

Interplay between Ligand Field Strength and the Nephelauxetic Effect in Chromium(III) Complexes with Anionic Amido Ligands

- Supporting Information -

Polina Yaltseva,[‡] Benjamin Wittwer,[‡] Daniel Leitner, Florian Neururer, Frank Tambornino, Alina Schmidt, Dominik Munz,^{*} Oliver S. Wenger^{*} and Stephan Hohloch^{*}

Table of Contents

1. Experimental Procedures	3
2. NMR Spectroscopy	6
3. IR Spectroscopy.....	10
4. Mass spectrometry	11
5. Cyclic Voltammetry	13
6. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$	18
UV-vis transient absorption.....	18
Alternative Rehm-Weller fitting analysis	25
7. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$	26
Ground state UV-vis absorption	26
UV-vis transient absorption.....	26
8. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{PY}})_2]^+$	29
Ground state UV-vis absorption	29
UV-Vis transient absorption	29
9. Dependence of the non-radiative deactivation rate constant on the experimental and theoretical/calculated energy gaps	31
10. Photoredox catalysis with $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$	32
11. Crystallographic Information.....	38
13. Computational Details.....	42
Chromium MIC Complex $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$	43
XYZ Coordinates	62
12. References	79
13. Author Contributions	80

1. Experimental Procedures

Methods and experimental procedures

All chemicals for synthesis were purchased from commercial suppliers in reagent grade and used without any further purification. 3,6-di-*tert*-butyl-1,8-bis(3-methylimidazolin-2-yliden-1-yl)carbazolide bis(hexafluorophosphate) (H_3L^{NHC}),^[1] 3,6-di-*tert*-butyl-1,8-bis(4,5,6,7-tetrahydro-2H-[1,2,3]triazolo[1,5-a]pyridin-8-ium)carbazolide bisiodide (H_3L^{MIC}),^[2,3] 3,6-di-*tert*-butyl-1,8-di(pyridine-2-yl)-carbazole (H_3L^{PY}) and $[Cr(L^{PY})_2]PF_6$ were synthesized according to literature procedures.^[4] Solvents for synthesis and spectroscopy were purchased in extra dry (>99.5% purity) and HPLC grades, solvents for synthesis were additionally degassed via freeze-pump-thaw cycles.

NMR spectra were recorded on Bruker Avance III instruments with 250 or 400 MHz proton frequency. Deuterated solvents were purchased from Eurisotop (Cambridge Isotope Laboratories). Chemical shifts were reported in δ values in ppm and were referenced to the solvent residue peak.^[5]

Cyclic voltammetry was conducted under Ar atmosphere in an electrochemical cell containing a glassy carbon disk as the working electrode, a silver wire as the counter electrode, and a saturated calomel electrode (SCE) as the reference electrode. In case of the ferrocene/ferrocenium referenced CVs, they were measured using a three-electrode setup using a glassy carbon working electrode, a platinum counter electrode and a silver-wire pseudo reference electrode. Ferrocene was used an internal standard.

Steady-state absorption spectroscopy was measured on a Varian Cary 5000 UV-Vis-NIR instrument. UV-vis transient absorption measurements on the nanosecond timescale were carried out on an LP920-KS instrument from Edinburgh Instruments. A frequency-tripled pulsed Nd:YAG laser (Quantel Q-smart 450, ca. 10 ns pulse width) with a beam expander (BE02-355 from Thorlabs) in the beam path was used for excitation at 355 nm (pulse energy of ~100 mJ) and a frequency-doubled Nd:YAG laser (Quantel Brilliant b, ca. 10 ns pulse width) with a beam expander (GBE02-A from Thorlabs) in the beam path was used for excitation at 532 nm (pulse energy of ~70 mJ). An iCCD camera from Andor was used to detect transient absorption spectra, and single-wavelength kinetics were recorded with a photomultiplier tube (Hamamatsu). UV-vis transient absorption measurements on the picosecond timescale were carried out with a TRASS instrument from Hamamatsu and a mode-locked picosecond Nd:YVO₄/YAG laser from Ekspla (PL2251B-20-SH/TH/FH with PRETRIG option, ca. 30 ps pulse width) as excitation light source. The frequency-tripled (355 nm) output of this laser powered an Ekspla PG402-264 OPA with a resulting energy output of 6 mJ at 430 nm. UV-vis transient absorption measurements on the femtosecond timescale were carried out with a HARPIA-TA instrument (Light Conversion). Excitation light is generated by a PHAROS laser (Light Conversion, Yb:KGW laser, source wavelength of 1030 nm, pulse width of ca. 190 fs, pulse energy ~0.2 mJ), and the actual pump light wavelength was generated by an OPA ORPHEUS (Light Conversion, used ~ 90% of fundamental pulse). The probe light was generated by a sapphire (5 mm thickness; ~10% of the fundamental pulse were used to generate a white light super-continuum).

Elemental analysis was carried out by Sylvie Mittelheisser on a Vario Micro Cube instrument (University of Basel, Department of Chemistry) and by Roland Egger on a Vario Unicube Instrument (University of Innsbruck, Department of General, Inorganic and Theoretical Chemistry). Electrospray ionization high resolution mass spectra (ESI-HRMS) were recorded by Dr. Michael Pfeffer (University of Basel, Department of Chemistry) on a Bruker maxis 4G ESI-Q-TOF instrument and by Dr. Thomas Müller on a Thermo Fisher Scientific, Q Exactive hybrid quadrupole-Orbitrap mass spectrometer instrument (University of Innsbruck).

All photochemical transformations were carried out on an NMR scale. The typical experimental setup included: an NMR tube placed in a beaker with cold water and the light source - 520 nm Kessil LED lamp.

EPR measurements were performed on a Bruker Magnettech ESR5000 X-band spectrometer with a temperature control unit in 3 mm o.d. fused silica tubes. Spectro electrochemistry was performed using a BioLogic potentiostat with a three-electrode

array (working electrode: platinum, counter electrode: platinum, reference electrode: silver) with $\text{NBu}_4\text{BArF}_{24}$ as supporting electrolyte. Analysis was performed using the EasySpin package for MatLab. Values were obtained by least-squares fitting to the experimental spectra using the garlic and pepper functions.^[6]

X-ray diffraction crystallography was performed at the University of Innsbruck (Bruker D8 Quest) All crystals were kept at low temperatures throughout data collection. Data collection, refinement and reduction was performed using the ApexIV. All structures were solved with SHELXT^[7] and refined using the OLEX 2 software package^[8] using SHELXL^[9] least square refinements. Strongly disordered solvent molecules have been removed using the SQUEEZE operation.^[10] All nonhydrogen atoms were refined anisotropically, and hydrogen atoms were included at the geometrically calculated positions and refined using a riding model.

Synthesis of the Cr^{III} complexes

[Cr(L^{MIC})₂]BF₄: The pro-ligand azolium salt [H₃L^{MIC}][I]₂ (400 mg, 0.514 mmol, 2.0 eq) was dissolved in THF (5.0 mL) and stirred for one minute before being cooled to -40 °C. To this, LiHMDS (301 mg, 1.80 mmol, 7.0 eq) was added as a solution in THF (5.0 mL, cooled to -40 °C) and the reaction mixture turned first dark red in colour, followed by a colour change to vibrant green and strongly fluorescent. The deprotonation reaction is stirred for 30 min while warming to room temperature. During this time, CrCl₂ (31.6 mg, 0.257 mmol, 1.0 eq) was suspended in THF (5.0 mL) and cooled to -40 °C as well. The deprotonated ligand was then slowly added at -40 °C to the chromium chloride suspension, resulting in a dark red/ brown reaction mixture, which was stirred overnight at room temperature. The next day, the reddish-brown reaction mixture was evaporated to dryness and taken out of the glovebox. The residue was dissolved in acetone and NaBF₄ (329 mg, 3.00 mmol, 10 eq) was added as a solid. The mixture was stirred for 30 min in an open flask and then slowly diluted with water to form a brown-orange precipitate/suspension. The solid was filtered off, and re-dissolved in acetone. This procedure was repeated two more times, to ensure complete anion exchange to tetrafluoroborate. The orange precipitate is dried in air and purified by flash column chromatography using dichloromethane/methanol (99:1). It is recommended to use a long (30 cm) column to ensure good separation from the remaining impurities. Finally, the orange material is recrystallized by slow (vapour) diffusion of pentane into dichloromethane at room temperature to give the title compound as large, transparent orange blocks in a yield of 50% (151 mg, 0.127 mmol). Anal. calcd. for [Cr(L^{MIC})₂]BF₄ (%): C, 65.13; H, 6.49; N, 16.62. Found (%): C, 65.43; H, 6.75; N, 16.10. HRMS (ESI, positive mode): calcd. for [Cr(L^{MIC})₂]⁺ (m/z): 1092.5779. Found (m/z): 1092.5726.

[Cr(L^{NHC})₂]PF₆: The pro-ligand [H₃L^{NHC}][I]₂ (84.0 mg, 115 μmol, 2.0 eq) was charged into a 25 mL Schlenk flask, which was evacuated and refilled with nitrogen (3 cycles). Dry and deaerated THF (10 mL) was added to the flask and the solution was cooled down to -78 °C, followed by a dropwise addition of LiHMDS (1 M in THF, 559 μL, 559 μmol, 8 eq). After completing the addition, the mixture was stirred at -78 °C for 30 minutes, followed by the dropwise addition of a solution containing CrCl₂ (7.20 mg, 59.0 μmol, 1.02 eq) in dry and deaerated THF (5.0 mL). The mixture was subsequently allowed to gradually warm up to room temperature and was then stirred for 16 hours at this temperature. The resulting dark orange suspension was filtered through celite, and the celite layer was further washed with dichloromethane. The filtrate was concentrated *in vacuo*, and the resulting solid was suspended in 2 mL of THF. The bright orange precipitate was then filtered and washed with an additional 2 mL of cold THF. The crude product was dissolved in 1 mL of acetone, and saturated aqueous KPF₆ was added. (*Note: For the preparation of the [BF₄]⁻ salt, NaBF₄ is used instead of KPF₆*). The mixture was stirred at room temperature for 30 minutes, followed by filtration of the precipitate. The precipitate was then washed with 5 mL of diethyl ether and dried *in vacuo*. Finally, the product (15.0 mg, 13.9 μmol, 24%) was obtained as dark orange needle-like crystals after recrystallization via solvent layering (dichloromethane – diethyl ether).

Anal. calcd. for [Cr(L^{NHC})₂]PF₆·(H₂O) (%): C, 61.59; H, 6.09; N, 12.82. Found (%): C, 61.48; H, 5.86; N, 12.75. HRMS (ESI, positive mode): calcd. for [Cr(L^{NHC})₂]⁺ (m/z): 928.4720. Found (m/z): 928.4724.

[Cr(L^{NHC})₂]BF₄: Anal. calcd. for [Cr(L^{NHC})₂]BF₄·(CH₂Cl₂) (%): C, 62.19; H, 6.04; N, 12.72. Found (%): C, 61.89; H, 5.74; N, 12.42.

HRMS (ESI, positive mode): calcd. for [Cr(L^{NHC})₂]⁺ (m/z): 928.4720. Found (m/z): 928.4694.

2. NMR Spectroscopy

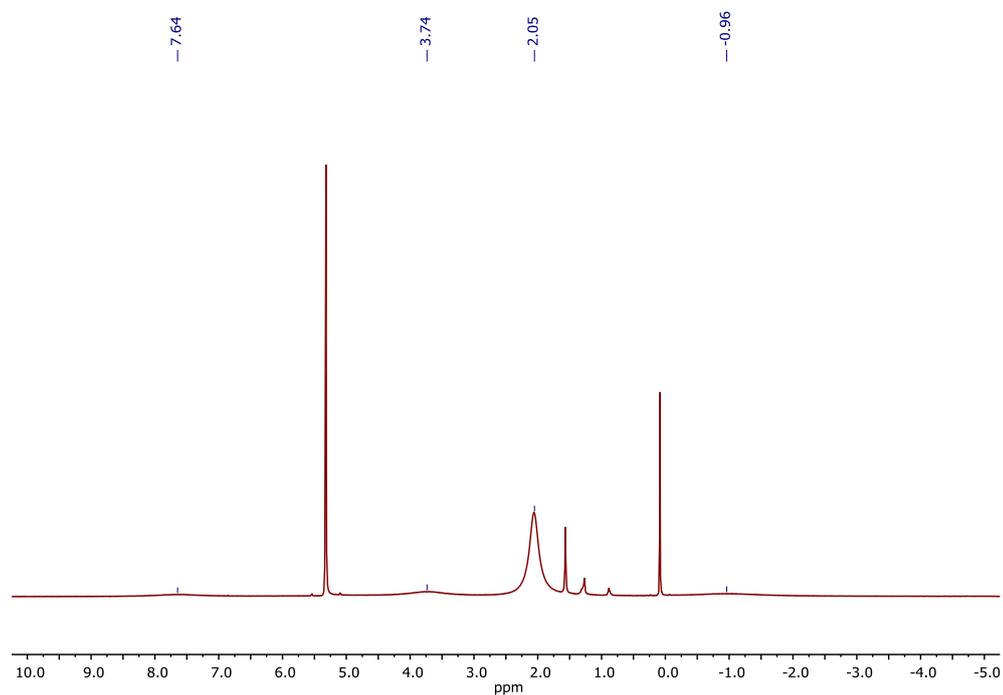


Figure S1: ^1H NMR of $[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from +10 – -5 ppm.

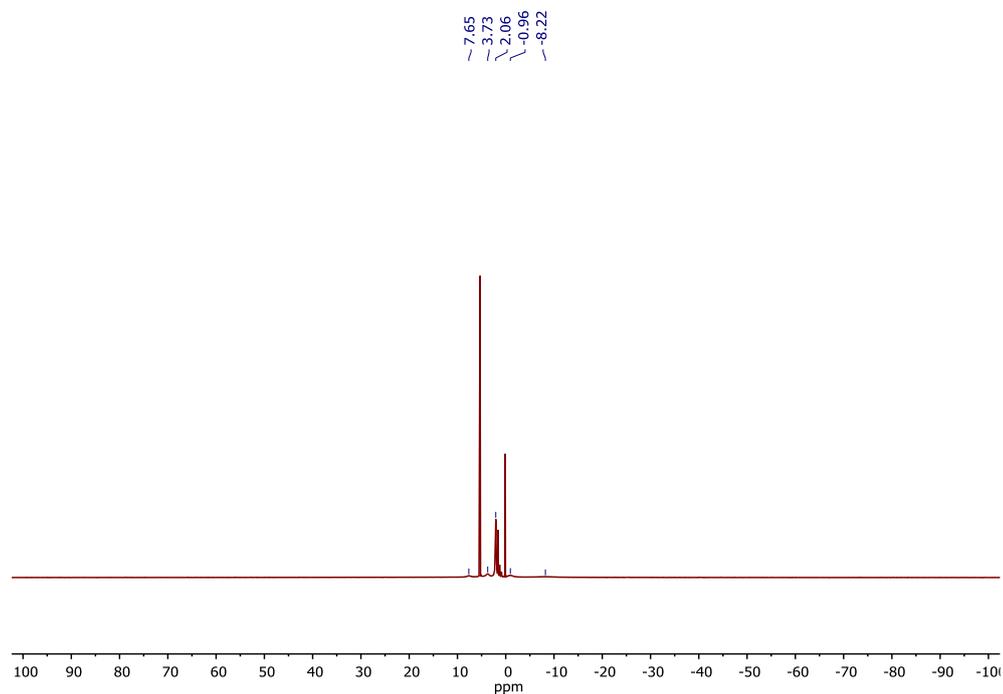
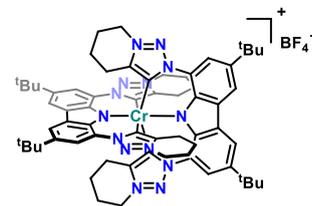
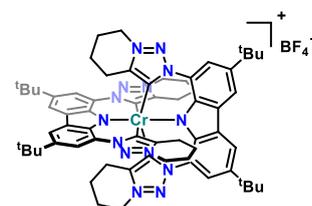


Figure S2: ^1H NMR of $[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from +100 – -100 ppm.



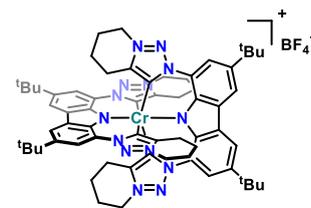
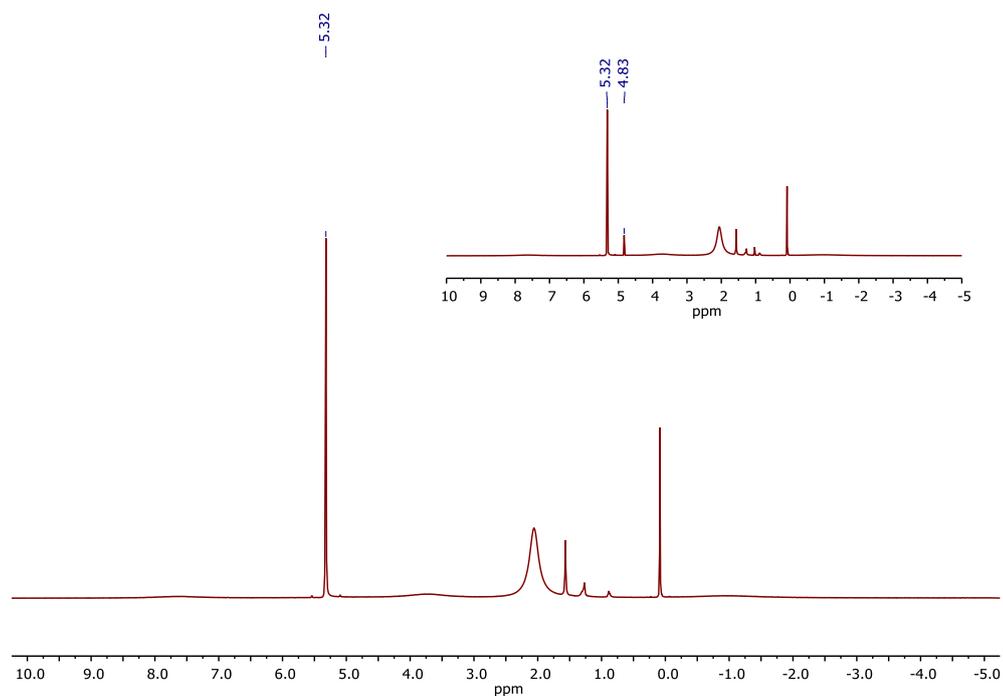


Figure S3: ^1H NMR of $[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from +10 – -5 ppm. Inlay shows the NMR from the Evans Method measurement showing the peak difference between the NMR solvent and the internal standard (NMR solvent in the capillary)

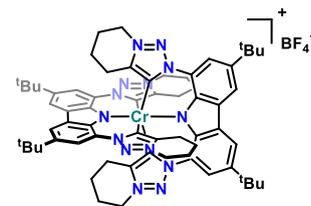
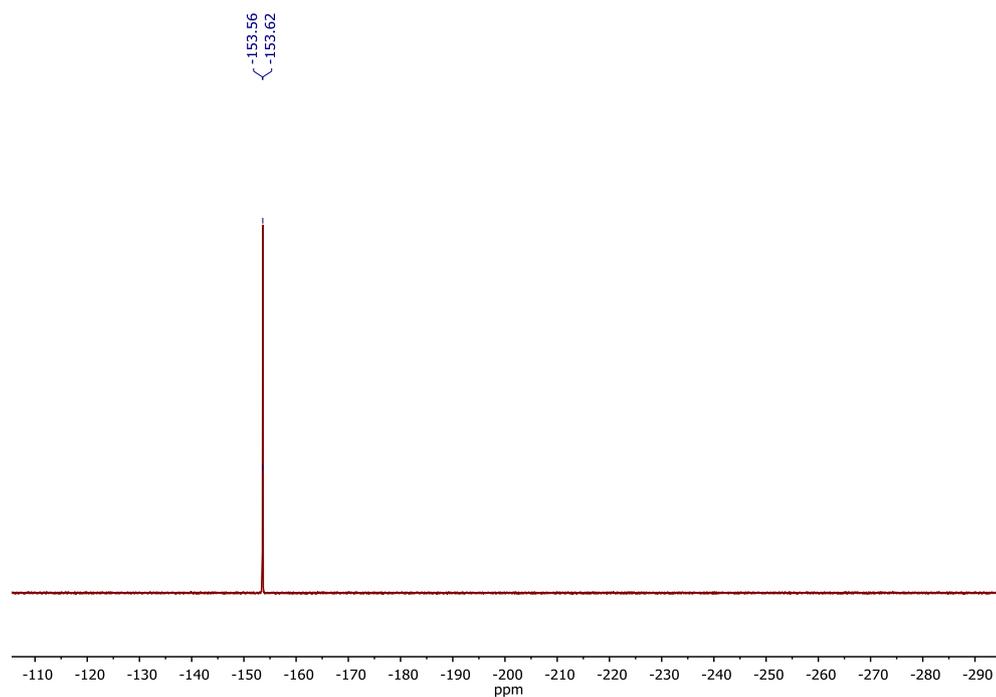


Figure S4: ^{19}F NMR of $[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from -110 – -290 ppm.

