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Supporting Information

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**Intervalent bis(μ -aziridinato) M^{II} - M^I Complexes (M = Rh, Ir)
Delocalized Metallo-Radicals or Delocalized Aminyl Radicals?**

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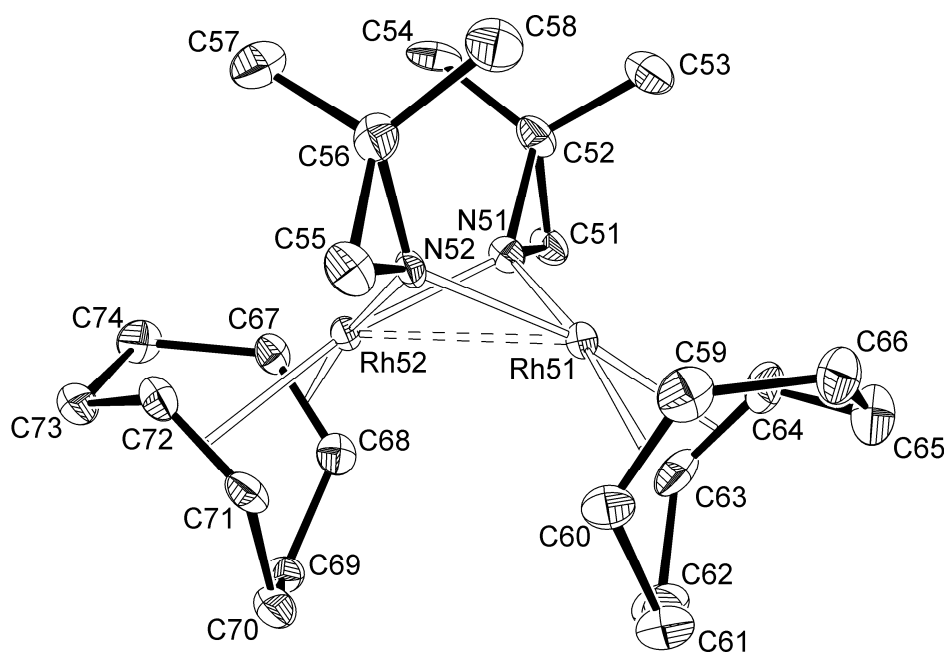


Figure S1. Structure (ORTEP at 50% level) of the second independent molecule of cation $[3]^+$

