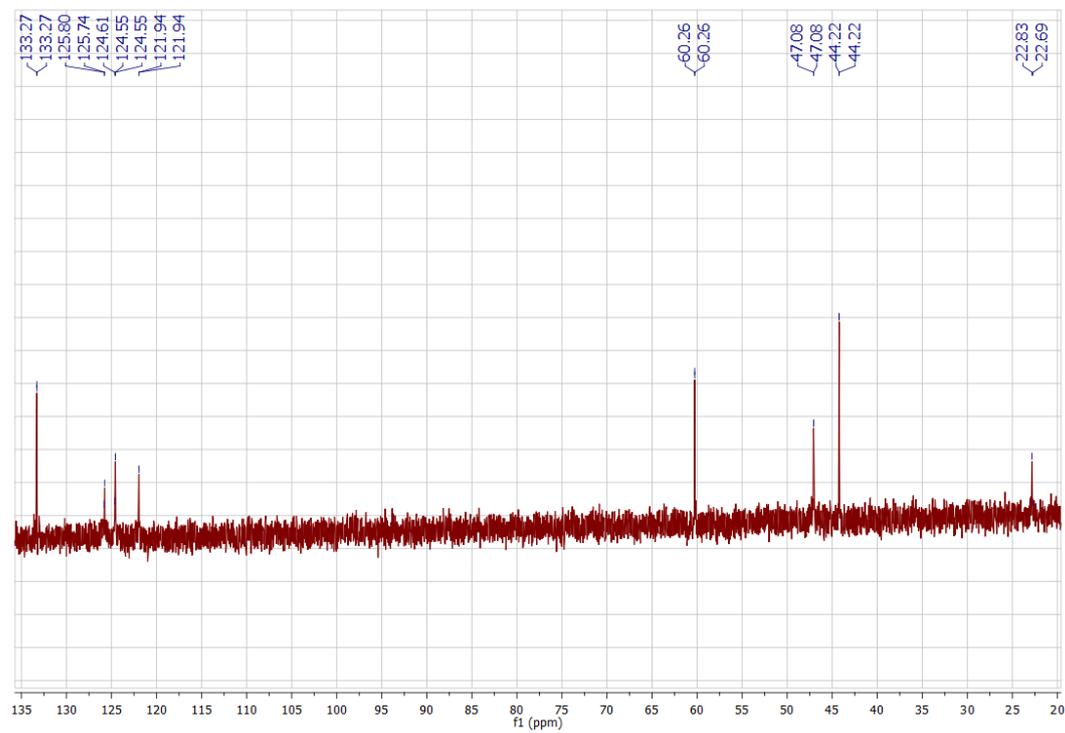


Figure S7. ^{13}C -NMR of **1**, measured in H_2O .

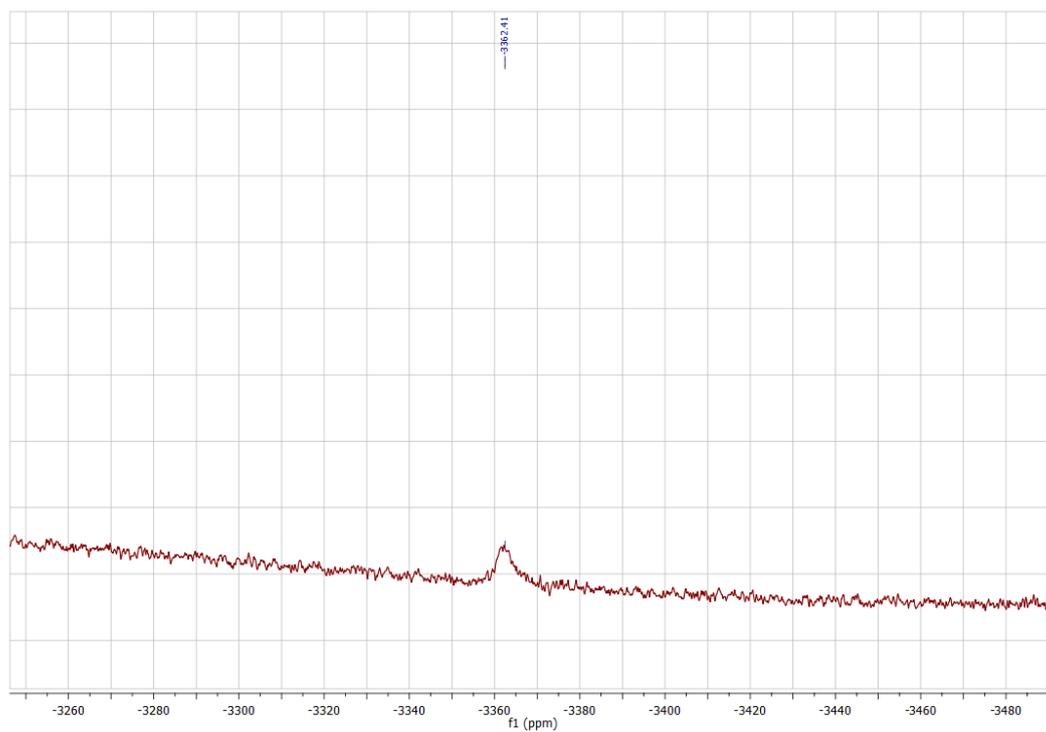


Figure S8. ^{195}Pt -NMR of **1**, measured in H_2O .

4. X-ray Powder Diffraction

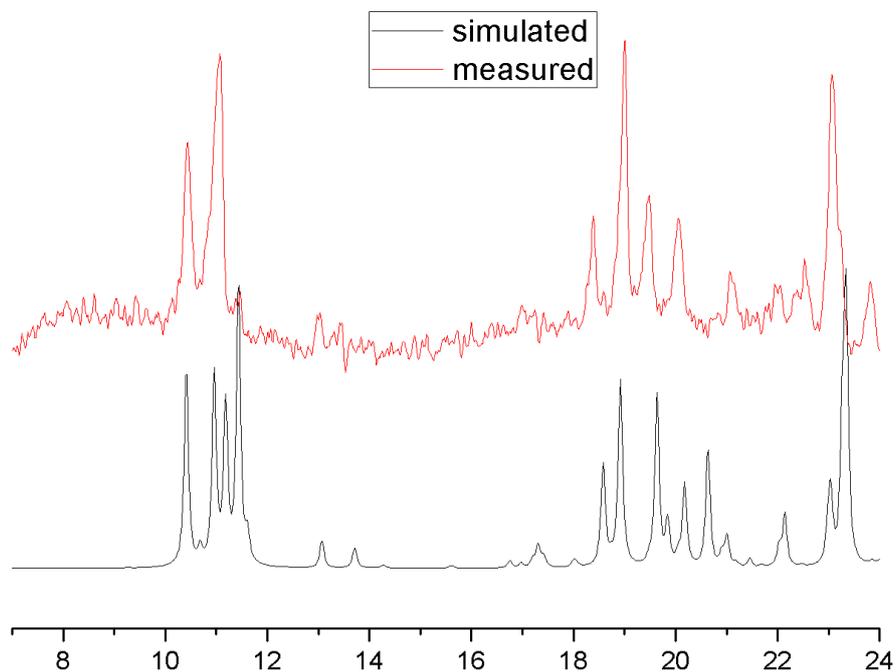


Figure S9. Powder diffraction pattern of **2** and simulated pattern based on the single crystal diffraction experiment. Small shifts between observed and simulated reflection positions are due to the temperature difference: The single crystal was measured at 100 K, whereas the experimental powder pattern was taken at room temperature.