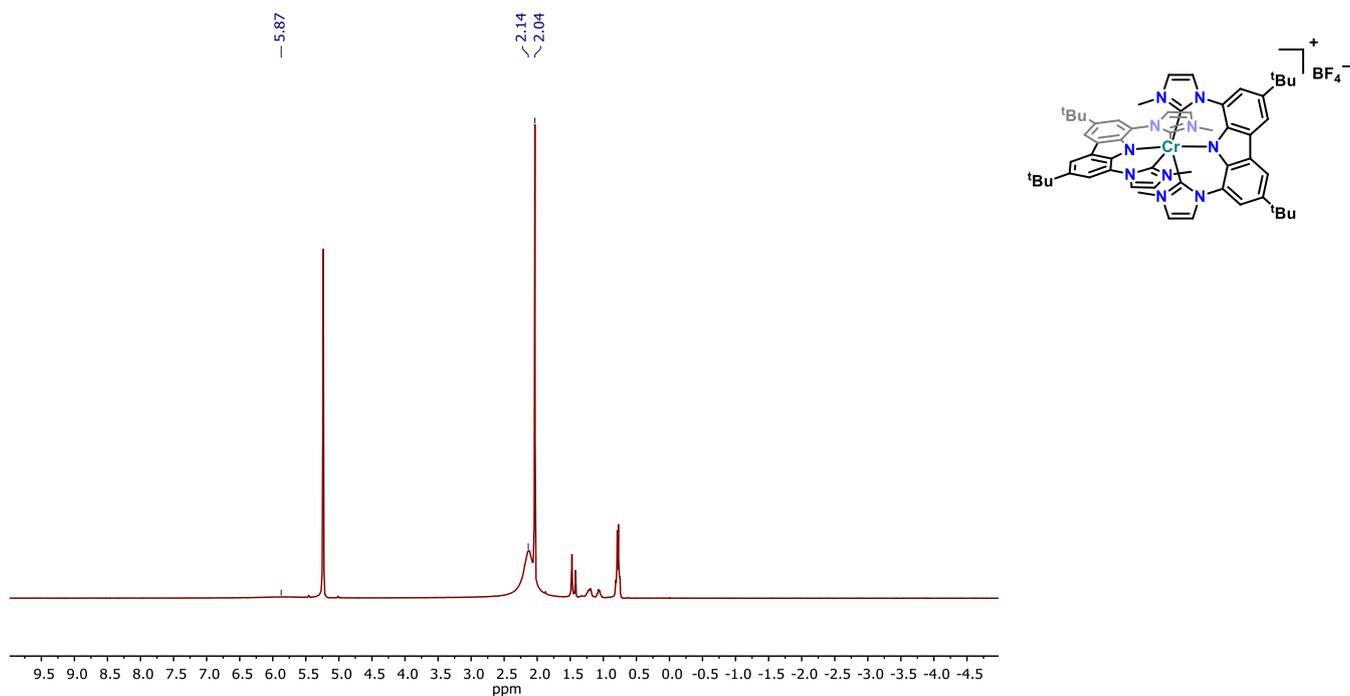


Figure S5: 1H NMR of $[Cr(L^{NHC})_2][BF_4]$ in CD_2Cl_2 at 298 K from +10 – –5 ppm.

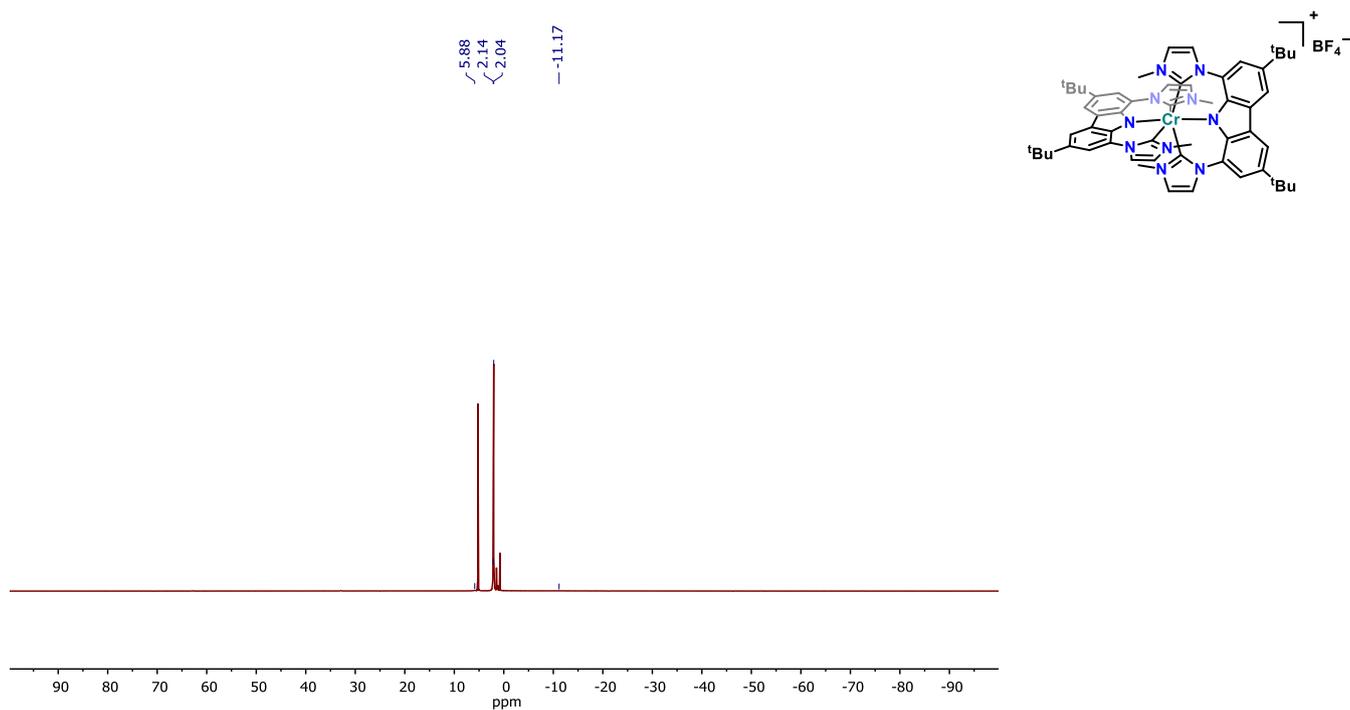


Figure S6: 1H NMR of $[Cr(L^{NHC})_2][BF_4]$ in CD_2Cl_2 at 298 K from +100 – –100 ppm.

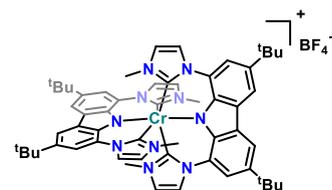
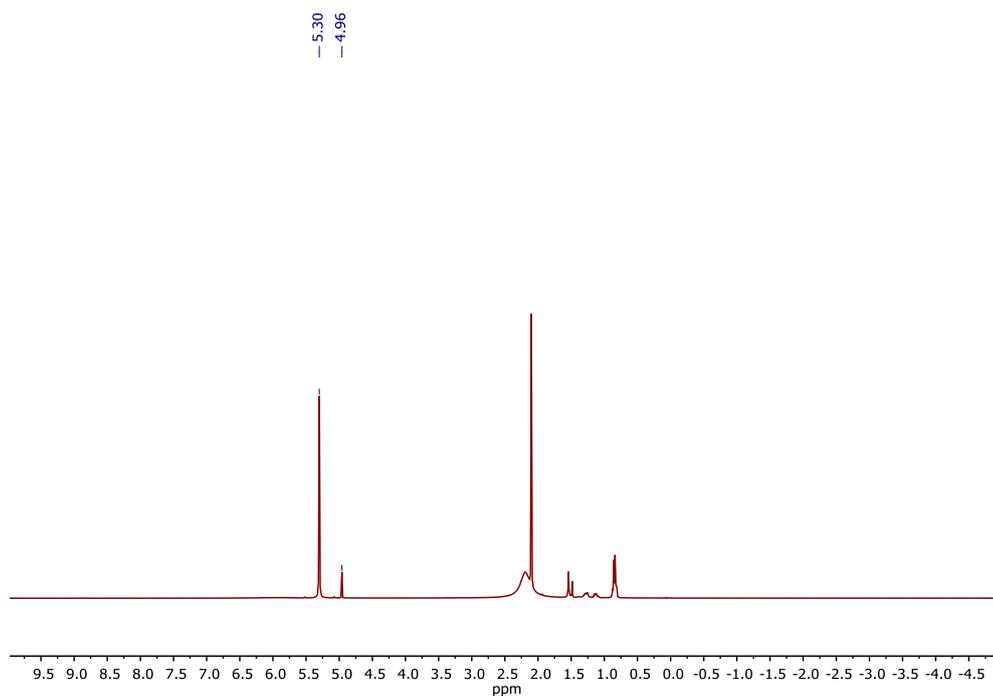


Figure S7: ^1H NMR of $[\text{Cr}(\text{L}^{\text{NHC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from +10 – –5 ppm. The Evans Method measurement showing the peak difference between the NMR solvent and the internal standard (NMR solvent in the capillary)

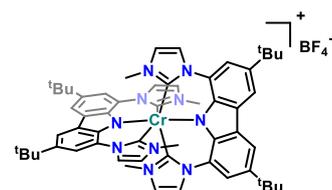
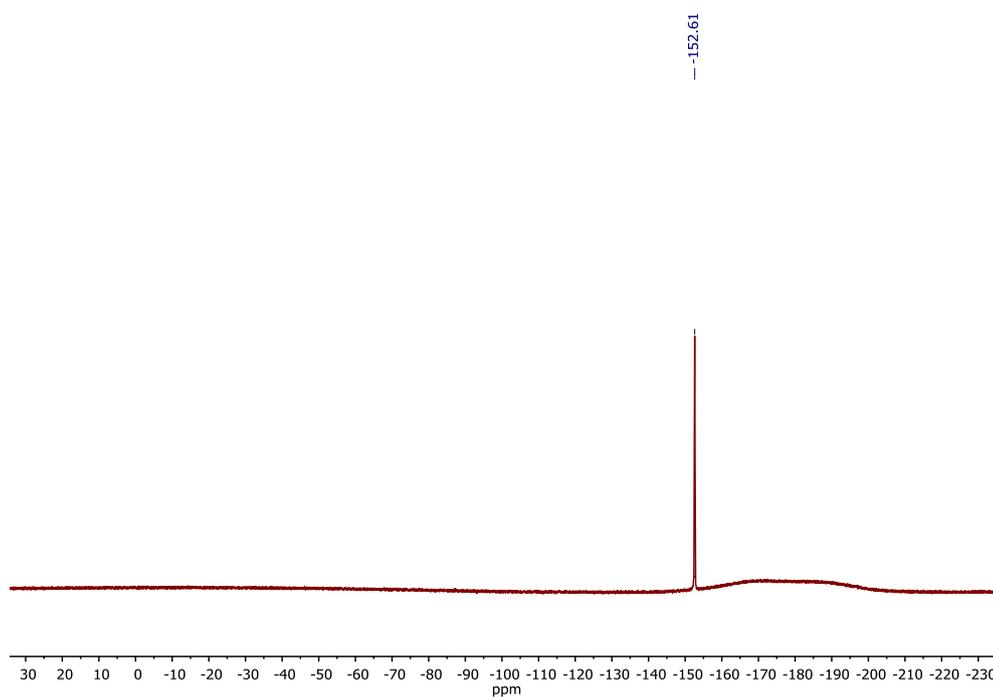


Figure S8: ^{19}F NMR of $[\text{Cr}(\text{L}^{\text{NHC}})_2][\text{BF}_4]$ in CD_2Cl_2 at 298 K from +30 – –230 ppm.

4. Mass spectrometry

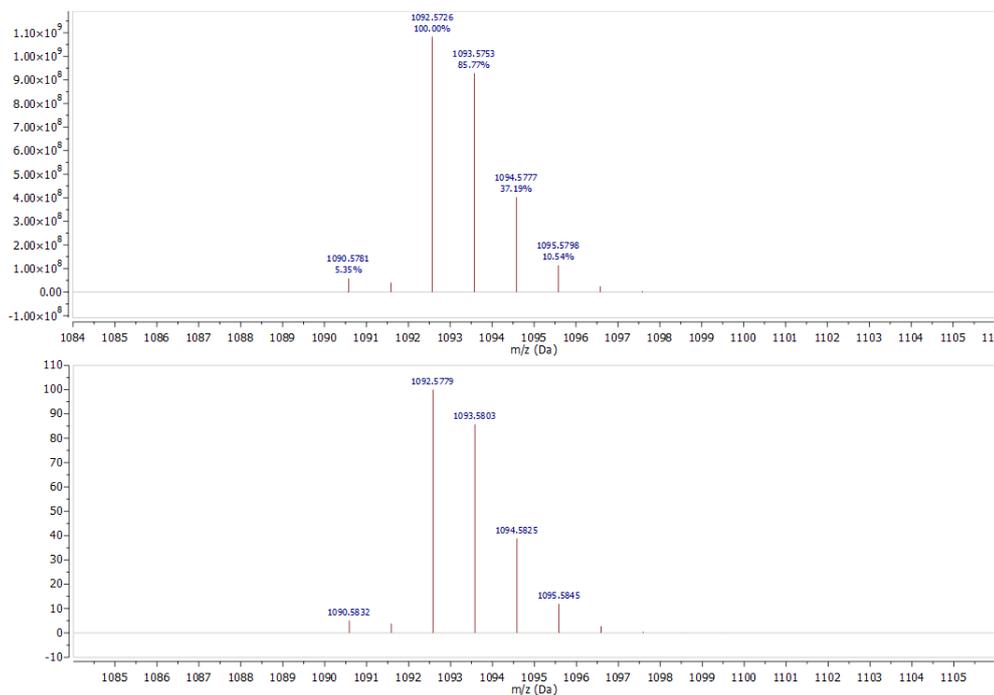


Figure S11: Experimental (top) and simulated (bottom) HR-ESI(+)-MS spectra of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$.

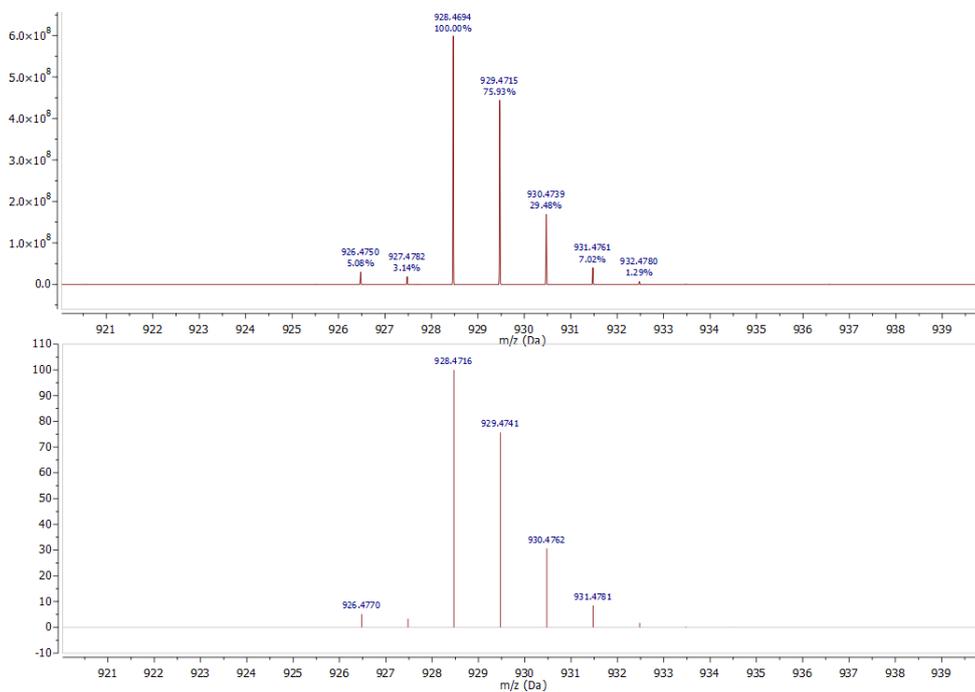


Figure S12: Experimental (top) and simulated (bottom) HR-ESI(+)-MS spectra of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$, from $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{BF}_4$ sample.