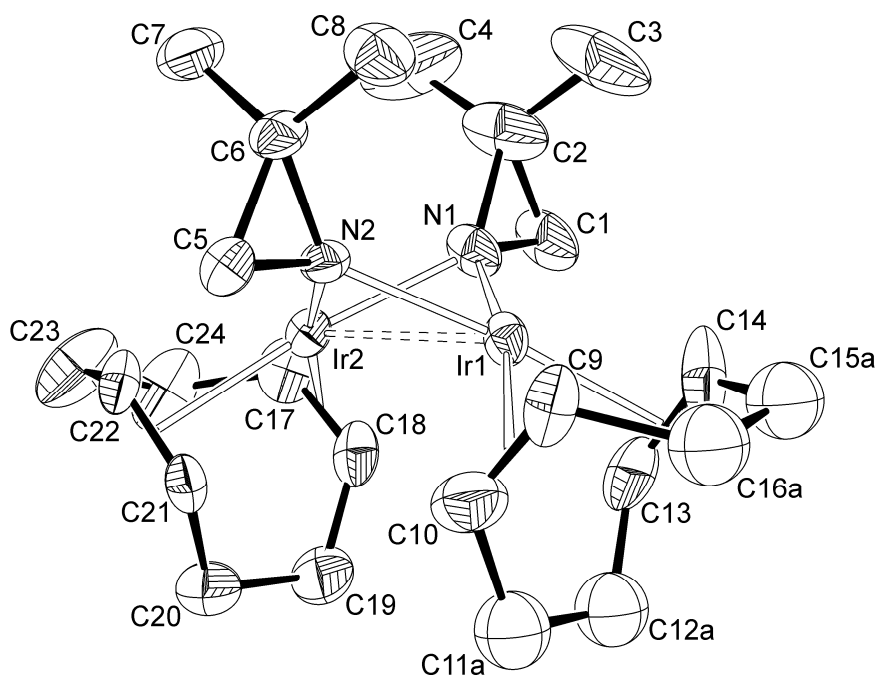


Figure S2. Structure (ORTEP at 50% level) of $[4]^+$

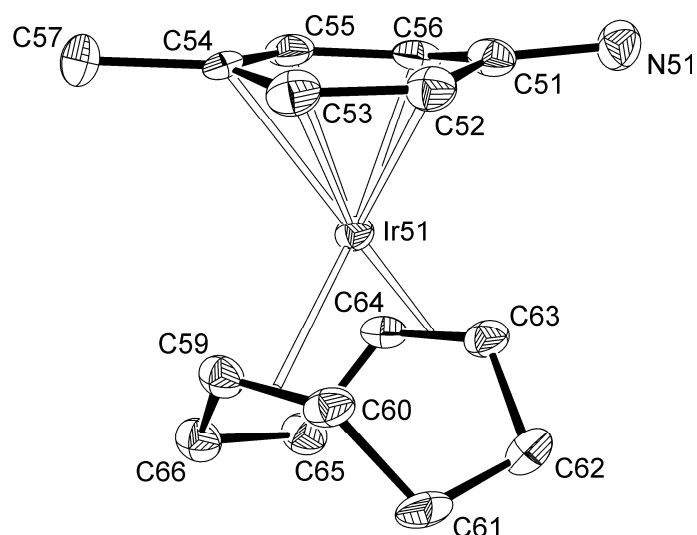


Figure S3. Structure (ORTEP at 50% level) of the second independent molecule of cation [7]⁺

Table S1. Selected bond distances (Å) and angles (°) of complex [7]⁺

| | | | |
|--|--------------------|----------------------------|--------------------|
| Ir1-C2 | 2.328(7), 2.305(8) | Ir1-Ct1 ^[a] | 2.017(8), 2.004(8) |
| Ir1-C3 | 2.247(8), 2.244(8) | Ir1-Ct2 ^[a] | 2.009(9), 1.983(9) |
| Ir1-C4 | 2.311(8), 2.320(7) | N1-C1 | 1.338(9), 1.370(9) |
| Ir1-C5 | 2.259(7), 2.280(7) | Ir1···C1 | 2.438(7), 2.416(7) |
| Ir1-C6 | 2.239(7), 2.235(7) | | |
| Ct1 ^[a] -Ir1-Ct2 ^[a] | 86.2(3), 86.7(3) | Ct1 ^[a] -Ir1-C3 | 100.8(3), 99.1(3) |
| C3-Ir1-C6 | 76.3(3), 76.7(3) | Ct2 ^[a] -Ir1-C6 | 99.0(3), 98.4(3) |

[a] Ct1 and Ct2 are the midpoints between C9-C10 and C13-C14, respectively.

