

Supporting Information for

Small Molecule Activation Mediated by a Uranium Bipyridyl

Metallocene

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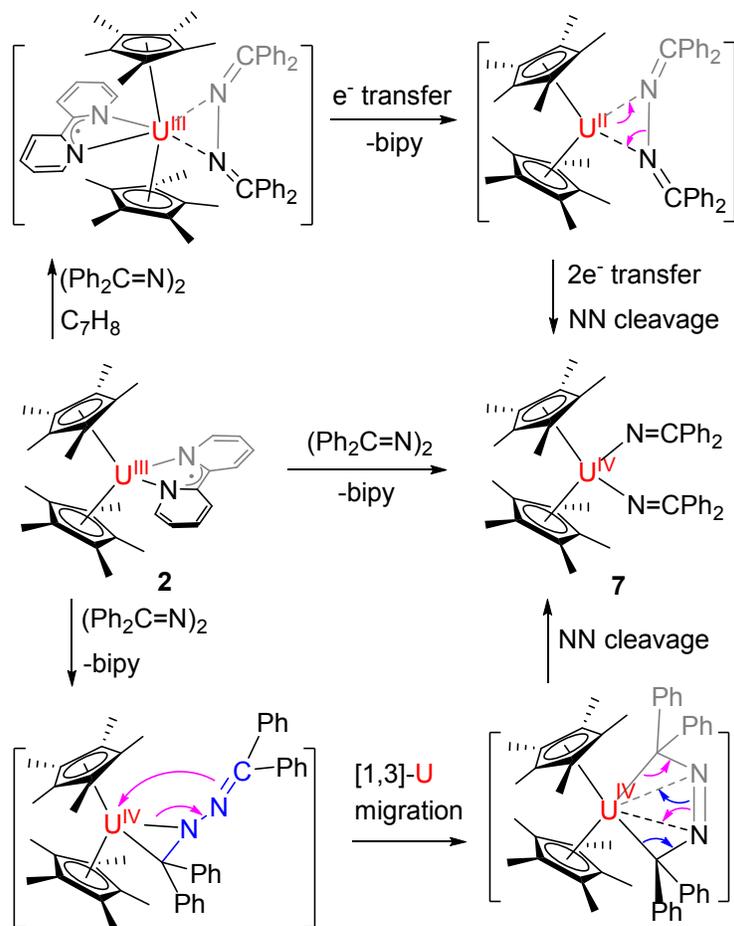
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Table of Content

| | |
|------------------------------|-----------|
| 1. Scheme and Figure | S2 |
| 2. Crystal parameters | S3 |

1. Scheme and Figure



Scheme S1. Synthesis of complex 7.

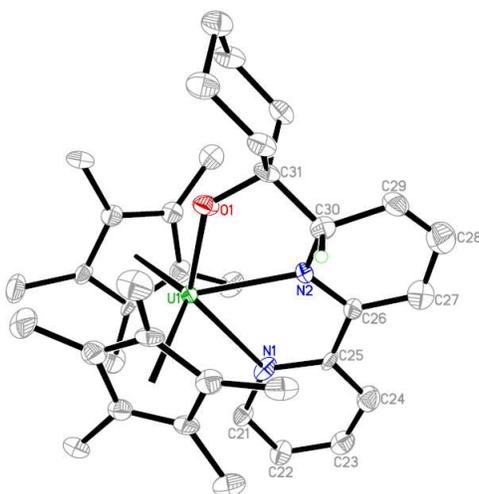


Figure S1. Molecular structure of **11** (thermal ellipsoids drawn at the 35% probability level).

Table S1. Crystal Data and Experimental Parameters for Compounds 8, 13b and 14

| Compound | 8 | 13b ·2C ₆ H ₆ | 14 |
|---------------------------------------------------------------|--------------------------------------------------|-------------------------------------------------------------------------------|---------------------------------------------------|
| Formula | C ₃₉ H ₆₃ N ₃ U | C ₈₂ H ₁₀₄ N ₄ O ₄ U ₂ | C ₃₀ H ₃₈ IN ₂ U |
| Fw | 811.95 | 1685.75 | 791.55 |
| crystal system | monoclinic | orthorhombic | monoclinic |
| space group | <i>P2₁/c</i> | <i>Pbcn</i> | <i>P2₁/c</i> |
| <i>a</i> (Å) | 10.051(1) | 11.796(1) | 10.552(1) |
| <i>b</i> (Å) | 20.195(1) | 16.927(1) | 14.422(1) |
| <i>c</i> (Å) | 17.898(1) | 36.159(1) | 18.308(1) |
| <i>α</i> (deg) | 90 | 90 | 90 |
| <i>β</i> (deg) | 90.03(1) | 90 | 90.39(1) |
| <i>γ</i> (deg) | 90 | 90 | 90 |
| <i>V</i> (Å ³) | 3632.98(18) | 7220.1(4) | 2786.03(4) |
| <i>Z</i> | 4 | 4 | 4 |
| <i>D</i> _{calc} (g/cm ³) | 1.484 | 1.551 | 1.887 |
| <i>μ</i> (Mo/Kα) _{calc} (cm ⁻¹) | 4.497 | 4.533 | 25.236 |
| size (mm) | 0.30 × 0.20 × 0.10 | 0.13 × 0.12 × 0.10 | 0.20 × 0.20 × 0.15 |
| <i>F</i> (000) | 1640 | 3360 | 1508 |
| 2θ range (deg) | 6.47 to 59.59 | 6.76 to 59.61 | 7.80 to 146.55 |
| no. of reflns, collected | 29733 | 47368 | 12222 |
| no of obsd reflns | 8959 | 9246 | 5434 |
| no of variables | 398 | 427 | 317 |
| abscorr (<i>T</i> _{max} , <i>T</i> _{min}) | 1.00, 0.68 | 1.00, 0.68 | 1.00, 0.57 |
| <i>R</i> | 0.036 | 0.044 | 0.028 |
| <i>R</i> _w | 0.057 | 0.064 | 0.067 |
| <i>R</i> _{all} | 0.058 | 0.097 | 0.031 |
| Gof | 1.03 | 1.02 | 1.05 |