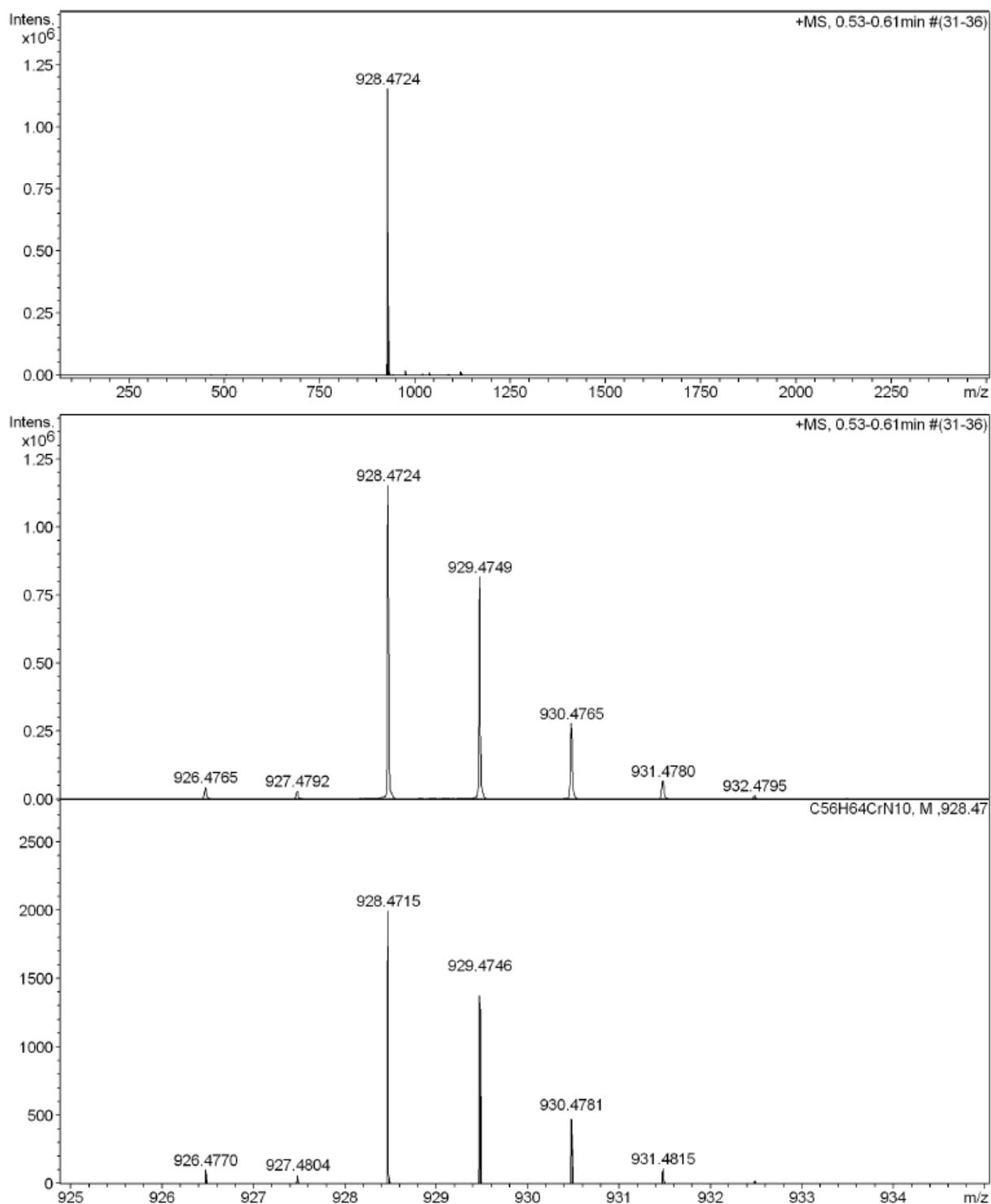


Figure S13: Experimental (top) and simulated (bottom) HR-ESI(+)-MS spectra of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$, from $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{PF}_6$ sample.

5. Cyclic Voltammetry

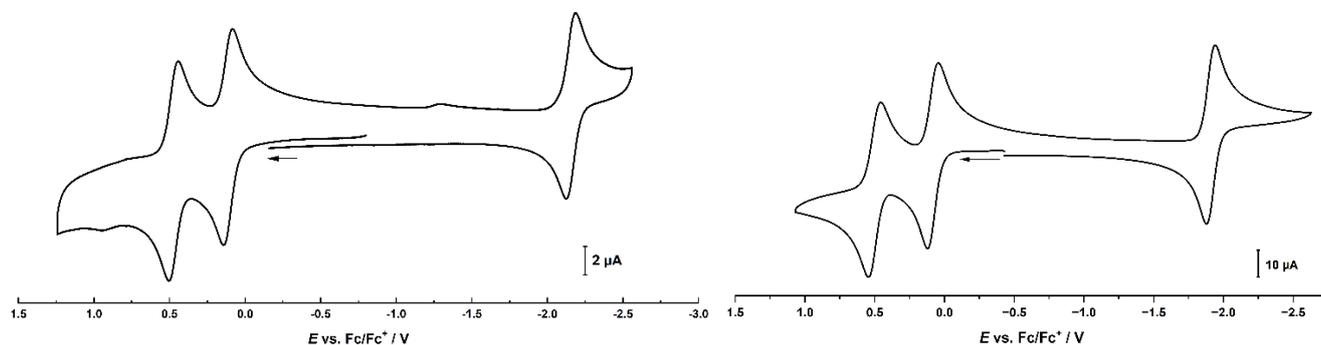


Figure S14: Cyclic voltammogram of 1 mM $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$ (left) and $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{PF}_6$ (right) in dry and deaerated acetonitrile with 0.2 M NBu_4PF_6 as the supporting electrolyte measured against ferrocene as an internal standard. A glassy carbon disk was used as the working electrode, platinum wire was used as a counter electrode and a silver wire was used as a pseudo-reference electrode.

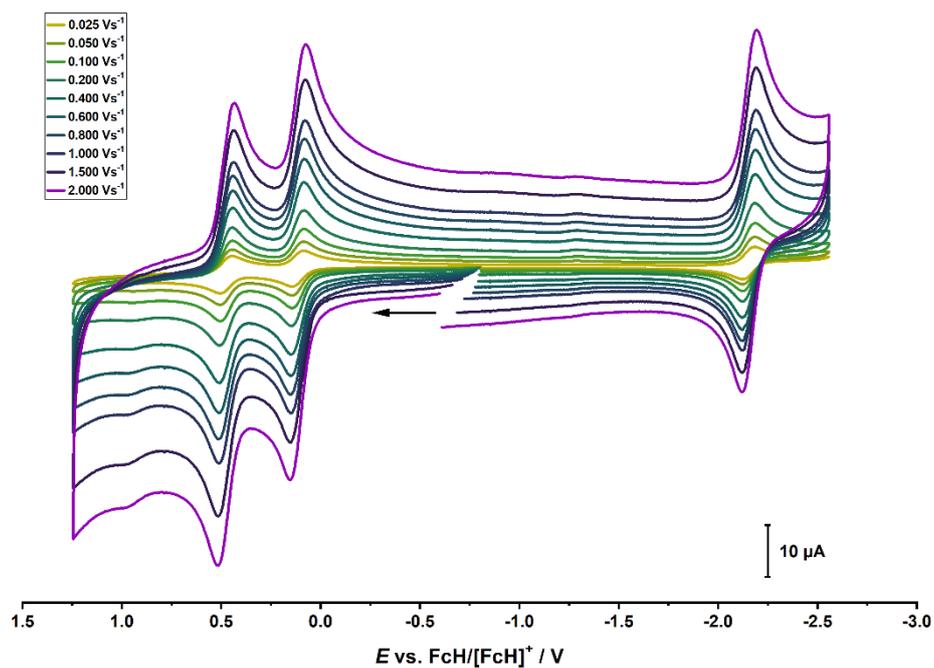


Figure S15: Cyclic voltammogram of 1 mM $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$ recorded at various scan rates between 25 – 2000 mV s^{-1} in 0.2 M NBu_4PF_6 in MeCN at 298 K.

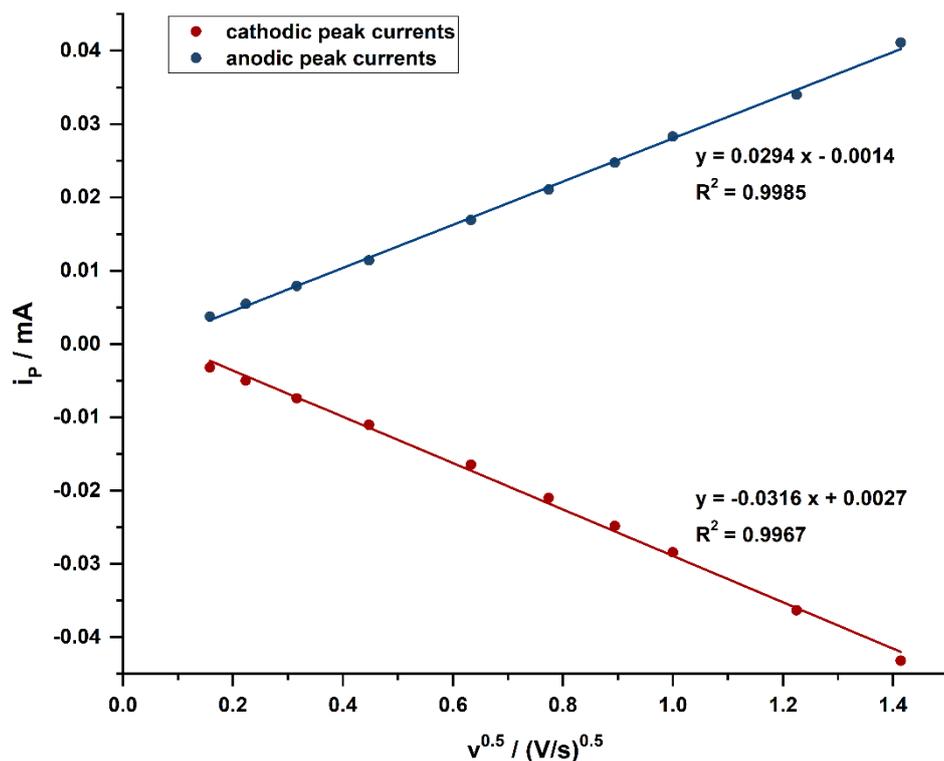


Figure S16: Randles-Sevcik plot of the first oxidation process for $[Cr(L^{MIC})_2]BF_4$.

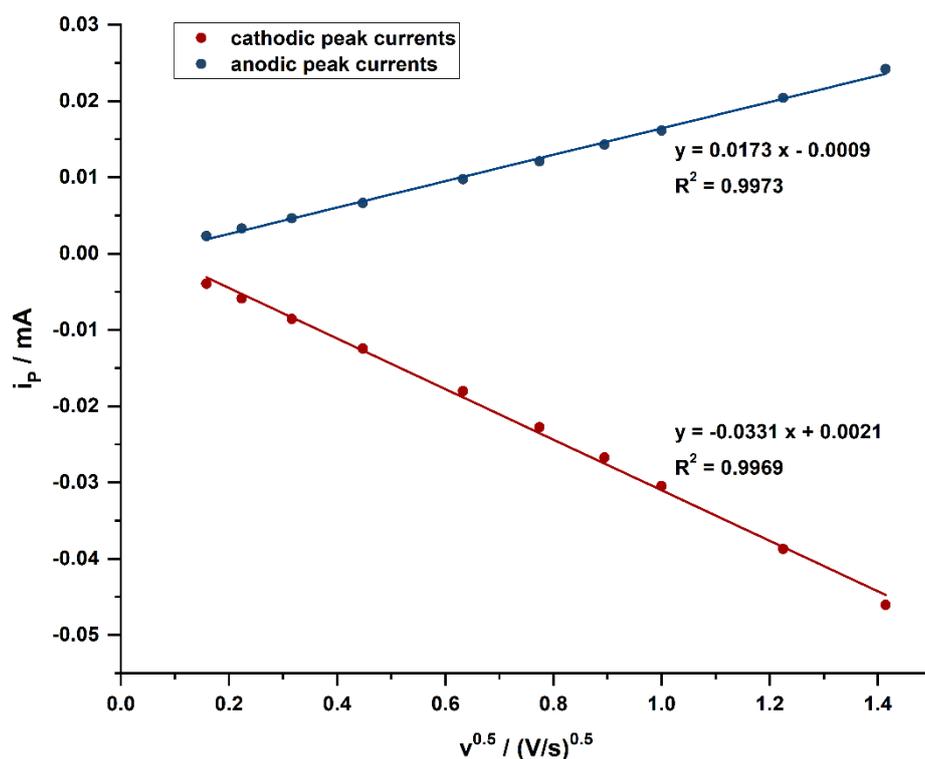


Figure S17: Randles-Sevcik plot of the second oxidation process for $[Cr(L^{MIC})_2]BF_4$.

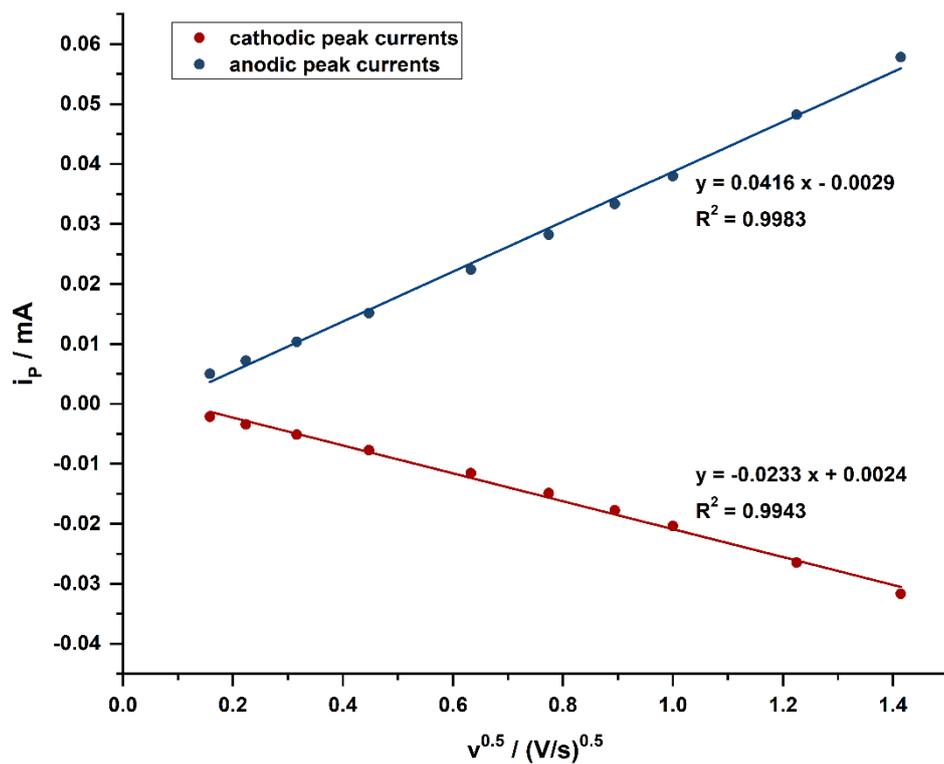


Figure S18: Randles-Sevcik plot of the first reduction process for $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$.

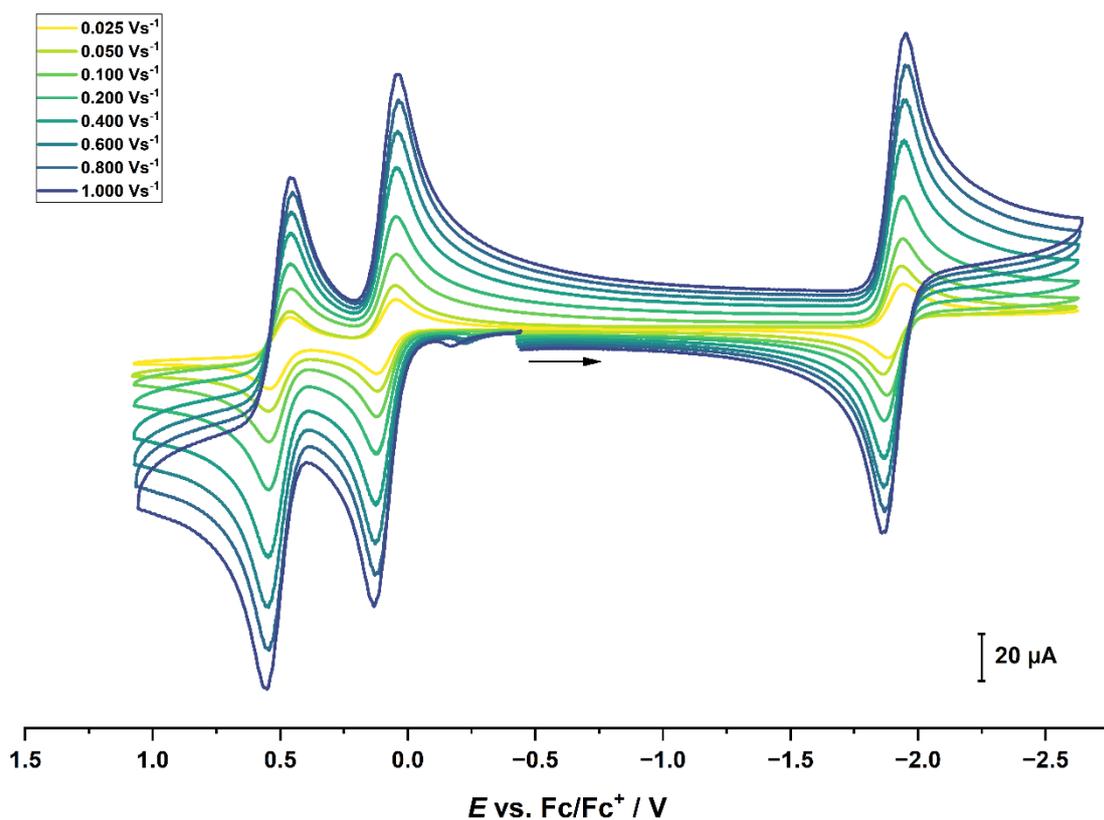


Figure S19: Cyclic voltammogram of $1 \text{ mM } [\text{Cr}(\text{L}^{\text{NHC}})_2]\text{BF}_4$ recorded at various scan rates between $25 - 2000 \text{ mV s}^{-1}$ in $0.2 \text{ M NBu}_4\text{PF}_6$ in MeCN at 298 K .