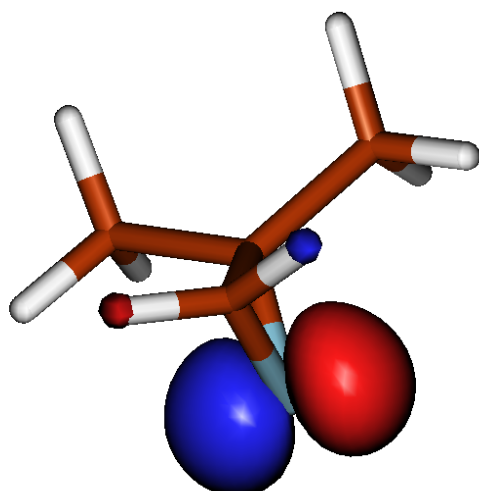


Figure S4. HOMO of the 2,2-dimethylaziridine anion

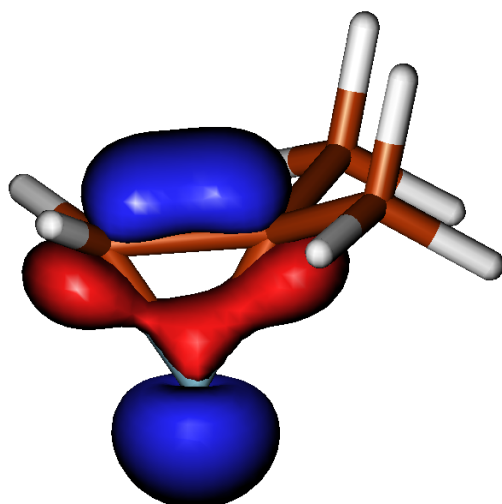


Figure S5. HOMO-1 of the 2,2-dimethylaziridine anion