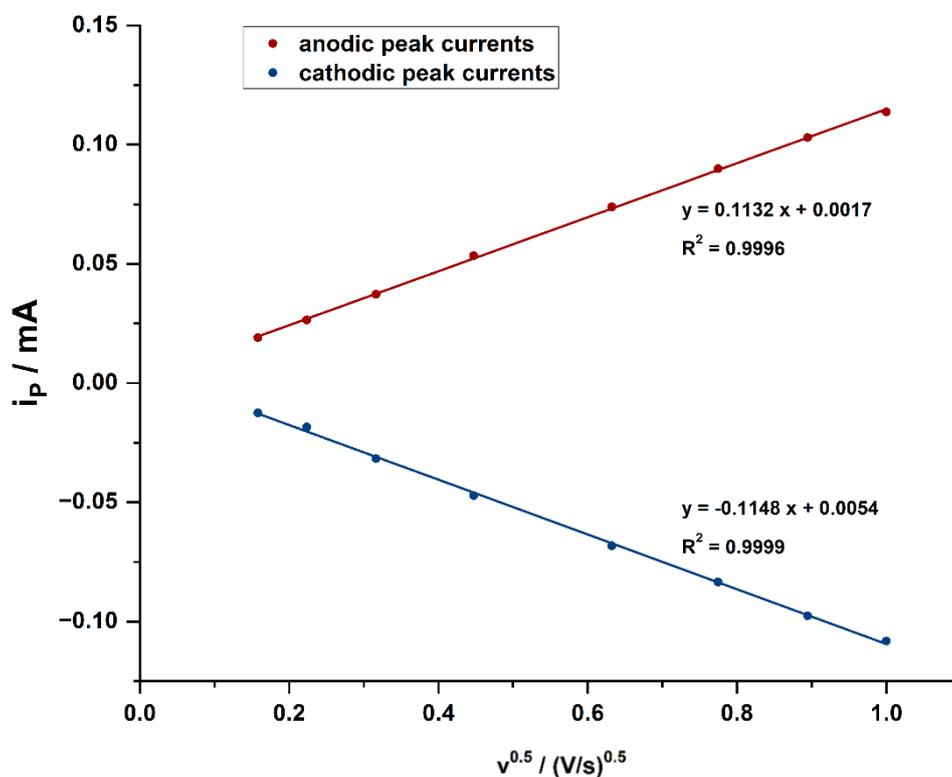


Figure S20: Randles-Sevcik plot of the first oxidation process for $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{BF}_4$.

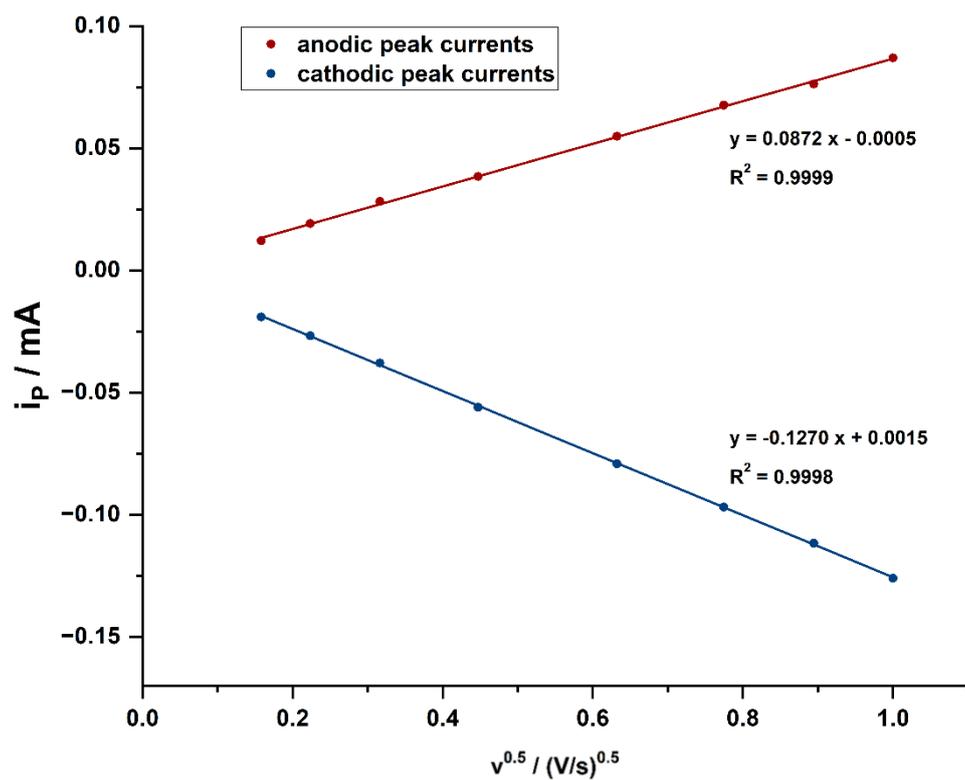


Figure S21: Randles-Sevcik plot of the first reduction process for $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{BF}_4$.

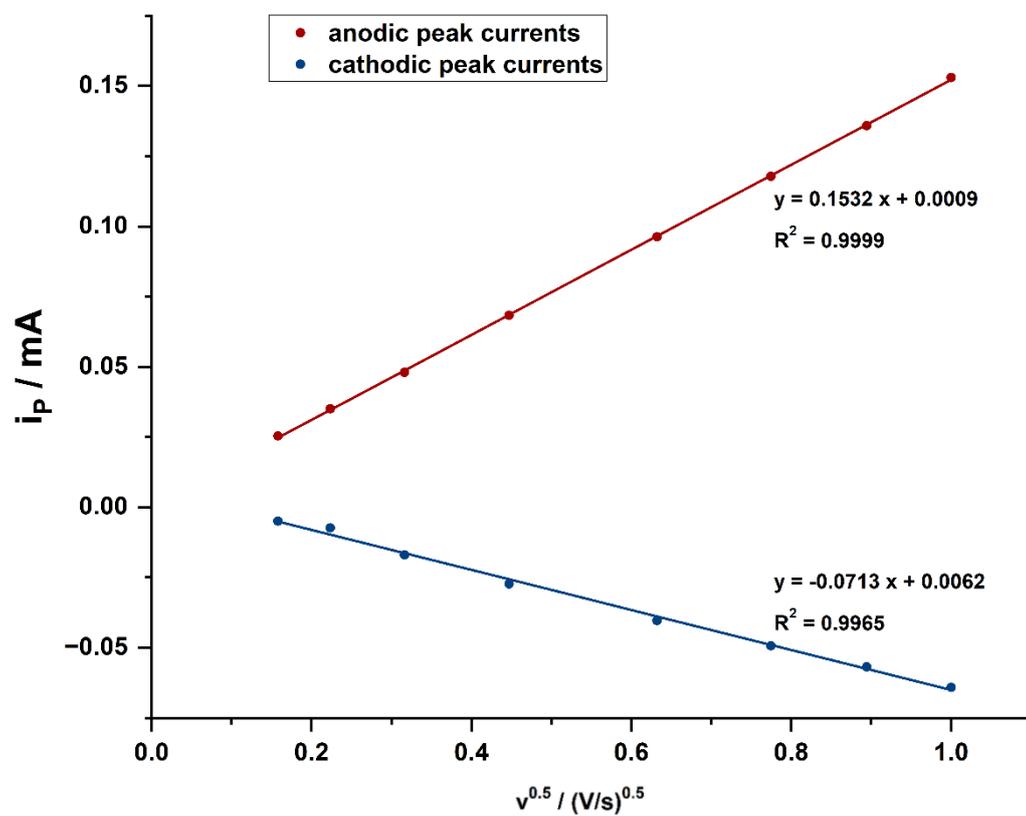


Figure S22: Randles-Sevcik plot of the second oxidation process for $[\text{Cr}(\text{L}^{\text{NHC}})_2]\text{BF}_4$.

6. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$

UV-vis transient absorption

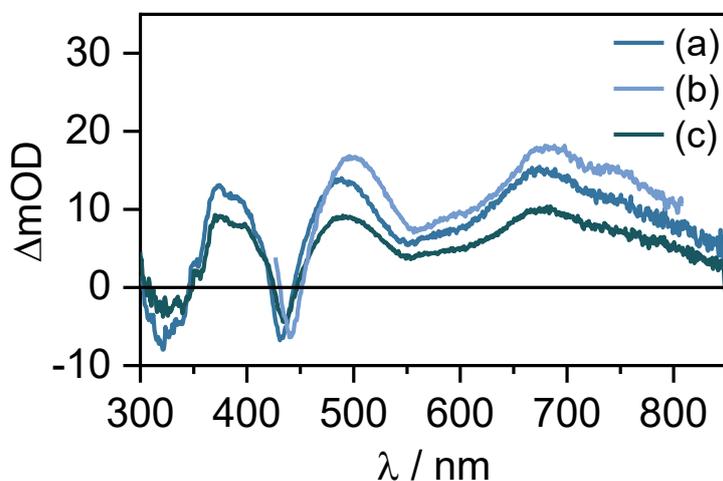


Figure S23: Transient UV-vis absorption spectra of $100 \mu\text{M} [\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$ in deaerated acetonitrile at 293 K, recorded following excitation at: **a.** 355 nm (~ 100 mJ per pulse) and **c.** 532 nm (~ 70 mJ per pulse) with nanosecond pulses (pulse duration ~ 10 ns), time-integrated over 200 ns; **b.** 430 nm (6 mJ per pulse) with picosecond pulses (pulse duration ~ 30 ps), time-integrated over 20 ns.

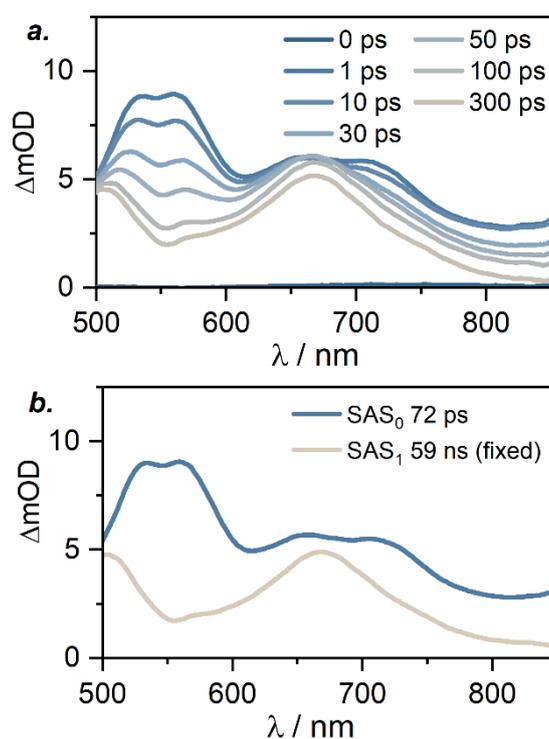


Figure S24: **a.** UV-vis transient absorption spectra of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ in acetonitrile at 293 K, recorded at different delay times (shown in the inset) following excitation at 430 nm with femtosecond pulses; **b.** result of the global fit analysis. For the fitting a sequential excited state population model was used. Obtained species-associated spectra SAS0-1 and corresponding excited state lifetimes are indicated in the inset.

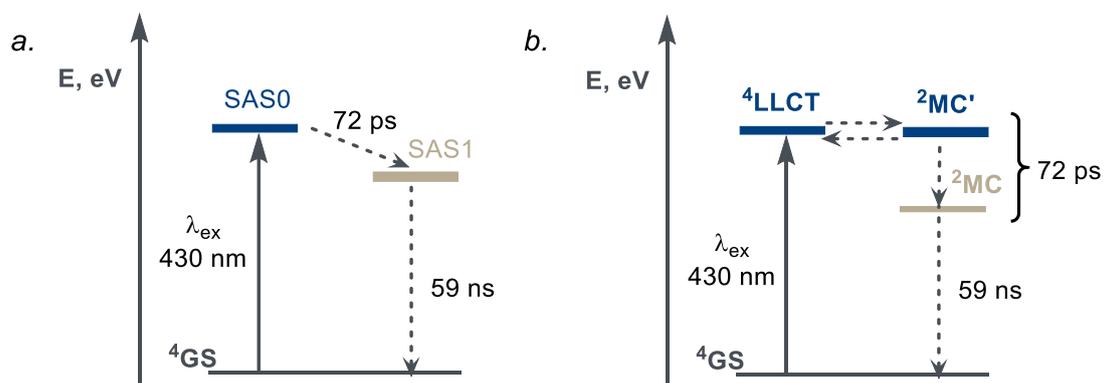


Figure S25: **a.** Scheme of the global fit analysis sequential excited state population model for $[\text{Cr}(\text{L}^{\text{M}^{\text{C}}})_2]^+$, SAS0 was assumed to be equilibrated ^4CT and higher-lying ^2MC state, SAS1 – lowest ^2MC state. **b.** Schematic excited state relaxation model proposed based on the global fit model in **a.** with excited state character assignment supported by spectro-electrochemistry data in Figure S24 and calculations (Table S15-16).

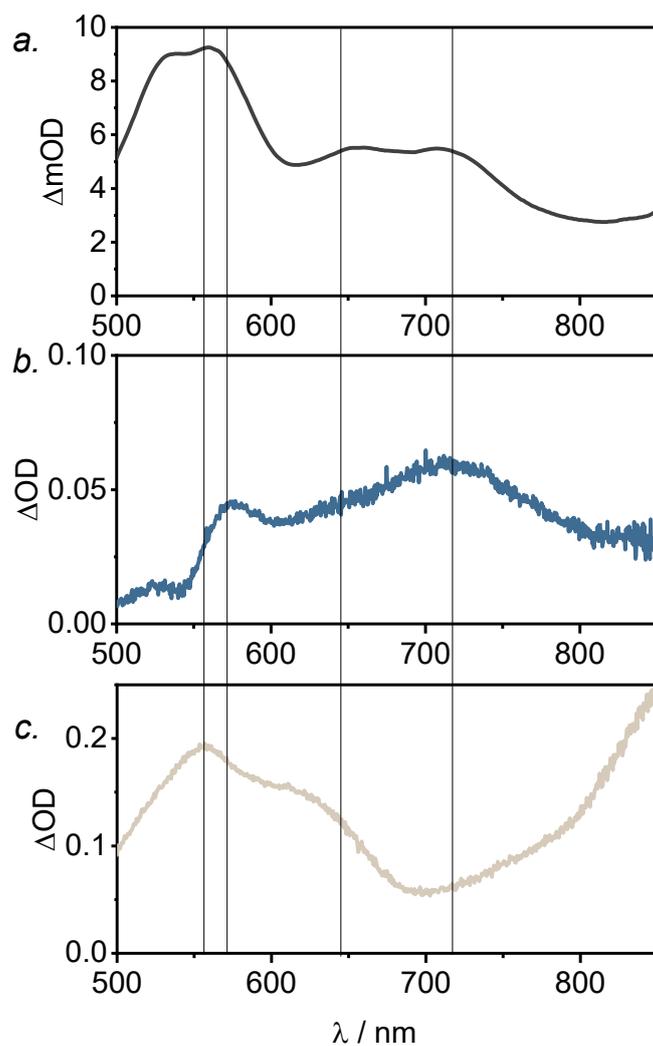


Figure S26: **a.** UV-vis transient absorption spectra of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ in acetonitrile at 293 K, recorded at different delay time of 1 ps following excitation at 430 nm with femtosecond pulses; **b.** UV-vis differential (ground-state) absorption spectrum of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ in deaerated CH_3CN at room temperature with -1.9 V vs SCE potential applied, corresponding to a ligand-based L^0/L^- reduction process; **c.** UV-vis differential (ground-state) absorption spectrum of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ in deaerated CH_3CN at room temperature with 0.5 V vs SCE potential applied, corresponding to a ligand-based L^0/L^+ oxidation process.

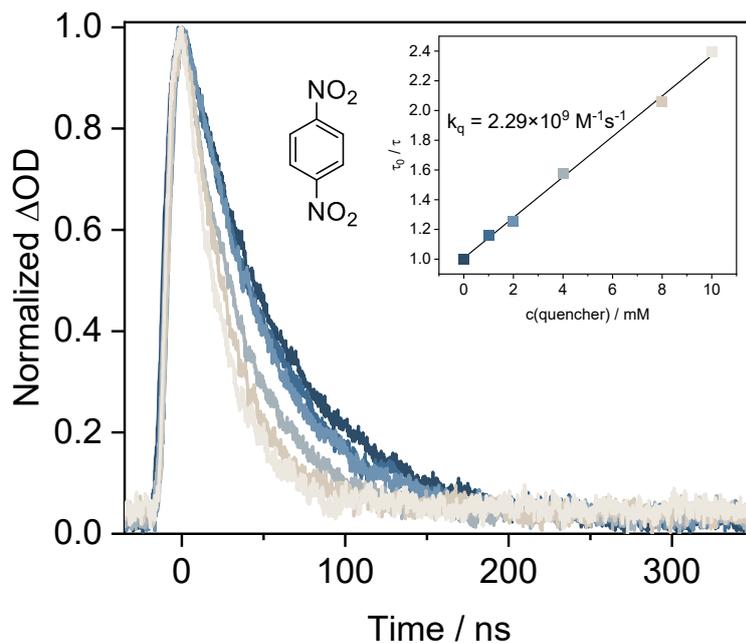


Figure S27: Main plot: Decay of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($30 \mu\text{M}$) excited state absorption band at 700 nm in the presence of increasing concentrations of 1,4-dinitrobenzene after excitation at 532 nm with nanosecond pulsed-laser ($\sim 70 \text{ mJ}$ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

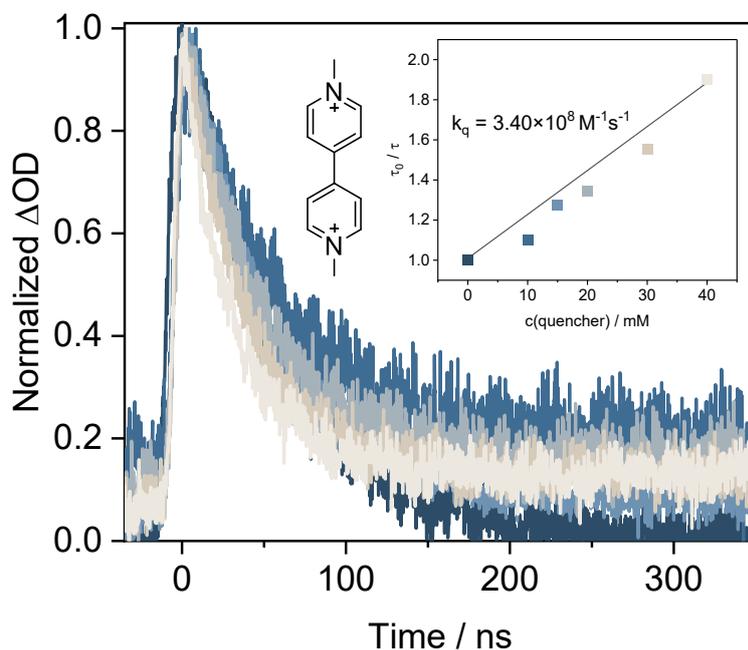


Figure S28: Main plot: Decay of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($30 \mu\text{M}$) excited state absorption band at 700 nm in the presence of increasing concentrations of methyl viologen hexafluorophosphate after excitation at 532 nm with nanosecond pulsed-laser ($\sim 70 \text{ mJ}$ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

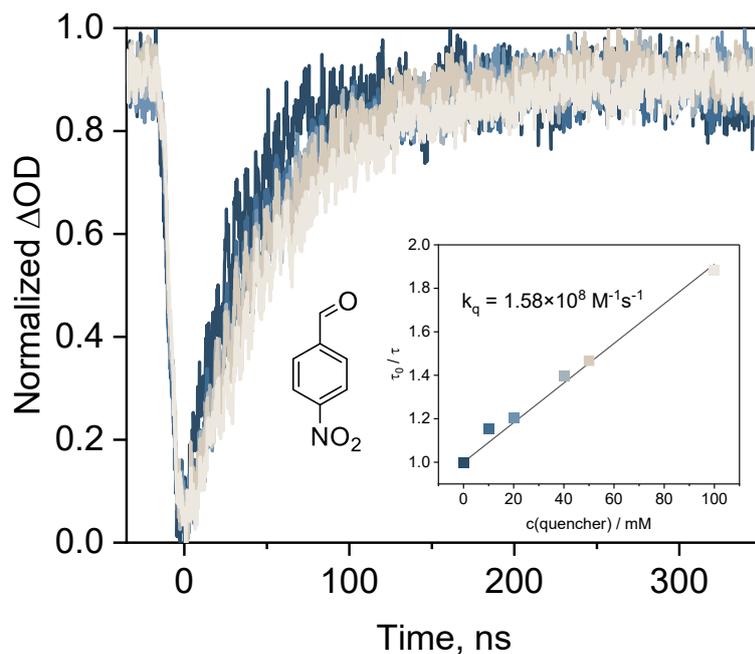


Figure S29: Main plot: Recovery of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($30 \mu\text{M}$) ground state bleach at 434 nm in the presence of increasing concentrations of 4-nitrobenzaldehyde after excitation at 532 nm with nanosecond pulsed-laser ($\sim 70 \text{ mJ}$ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

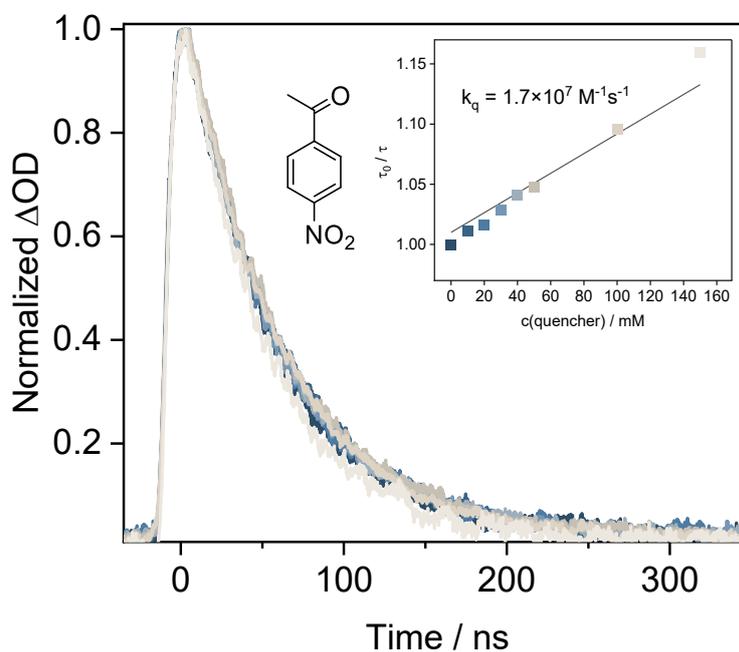


Figure S30: Main plot: Decay of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($30 \mu\text{M}$) excited state absorption band at 700 nm in the presence of increasing concentrations of 4-nitroacetophenone after excitation at 532 nm with nanosecond pulsed-laser ($\sim 70 \text{ mJ}$ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

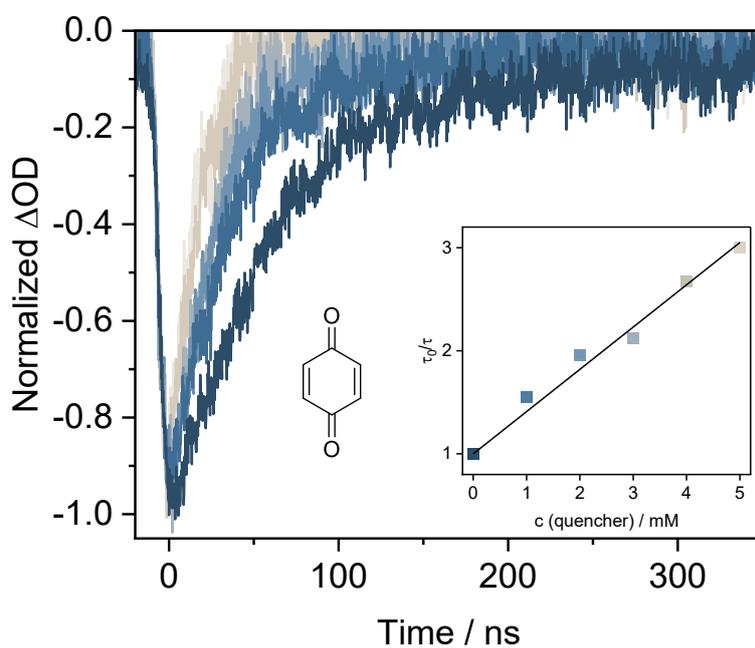
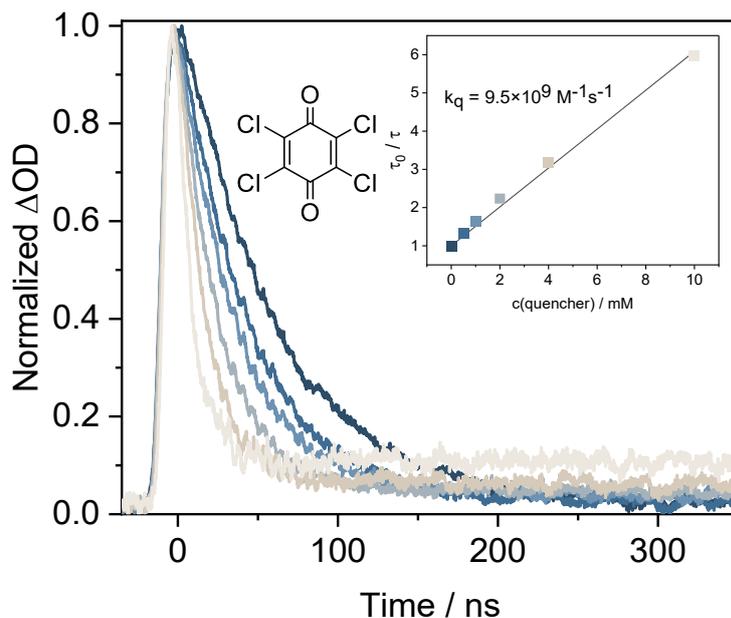


Figure S32: Main plot: Recovery of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($30 \mu\text{M}$) ground state bleach at 434 nm in the presence of increasing concentrations of 1,4-benzoquinone after excitation at 532 nm with nanosecond pulsed-laser ($\sim 70 \text{ mJ}$ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

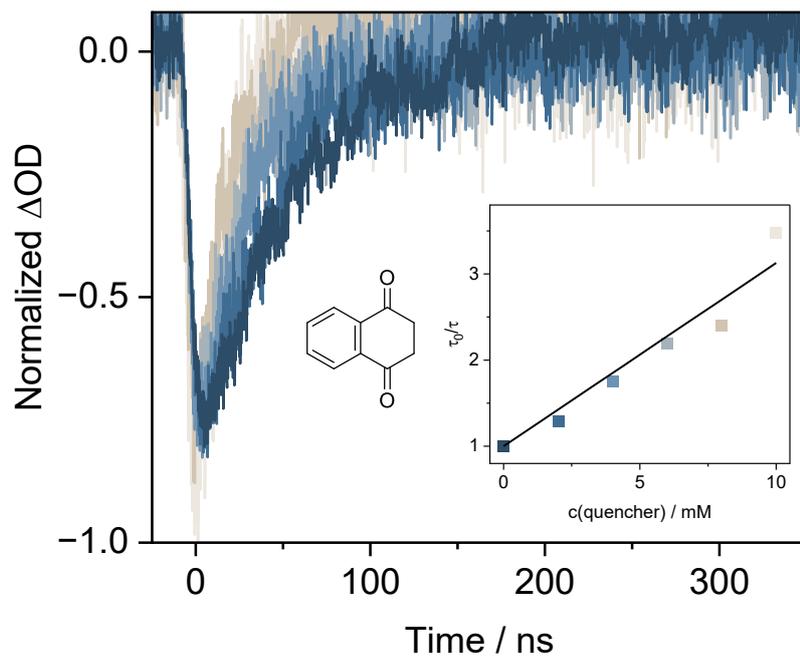


Figure S33: Main plot: Recovery of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ (30 μM) ground state bleach at 434 nm in the presence of increasing concentrations of 1,4-naphthoquinone after excitation at 532 nm with nanosecond pulsed-laser (~ 70 mJ per pulse). Inset: Stern-Volmer plot (color-coding corresponds to the kinetic plots).

Alternative Rehm-Weller fitting analysis

It is important to note that in the Rehm-Weller equation (Eq. S3) the pre-exponential factor, which we fixed as constant of 0.25 in Eq.3 for fitting simplicity (Figure 10), is in fact a function of the dissociation rate constant of the donor-acceptor encounter complex back to the initial reactants (k_{d-1}). The value of 0.25 in Eq.3 was originally assumed by Rehm and Weller for an onward reaction with $k_d = 2 \cdot 10^{10} \text{ M}^{-1}\text{s}^{-1}$.^[11] Clearly, in our case that value would change together with k_d and k_{d-1} . To account for this, advanced data fitting included treating the pre-exponential factor as a function of k_d in Eq. S3, compared to Eq. 3 in the main paper. Parameter a in Eq. S3 includes the dissociation rate constant of the donor-acceptor encounter complex back to the initial reactants (k_{d-1}) and a constant related to the dielectric relaxation time of the solvent (k^0). See Figure 10 for the fit results comparison. According to the fitting results (Figure S34), we obtained a lower k_q value of $1.17 \cdot 10^{10} \text{ M}^{-1}\text{s}^{-1}$, compared to the $1.49 \cdot 10^{10} \text{ M}^{-1}\text{s}^{-1}$ from the simplified fit. We also observed a higher $\Delta G_{ET}^\ddagger(0)$ of 0.16 eV, as opposed to 0.13 eV. However, ultimately, that approach gave a similar $E^0(D^+/D^{2+})$ value of -0.84 V .

$$E_0(D^+ / D^{2+}) = E_0(D^+ / D^{2+}) - E_{00} / e \quad (\text{S1})$$

$$\Delta G_{ET} = [E^0(D^{2+} / D^+) - E^0(A / A^-)] \times e \quad (\text{S2})$$

$$k_q = \frac{k_d}{1 + a \cdot [\exp(\Delta G_{ET}^\ddagger/k_b T) + \exp((\Delta G_{ET}/k_b T)]} \quad \text{where: } a = k_{d-1}/k^0 \quad (\text{S3})$$

$$\Delta G_{ET}^\ddagger = \left[(\Delta G_{ET}/2)^2 + \Delta G_{ET}^\ddagger(0)^2 \right]^{1/2} + \Delta G_{ET}/2 \quad (\text{S4})$$

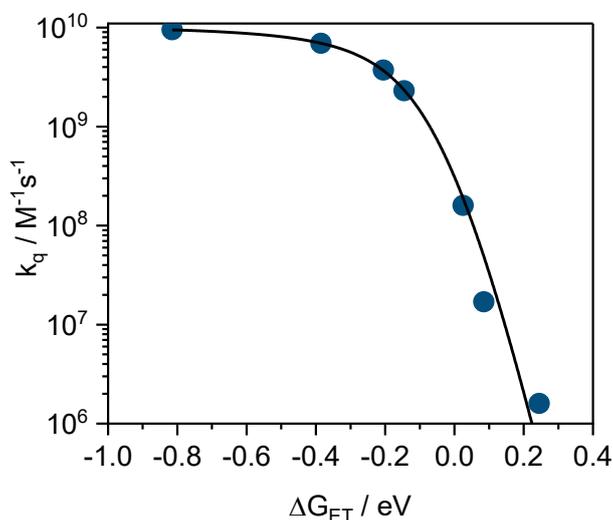


Figure S34: Rehm-Weller plot, showing a dependency between the bimolecular electron transfer rate constants (k_q) for $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ with selected electron acceptors and free energy (ΔG_{ET}). Best fit for $E^0(D^+/D^{2+}) = -0.84 \text{ V}$; $k_d = (1.17 \pm 0.03) \cdot 10^{10} \text{ M}^{-1}\text{s}^{-1}$; $\Delta G_{ET}^\ddagger(0) = 0.15 \pm 0.01 \text{ eV}$; $a = (1.6 \pm 0.3) \cdot 10^{11} \text{ M}^{-1}\text{s}^{-1}$.

7. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$

Ground state UV-vis absorption

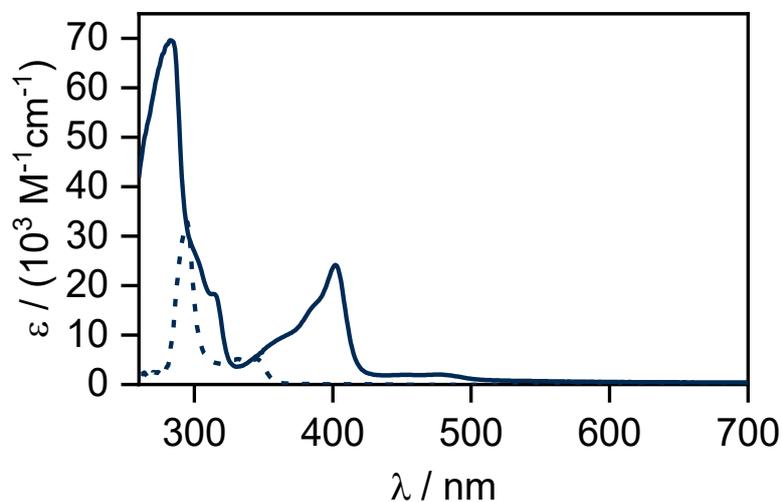


Figure S35: UV-vis absorption of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ (solid line) and $[\text{H}_3(\text{L}^{\text{NHC}})_2]^{2+}$ pro-ligand (dashed line) in acetonitrile at 293 K.

UV-vis transient absorption

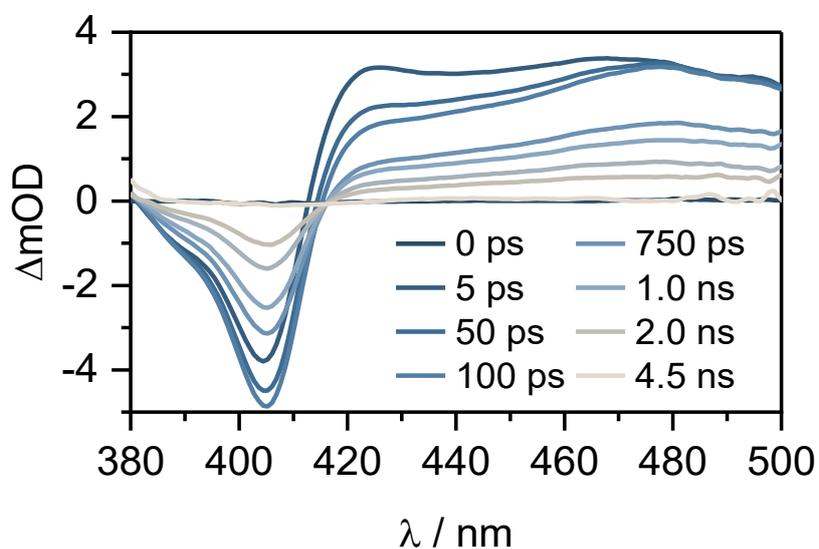


Figure S36: UV-Vis transient absorption spectra of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ in acetonitrile at 293 K, recorded at different delay times (shown in the inset) following excitation at 355 nm with femtosecond pulses.

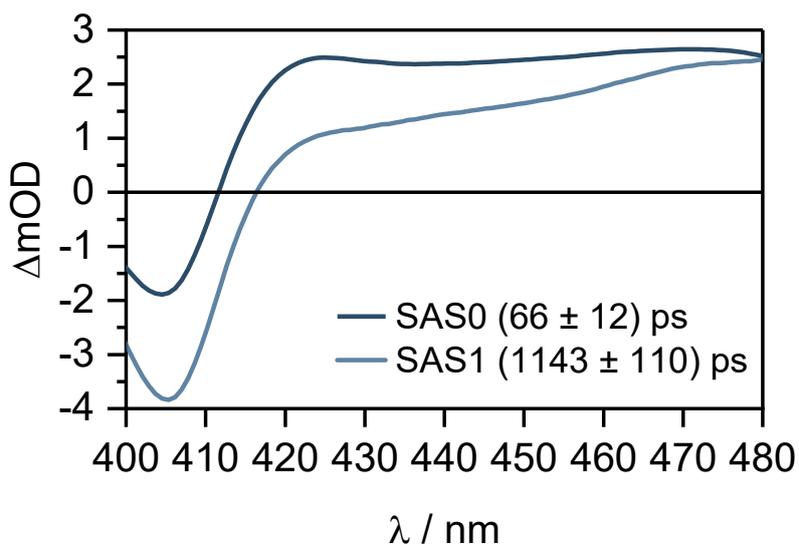


Figure S37: Result of the global fit analysis of the UV-Vis transient absorption spectra for $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ (see Figure S36). For the fitting a sequential excited state population model was used. Obtained SAS and corresponding lifetimes are indicated in the inset.