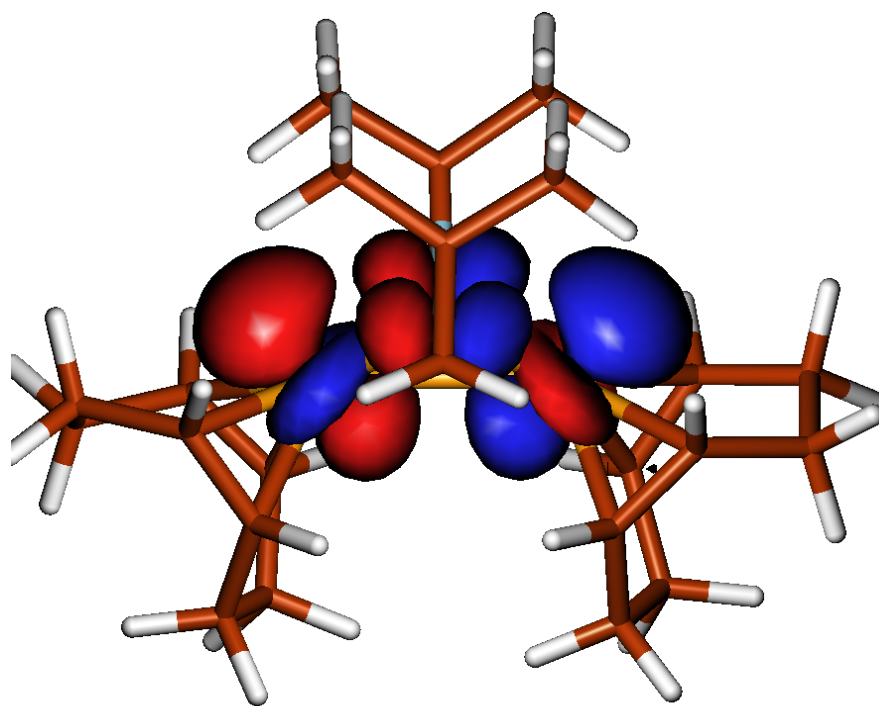


Figure S6. HOMO of complex $[3]^+$

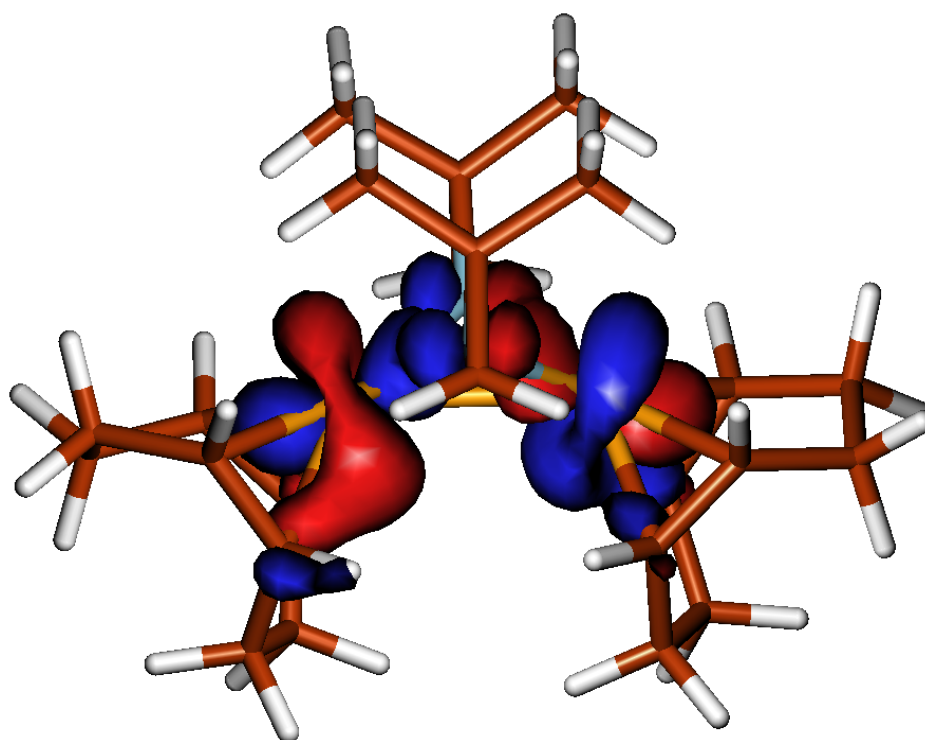


Figure S7. HOMO-2 of complex $[3]^+$

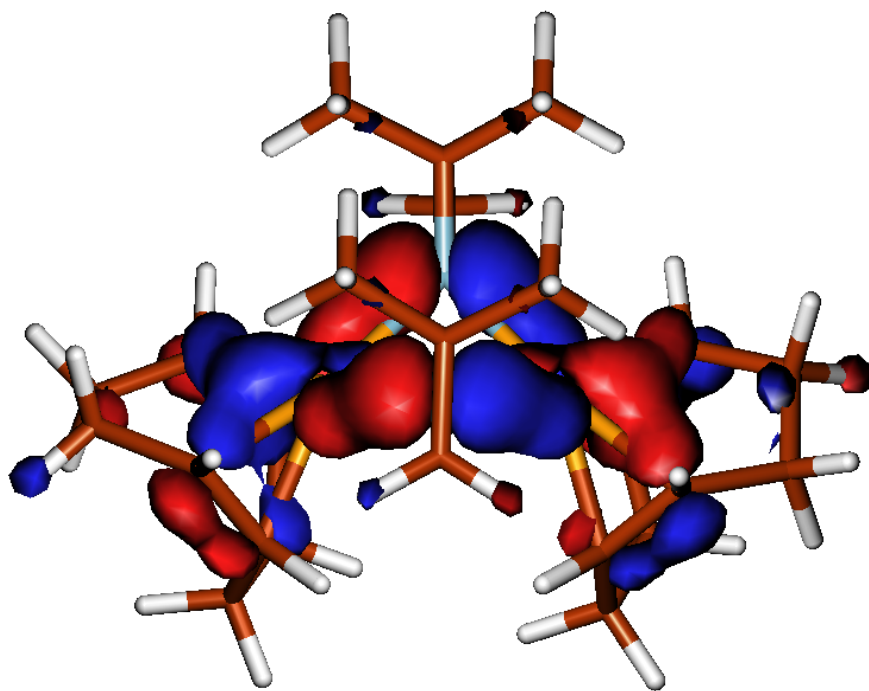