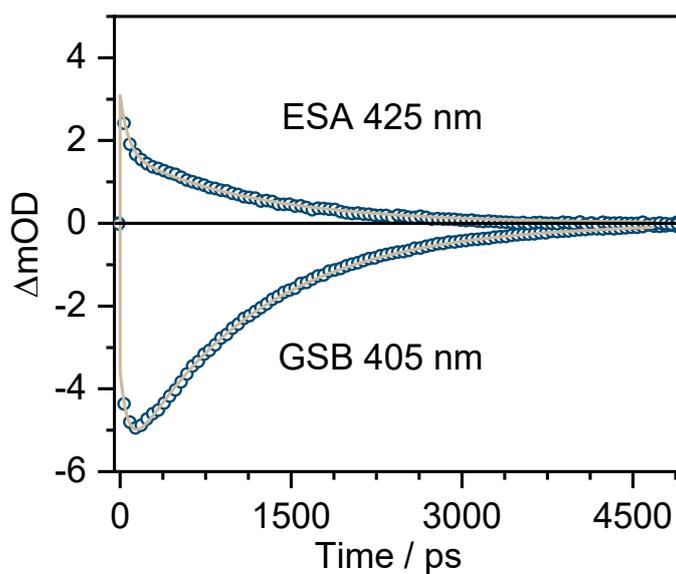


Figure S38: Decay of the ESA signal at 425 nm and the GSB at 405 nm for $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ in acetonitrile at 293 K following excitation at 355 nm with femtosecond pulses. The experimental data are depicted by circles, while the fits are represented by lines.

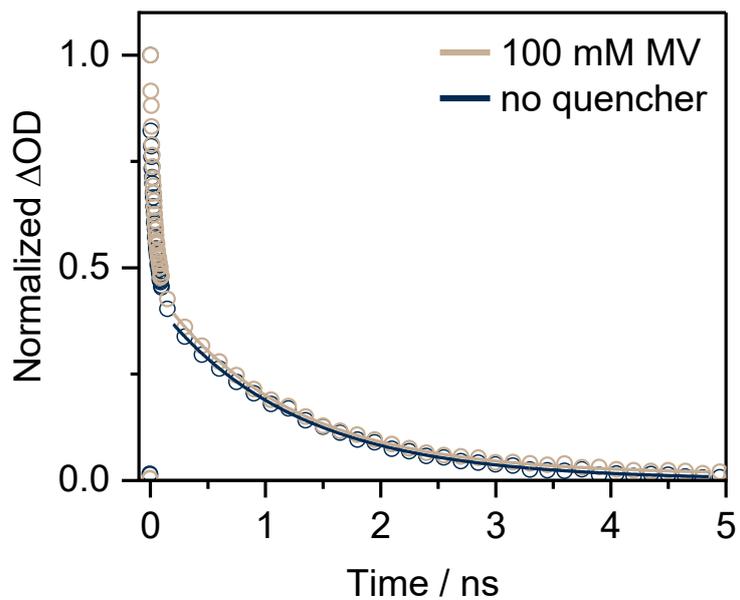


Figure S39: Decay of the ESA signal at 425 nm of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ in acetonitrile at 293 K in the absence of the quencher (blue) and presence of 100 mM of methyl viologen (brown) after the excitation at 355 nm with femtosecond pulses. The experimental data are depicted by circles, while the fits are represented by lines.

8. Photophysical Properties of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$

Ground state UV-vis absorption

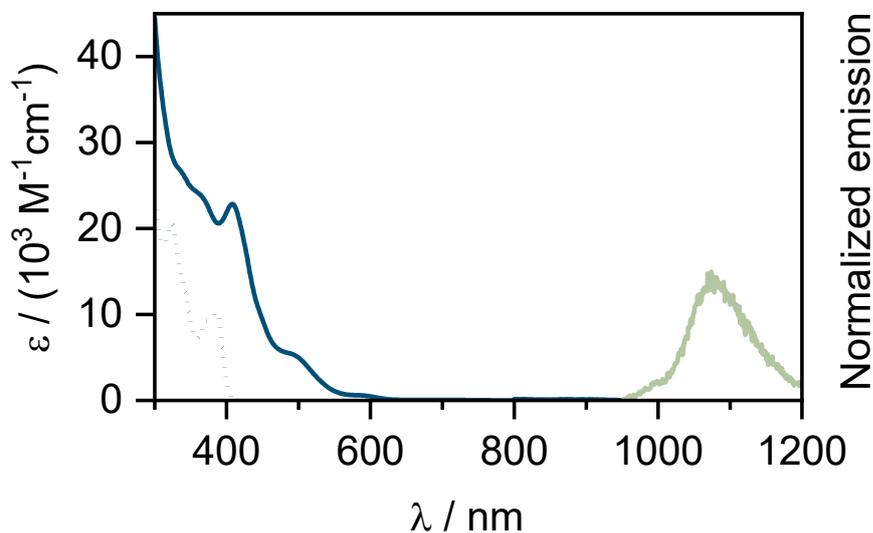


Figure S40: UV-vis absorption of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ (blue solid line) and HL^{Py} pro-ligand (dashed line) in acetonitrile; emission of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ (green solid line) in 2-methyl tetrahydrofuran at 77 K.

UV-Vis transient absorption

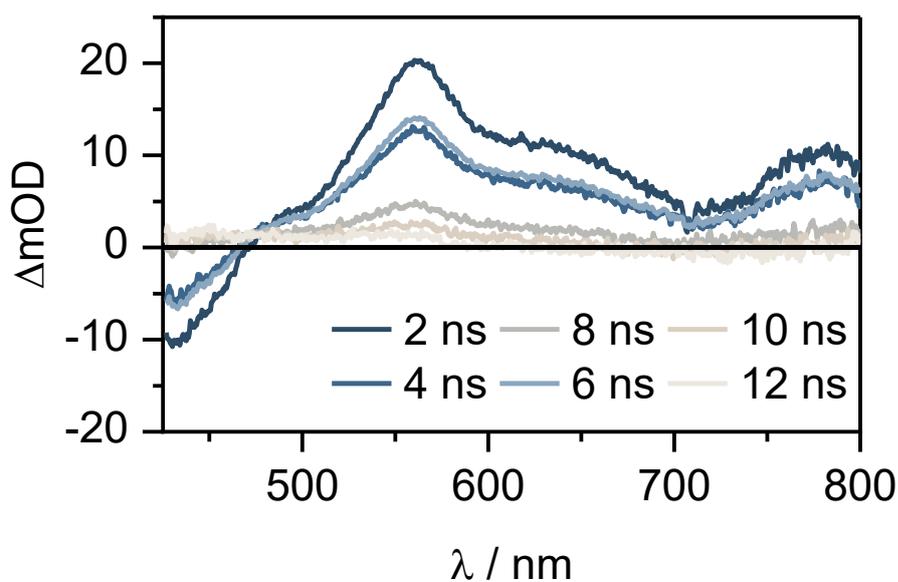


Figure S41: UV-Vis transient absorption spectra of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ in deaerated acetonitrile at 293 K, recorded at different delay times (shown in the inset) following excitation at 355 nm with picosecond pulses.

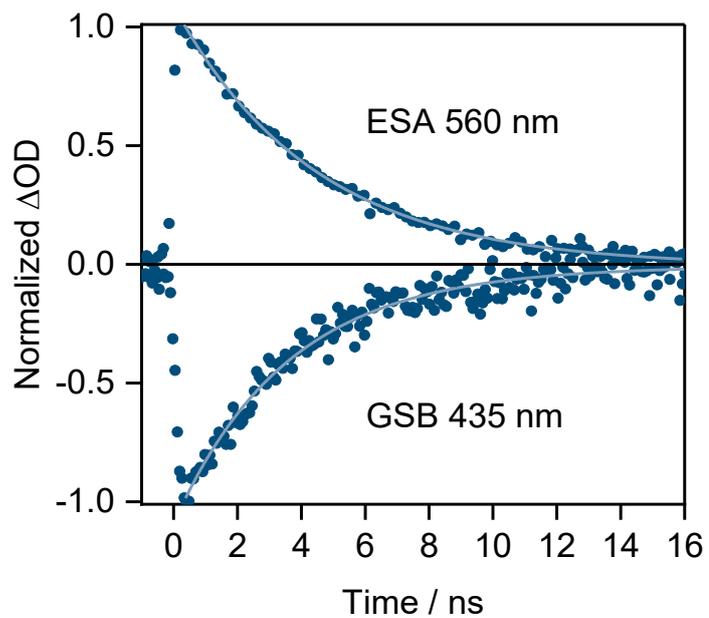


Figure S42: Decay of the ESA at 560 nm and recovery of the GSB at 435 nm after excitation of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ with picosecond pulses at 355 nm. A monoexponential fitting for both data sets provides a time constant of (4.4 ± 0.1) ns. The experimental data are depicted by circles, while the fits are represented by lines.

9. Dependence of the non-radiative deactivation rate constant on the experimental and theoretical/calculated energy gaps

Table S1. Dependence of the non-radiative deactivation rate constant (k_{nr}) on the experimental and theoretical/calculated energy gaps (ΔE) between key excited states (${}^4MC\text{-}{}^2MC$ and ${}^4CT\text{-}{}^2MC$) in $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{PY}})_2]^+$ complexes.

Complex	$\ln k_{nr}$	$\Delta E_{\text{exp}}({}^4MC\text{-}{}^2MC)$ / eV	$\Delta E_{\text{theor}}({}^4MC\text{-}{}^2MC)$ / eV	$\Delta E_{\text{exp}}({}^4CT\text{-}{}^2MC)$ / eV	$\Delta E_{\text{theor}}({}^4CT\text{-}{}^2MC)$ / eV
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$	16.64	1.68	1.33	1.01	0.66
$[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$	20.62	n/a	1.50	n/a	0.36
$[\text{Cr}(\text{L}^{\text{PY}})_2]^+$	19.25	1.01	0.37	1.09	0.45

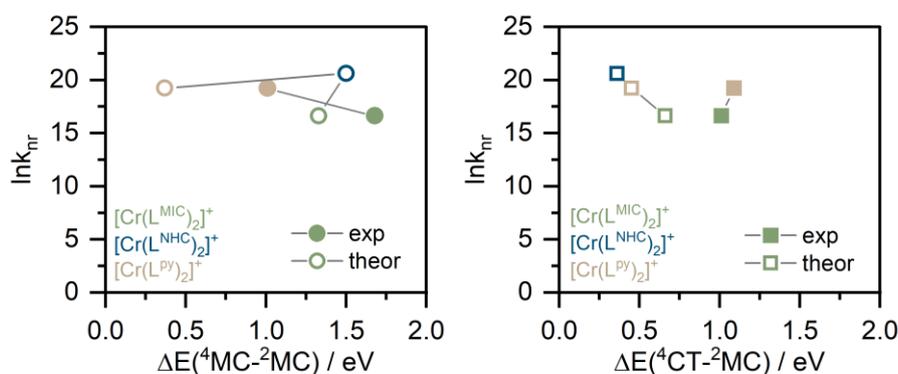


Figure S43. Data of Table S1 illustrated as plot of logarithmic non-radiative deactivation rate constant against energy gap between ${}^4MC\text{-}{}^2MC$ excited states (left) and ${}^4CT\text{-}{}^2MC$ excited states (right) in $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{PY}})_2]^+$ complexes, see legend for color coding.

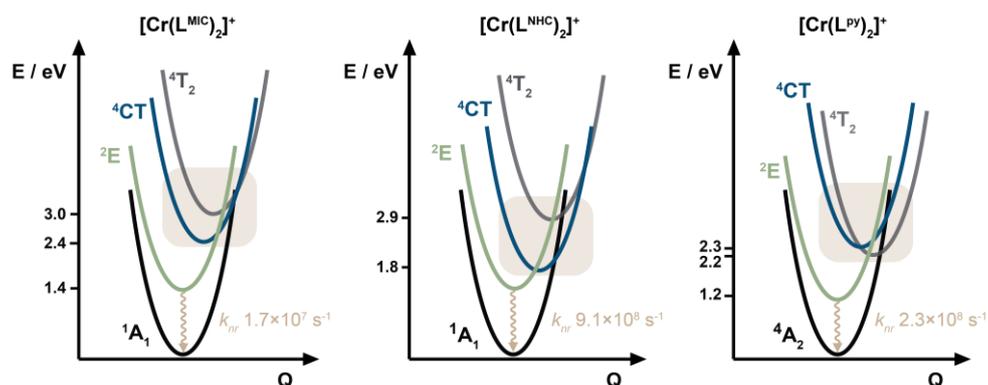


Figure S44. Proposed excited-state ordering in $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$, $[\text{Cr}(\text{L}^{\text{PY}})_2]^+$ complexes depicted with simplified potential well diagram based on the combination of experimental and computational data (for latter see Computational Details).

10. Photoredox catalysis with $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$

Photocatalytic C-H arylation of furan with 4-methoxyphenyl diazonium tetrafluoroborate

The procedure was adapted from a previously published method.^[12] 1,3,5-Trimethoxybenzene was used as internal standard. In an NMR tube 4-methoxyphenyl diazonium tetrafluoroborate (15 mg, 67.6 μmol , 1 eq.), $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$ (1 mol.%), 1,3,5-trimethoxybenzene (11.4 mg, 67.6 μmol , 1 eq.) and furan (41.9 μL , 676 μmol , 10 eq.) were dissolved in 0.6 mL of dry DMSO-d_6 , then the solution was deaerated. The sample was continuously irradiated with a 520 nm Kessil LED lamp for 3 hours, ^1H NMR spectra were measured every 30 min to monitor the reaction progress. A yield of 66% and conversion of >95% were determined relative to the internal standard.

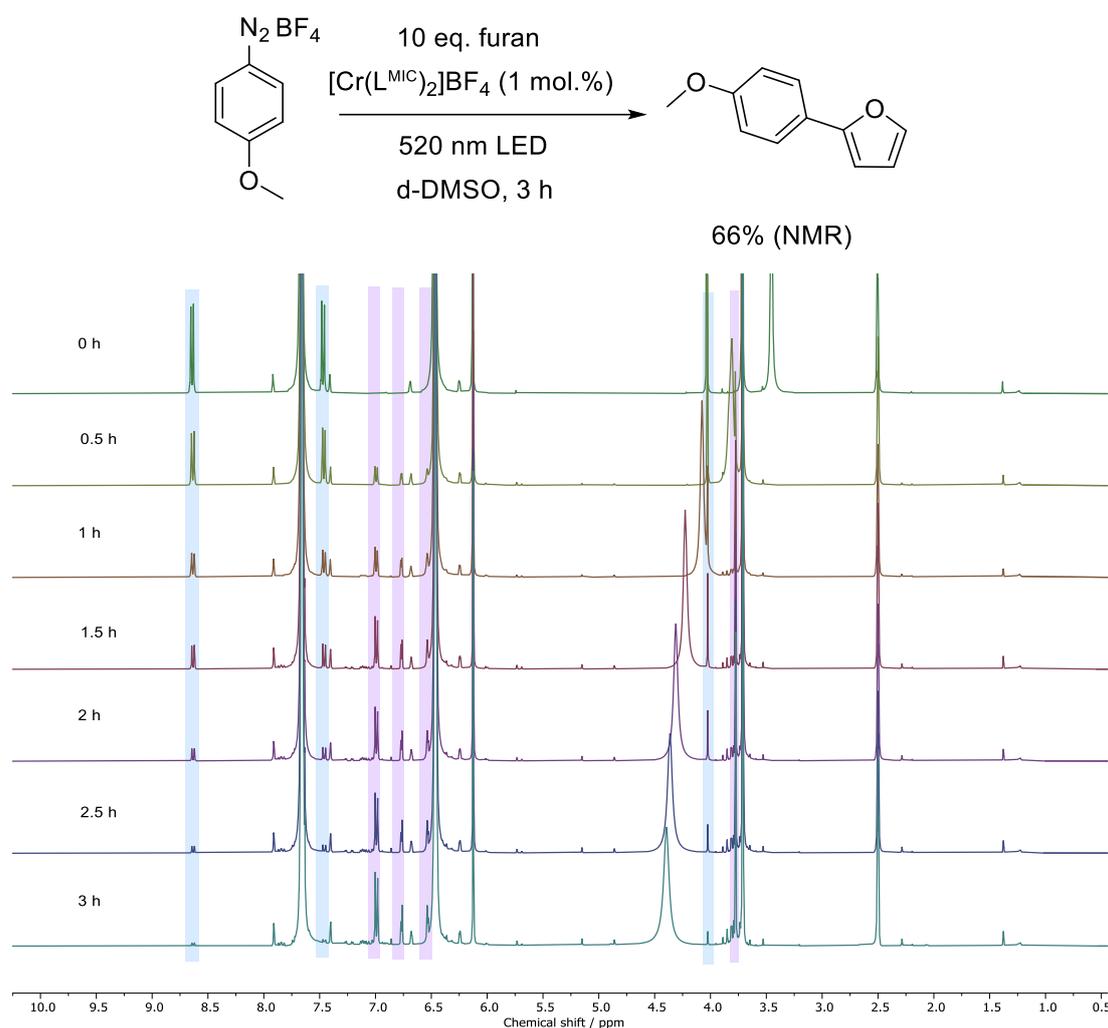


Figure S45: The C-H arylation of furan with 4-methoxyphenyl diazonium tetrafluoroborate was monitored via ^1H -NMR spectroscopy over the indicated irradiation periods. Signals corresponding to the starting material and product are highlighted in blue and purple, respectively.

A control experiment was performed to assess the photocatalytic activity of $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$. The same experiment as described above was repeated in the absence of the photocatalyst. The experiment revealed a product yield of 18% and a starting material conversion of 28%.

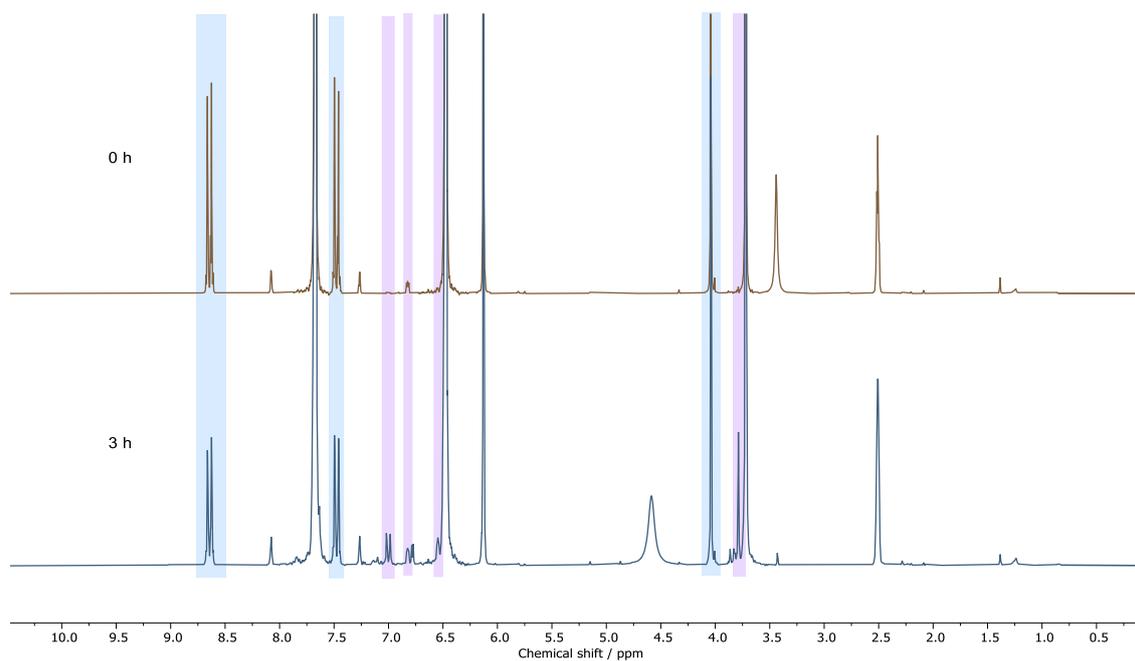


Figure S46: Control experiment in the absence of the photocatalyst. ^1H -NMR spectra measured after the indicated irradiation periods. Signals corresponding to the starting material and photoproduct are highlighted in blue and purple, respectively.