Figure S8. HOMO-8 of complex $[3]^+$

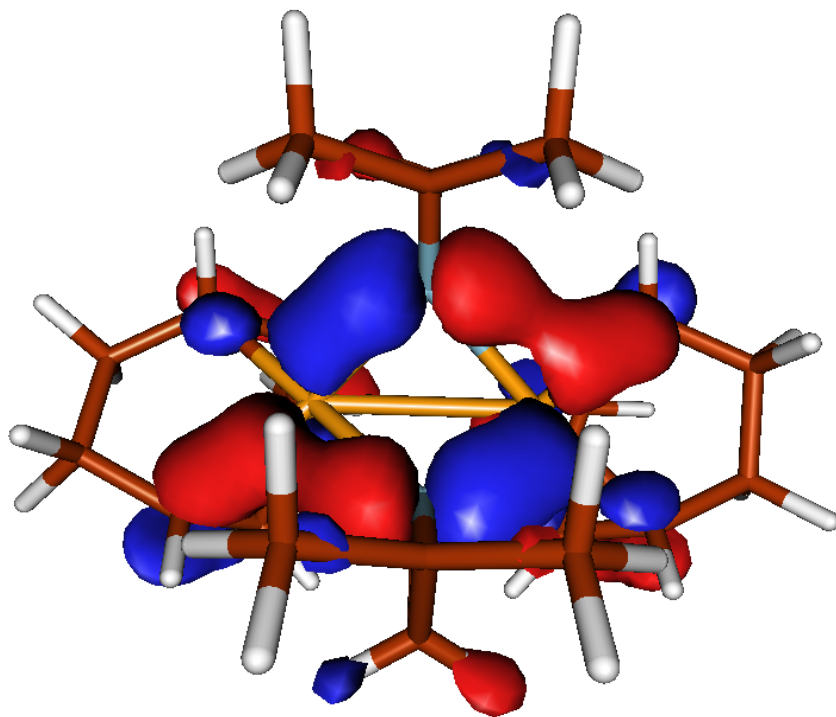


Figure S9. HOMO-9 of complex $[3]^+$

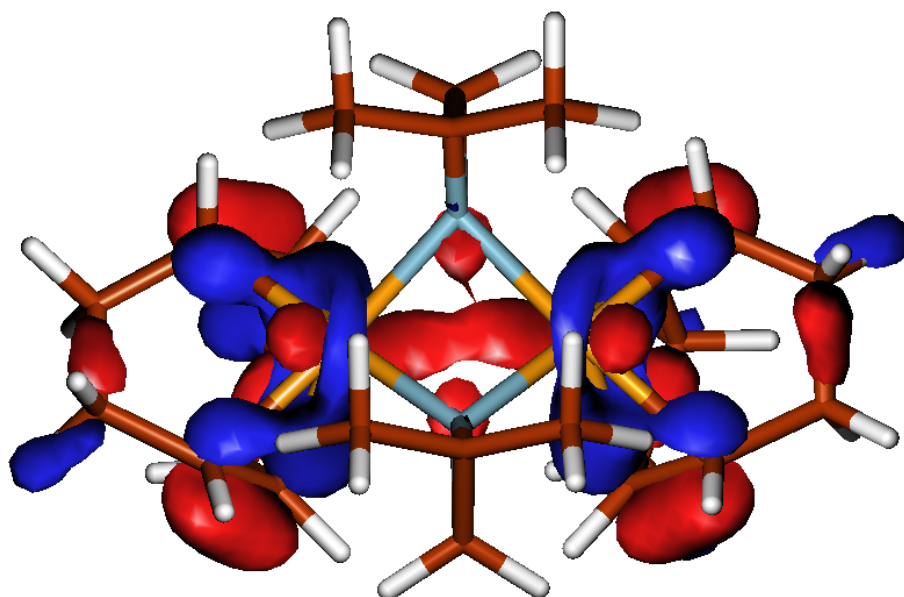


Figure S10. HOMO-11 of complex $[3]^+$

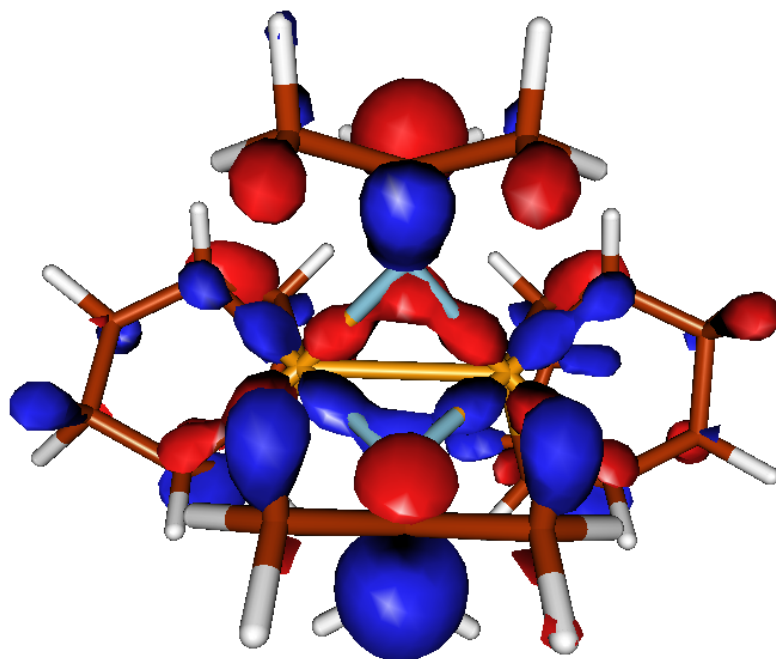


Figure S11. HOMO-12 of complex $[3]^+$

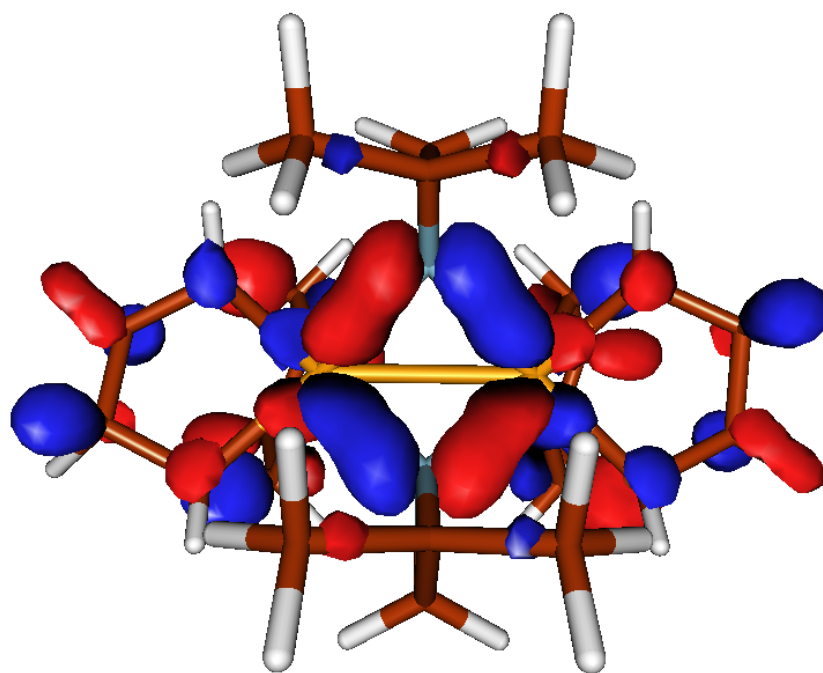


Figure S12. HOMO-13 of complex $[3]^+$