A control experiment was performed to assess the photocatalytic activity of $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$. The same experiment as described above was repeated in the presence of the photocatalyst and in the absence of light. The experiment revealed a product yield of 4.7% and a starting material conversion of 11%.

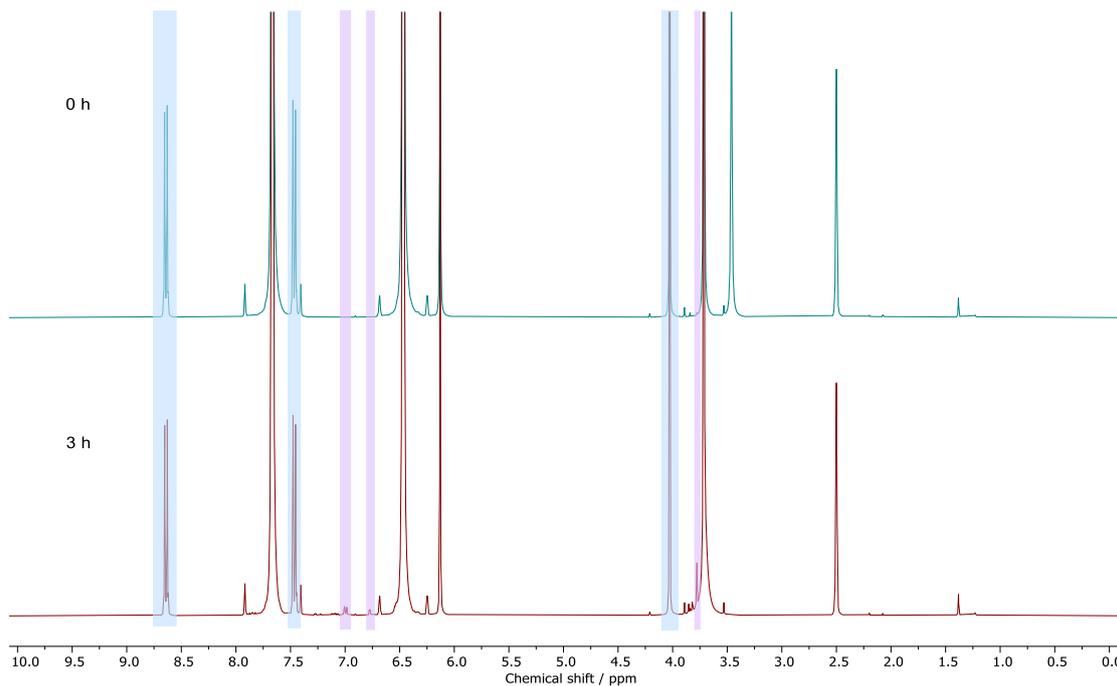


Figure S47: Control experiment in the presence of photocatalyst and in the absence of light. $^1\text{H-NMR}$ spectra measured after the indicated irradiation periods. Signals corresponding to the starting material and photoproduct are highlighted in blue and purple, respectively.

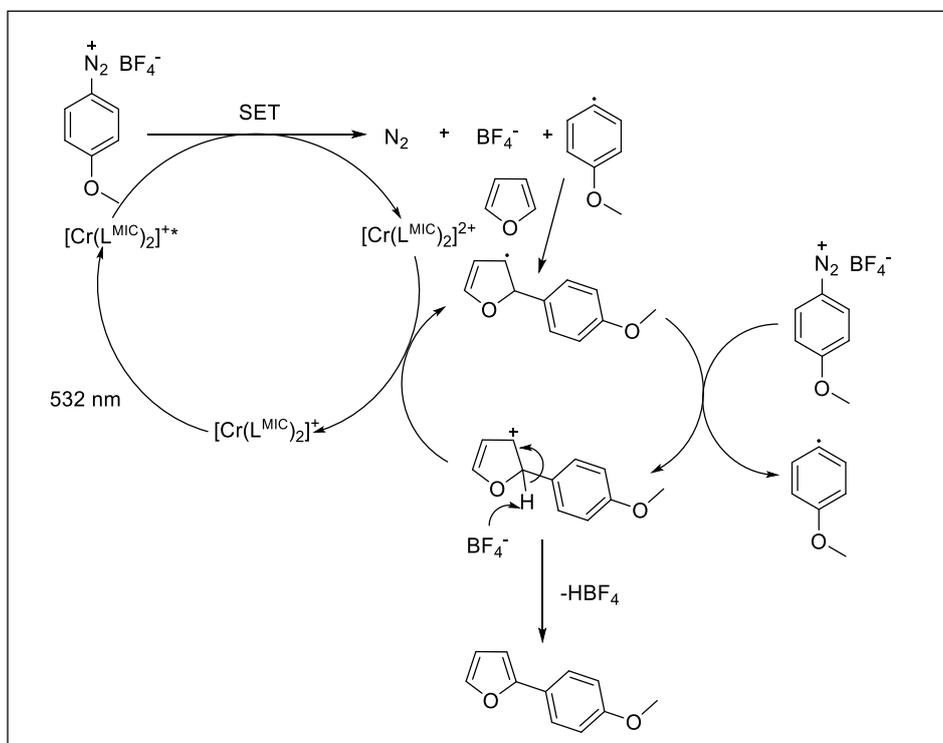


Figure S48: Mechanism of the photocatalytic C-H arylation of furan with 4-methoxyphenyl diazonium tetrafluoroborate, as reported in the literature.^[11]

Photocatalytic borylation of 4-methoxyphenyl diazonium tetrafluoroborate with bis(pinacolato)diboron

The procedure was adapted from a previously published method.^[12,13] 1,3,5-Trimethoxybenzene was used as internal standard. In an NMR tube 4-methoxyphenyl diazonium tetrafluoroborate (15 mg, 67.6 μmol , 1 eq.), $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$ (1 mol.%), 1,3,5-trimethoxybenzene (11.4 mg, 67.6 μmol , 1 eq.) and bis(pinacolato)diboron (52.0 mg, 203 μmol , 3 eq.) were dissolved in 0.6 mL of dry MeCN-d_3 , then the solution was deaerated. The sample was continuously irradiated with a 520 nm Kessil LED lamp for 16 hours, ^1H NMR spectra were measured every 2 hours to monitor the reaction progress. A yield of 74% and conversion of >99% were determined relative to the internal standard.

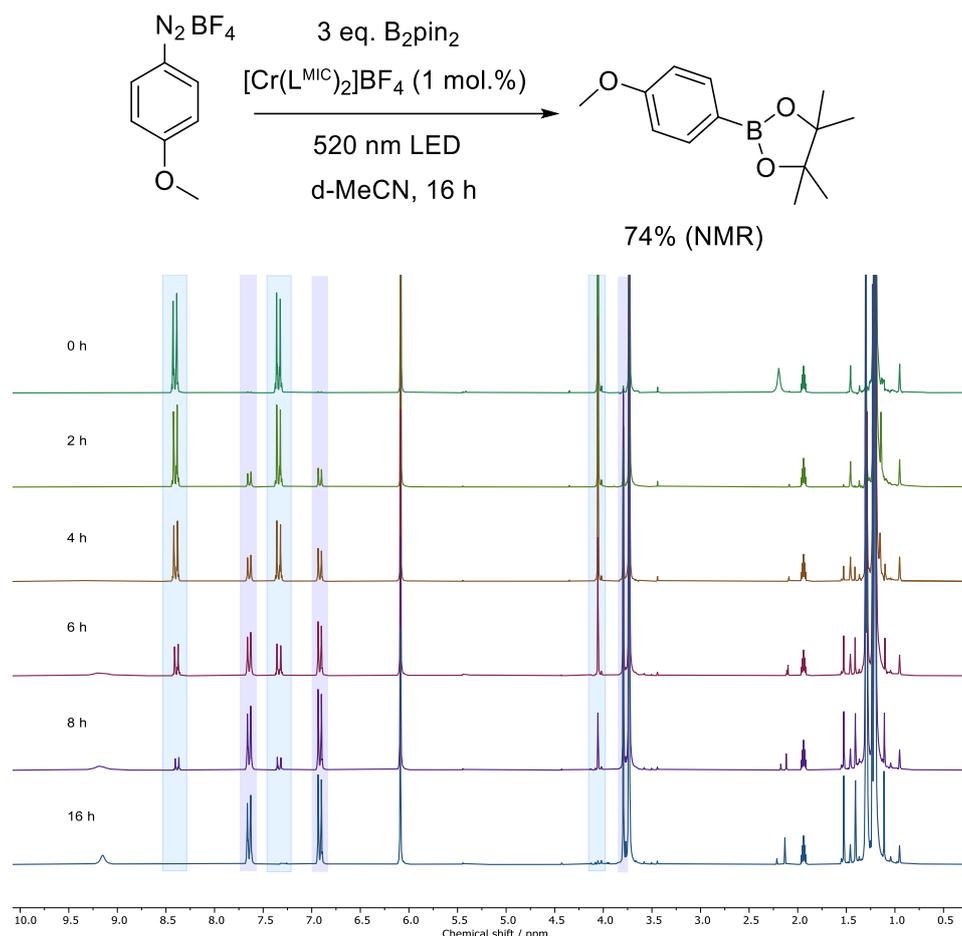


Figure S49: Borylation of 4-methoxyphenyl diazonium tetrafluoroborate with bis(pinacolato)diboron was monitored via ^1H -NMR spectroscopy over indicated irradiation periods. Signals corresponding to the starting material and photoproduct are highlighted in blue and purple, respectively.

A control experiment was performed to assess the photocatalytic activity of $[\text{Cr}(\text{L}^{\text{MIC}})_2]\text{BF}_4$. The same experiment as described above was repeated in the absence of the photocatalyst. The control experiment revealed a product yield of 10% and a starting material conversion of 22%.

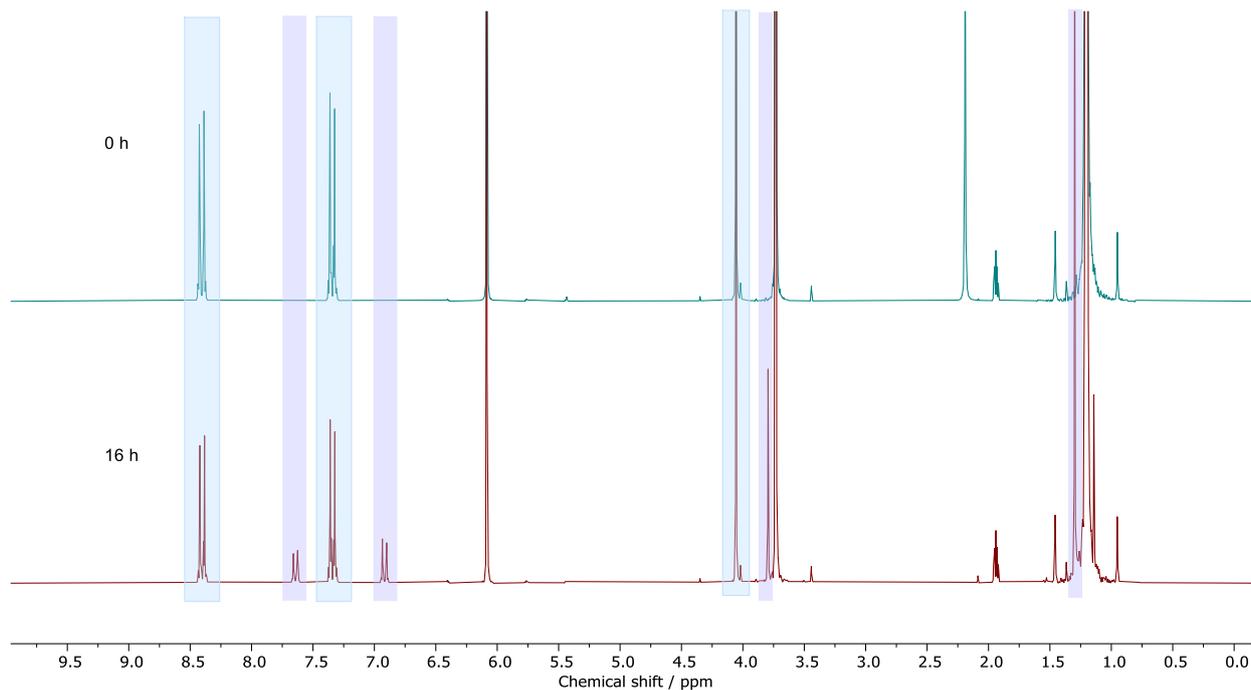


Figure S50: Control experiment in the absence of the photocatalyst. $^1\text{H-NMR}$ spectra measured after the irradiation periods. Signals corresponding to the starting material and photoproduct are highlighted in blue and purple, respectively.

A control experiment was performed to assess the photocatalytic activity of $[\text{Cr}(\text{L}^{\text{M}^{\text{C}}})_2]\text{BF}_4$. The same experiment as described above was repeated in the presence of photocatalyst and in the absence of light. The control experiment revealed that, in this case, trace signals of the product (<0.1 mM) were already detectable in the spectrum immediately after sample preparation (see 0 h panel in Figure S51), further after 16 h a product yield of 3.2% and a starting material conversion of 8.8% were achieved.

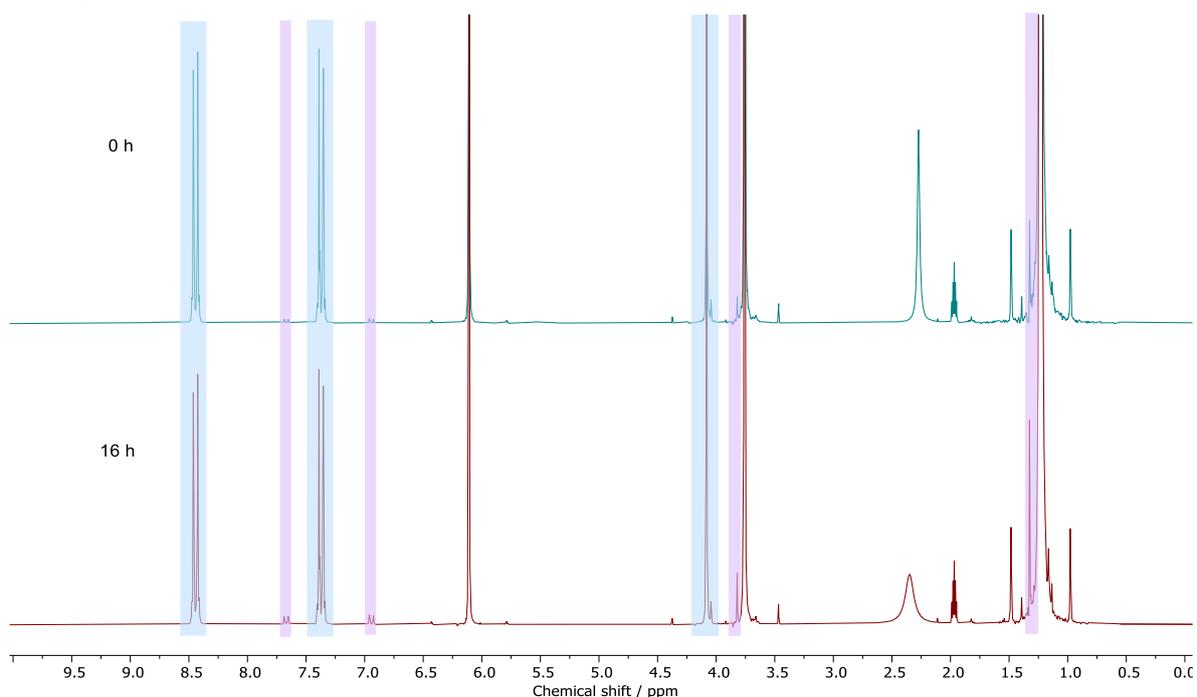


Figure S51: Control experiment in the presence of photocatalyst and in the absence of light. $^1\text{H-NMR}$ spectra measured after the irradiation periods. Signals corresponding to the starting material and photoproduct are highlighted in blue and purple, respectively.

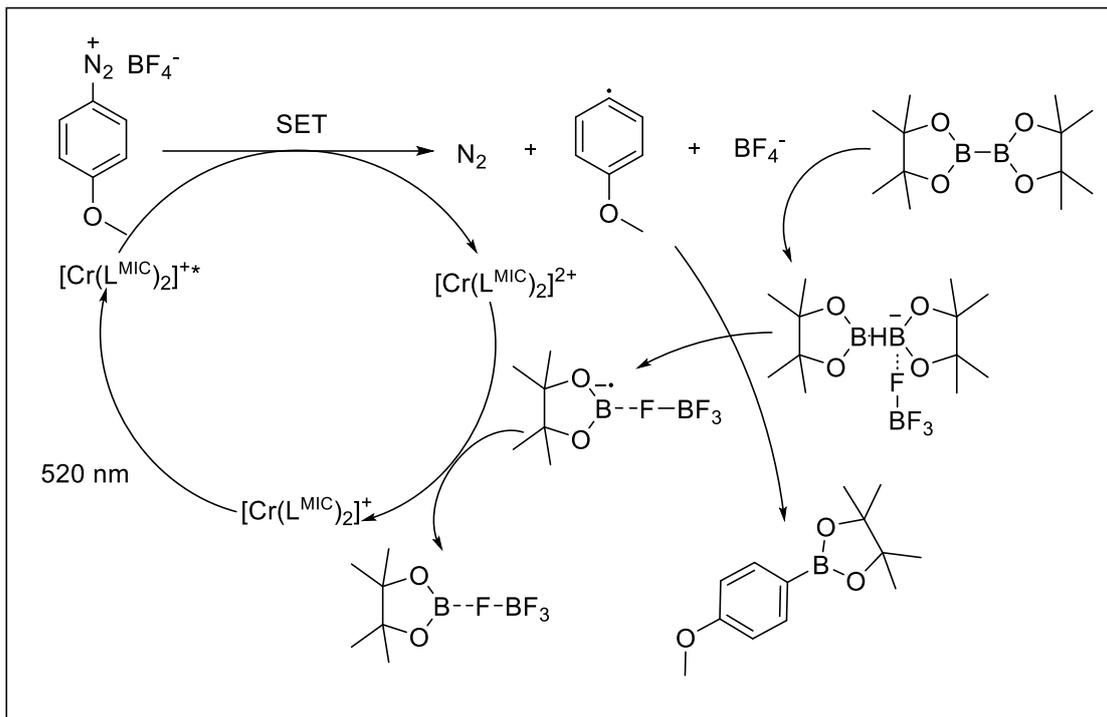


Figure S52: Mechanism of photocatalytic 4-methoxyphenyl diazonium tetrafluoroborate borylation with bis(pinacolato)diboron, reported in the literature.^[13,14]

11. Crystallographic Information

Table S2: Crystallographic data for complexes $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ and $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$.