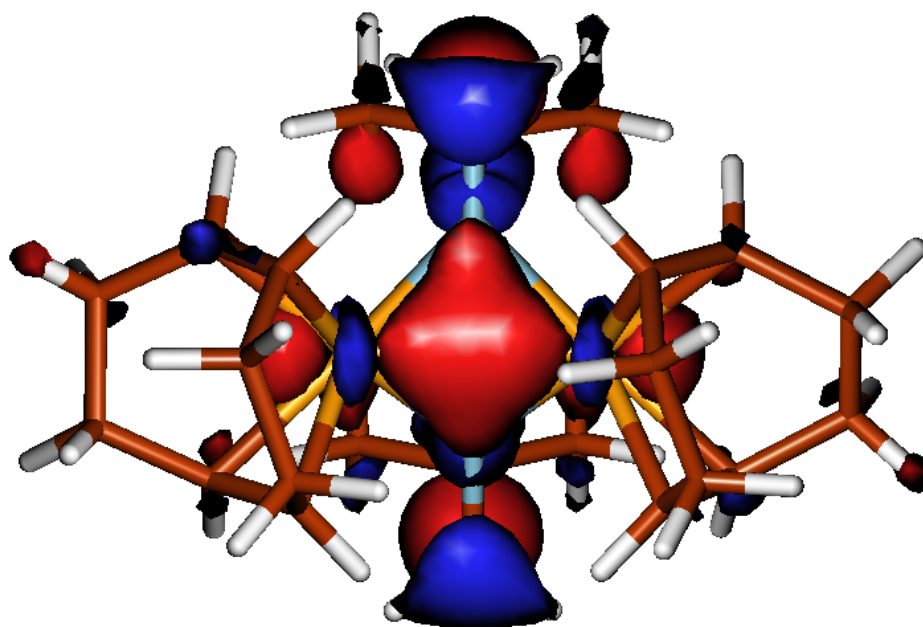


Figure S13. HOMO-15 of complex $[3]^+$ (top view).

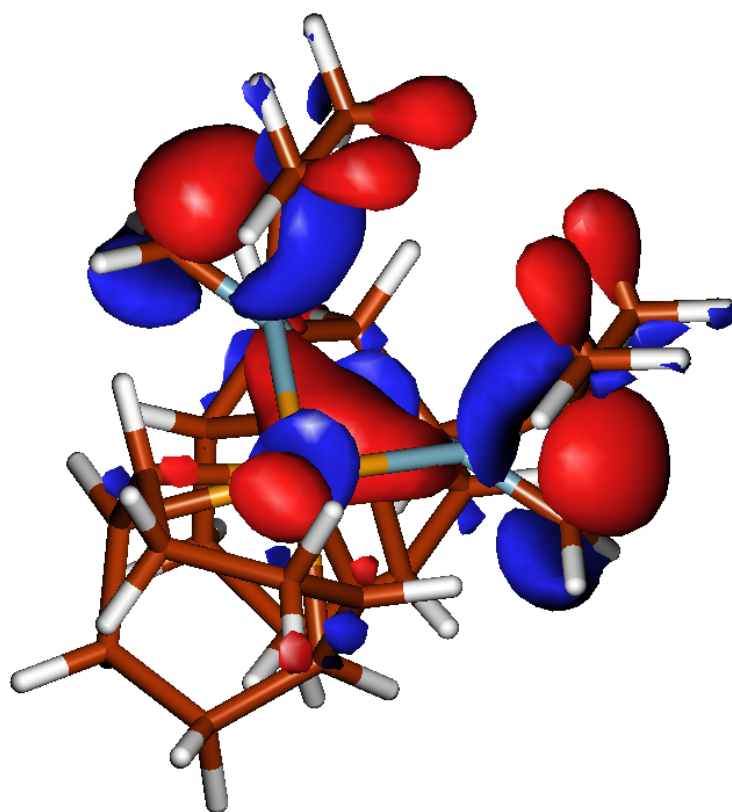


Figure S14. HOMO-15 of complex [3]⁺ (side view).