	$[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$	$[\text{Cr}(\text{L}^{\text{NHC}})_2][\text{BF}_4]$
Chemical formula	$\text{C}_{64}\text{H}_{76}\text{N}_{14}\text{Cr}_1 \text{B}_1\text{F}_4$ $3(\text{C}_6\text{H}_{14})$	$\text{C}_{56}\text{H}_{64}\text{N}_{10}\text{Cr}_1 \text{B}_1\text{F}_4$ $1.7(\text{C}_3\text{H}_6\text{O}_1)$
M_r	1438.71	1114.71
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a (Å)	13.9525(9)	10.6942(9)
b (Å)	32.012(3)	23.5231(19)
c (Å)	17.1974(14)	23.714(2)
α (°)	90	90
β (°)	99.868(2)	93.368(3)
γ (°)	90	90
V (Å ³)	7566.1(10)	5955.3(9)
Z	4	4
Density (g cm ⁻³)	1.263	1.243
F(000)	3092	2358
Radiation Type	MoK α	MoK α
μ (mm ⁻¹)	0.214	0.255
Crystal size (mm)	0.34x0.32x0.30	0.20x0.19x0.02
Meas. Refl.	173087	100688
Indep. Refl.	13290	10567
Obsvd. [$I > 2\sigma(I)$]	10488	6857
R_{int}	0.0845	0.1086
R_1 [$I > 2\sigma(I)$]	0.0732	0.0600
w $R_2(F^2)$	0.2138	0.1761
GooF	1.043	1.039
$\Delta\rho_{\text{max}}$ (e Å ⁻³)	1.183	0.299
$\Delta\rho_{\text{min}}$ (e Å ⁻³)	-0.436	-0.504
CCDC	2304955	2343870

Table S3: Selected bond lengths and angles for complex $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ and $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$

	$[\text{Cr}(\text{L}^{\text{MIC}})_2][\text{BF}_4]$	$[\text{Cr}(\text{L}^{\text{NHC}})_2][\text{BF}_4]$
Cr1-N10	2.026(2)	2.002(2)
Cr1-N10A	2.025(2)	2.004(2)
Cr1-C1	2.136(3)	2.127(3)
Cr1-C2	2.137(3)	2.159(3)
Cr1-C1A	2.144(3)	2.160(3)
Cr1-C2A	2.136(3)	2.141(3)
C1-Cr1-C2	176.38(11)	173.00(12)
C1A-Cr1-C2A	175.62(12)	172.57(12)
N10-Cr1-N10A	179.90(13)	178.85(11)

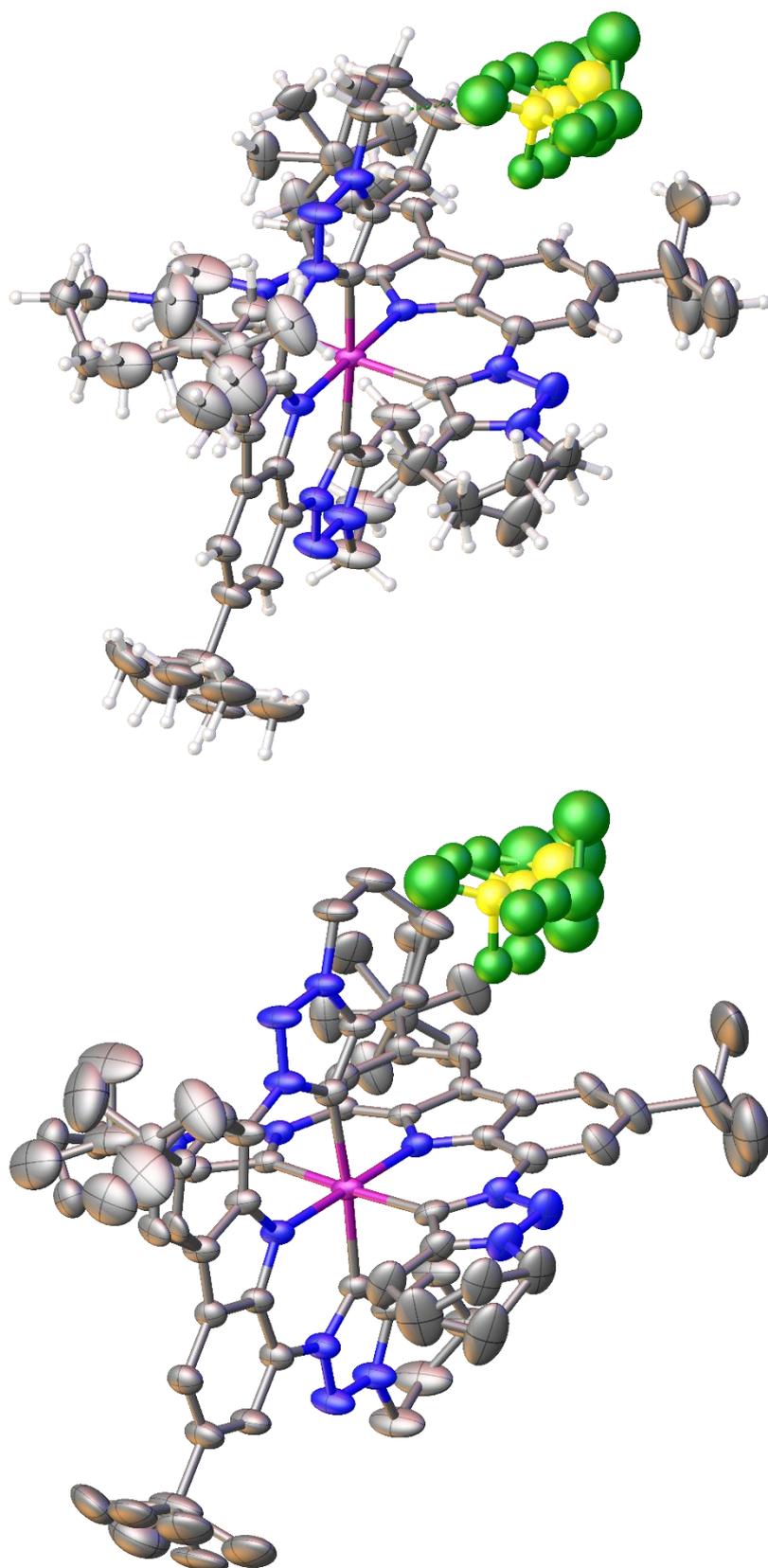


Figure S53: Molecular structure of complex $[\text{Cr}(\text{L}^{\text{M}^{\text{C}}})_2][\text{BF}_4]$ displayed with (top) and without (bottom) hydrogen atoms and full molecular disorders, including the positional disorder of the tetrafluoroborate counter ions.

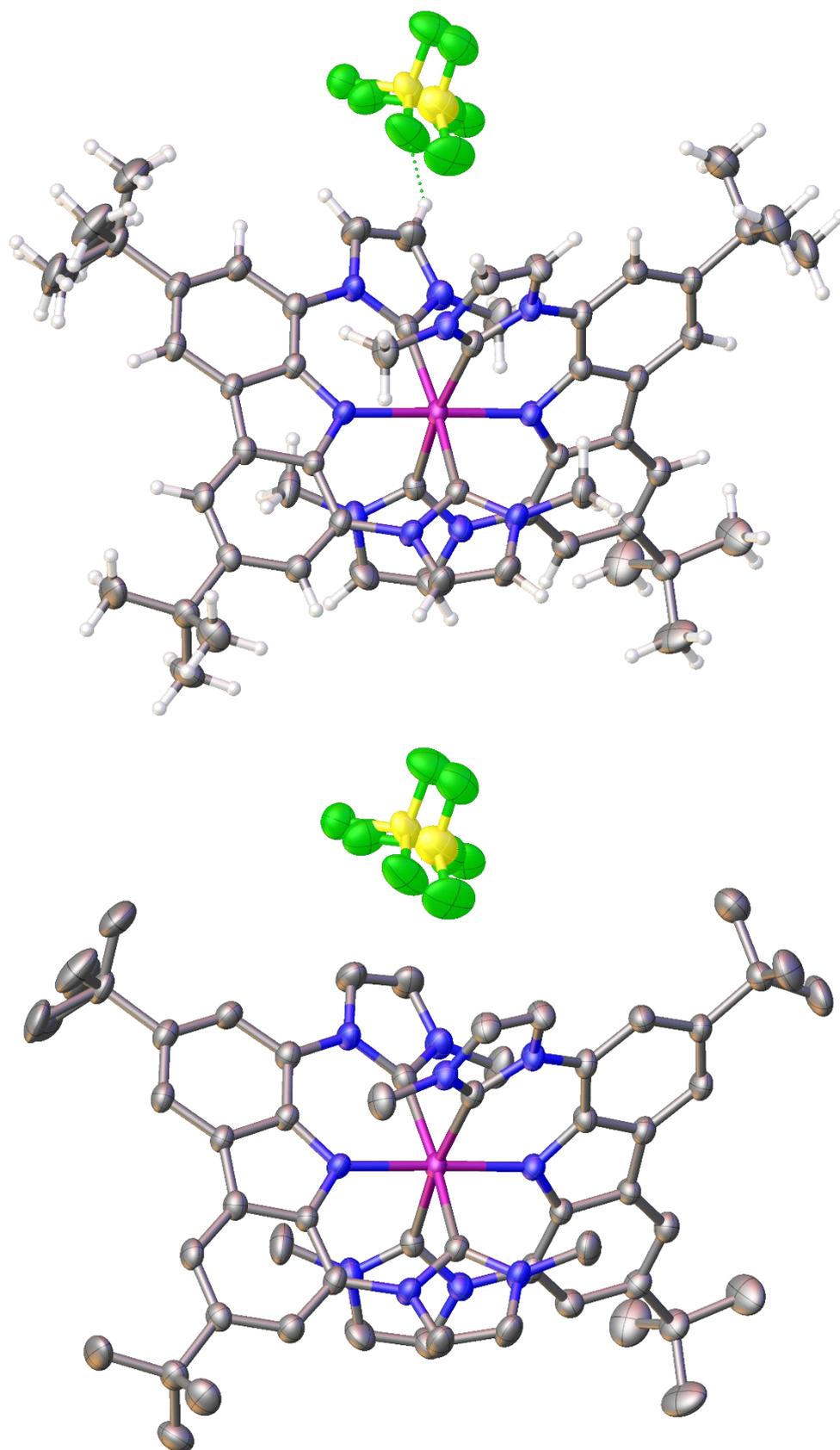


Figure S54: Molecular structure of complex $[\text{Cr}(\text{L}^{\text{NHC}})_2][\text{BF}_4]$ displayed with (top) and without (bottom) hydrogen atoms and full molecular disorders, including the positional disorder of the tetrafluoroborate counter ions.

12. EPR Spectroscopy

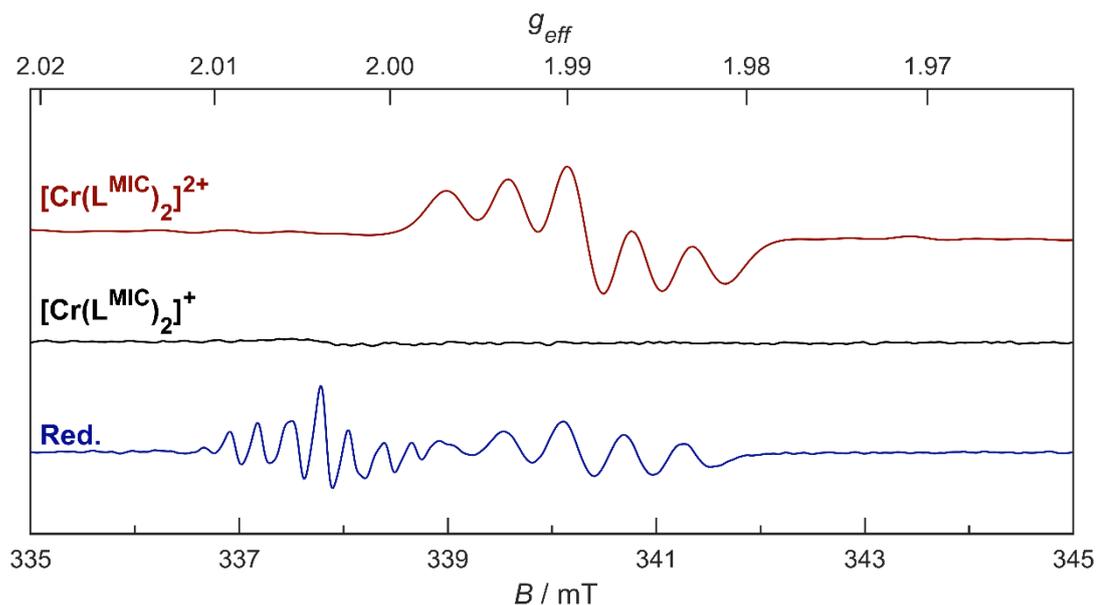


Figure S55: Solution (238 K) EPR spectra of the in-situ oxidation and reduction of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$. The oxidation shows one organic species, while the reduction shows (at least) two different signals, we attribute one to the chromium-bound ligand and the second to a free ligand radical ($g = 2.003$). We hence assume that the complex undergoes further chemical transformation upon reduction, including ligand dissociation.

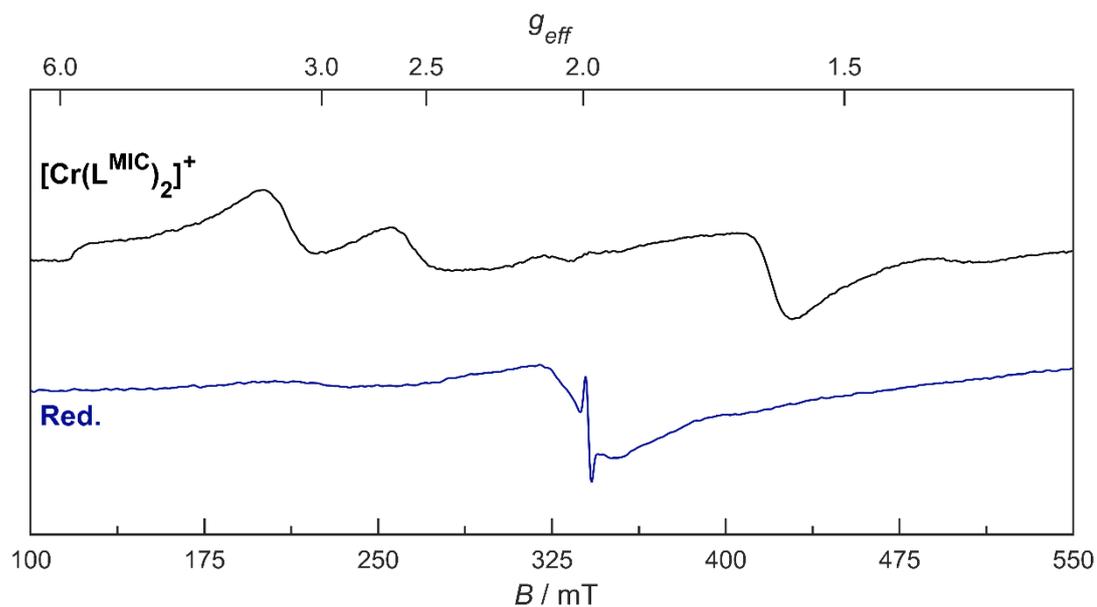


Figure S56: Frozen solution (98 K) EPR spectra of the in-situ reduction of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$. The chromium signal disappears and is mostly replaced by the organic signature (see Fig. S 50).

13. Computational Details

The calculations were performed with ORCA 5.0.4.^[15,16] All calculated structures were verified as true minima by the absence of imaginary eigenvalues in the harmonic vibrational frequency analysis. Tighter than default convergence criteria were chosen for both the optimization of the structural parameters (*tightopt*) and the scf (*tightscf*). The geometry optimizations for [Cr]⁺ were performed at the r²SCAN-3c,^[17] ZORA-PBE0-D4/ZORA-def2-SVP (Cr: ZORA-def2-TZVP),^[18–21] ZORA- ω B97X-V/ZORA-def2-SVP (Cr: def2-TZVP)^[22] and ZORA-cam-B3LYP/ZORA-def2-SVP (Cr: ZORA-def2-TZVP)^[23] level of theories. The geometry optimizations for [Cr] and [Cr]²⁺ were performed at the r²SCAN-3c and ZORA-PBE0-D4/ZORA-def2-SVP (Cr: ZORA-def2-TZVP) level of theories only. Where applicable, the zeroth-order regular approximation (ZORA) in conjunction with the related basis sets was used to include scalar relativistic effects, the RIJCOSX approximation^[24–26] and the related auxiliary basis set SARC/J^[26,27] (*autoaux*, respectively, for AuxC)^[28] were used to speed up the calculations. The r²SCAN-3c method was found to afford the best fit with the structural parameters found in the solid state (Table S4). Various low-spin (including broken-symmetry) states were computationally evaluated, yet did either not converge or were found to be higher in energy (Table S3). Population analyses were conducted with single-point calculations at the triple- ζ level of theory (ZORA-def2-TZVPP), Intrinsic Bond Orbitals (IBOs)^[29] were calculated at the triple- ζ level of theory as well. The absorption spectra were then modelled by time-dependent DFT (TD-DFT) as single point calculations using the r²SCAN-3c structural parameters ($S = 3/2$) using the ZORA-def2-TZVPP basis set (ZORA-TPSSH^[30], ZORA-cam-B3LYP, ZORA- ω B97X-D, Fig. S50). Solvation effects in acetonitrile were explored with the Conductor-like Polarizable Continuum Model (CPCM) module,^[31] yet were found to be small (Tables S9, 11).

Furthermore, CASSCF calculations were performed for [Cr(L^{MIC})₂]⁺, [Mn(L^{MIC})₂]²⁺ as well as the NHC- and pyridine congeners [Cr(L^{NHC})₂]⁺ and [Cr(L^{Py})₂]⁺. For these calculations, model systems were used with all ^tBu groups truncated with hydrogen atoms (*optimizehydrogens*). Also here, ZORA in combination with the ZORA-def2-TZVPP model system was used. The energies of states were refined using n-electron valence state perturbation theory (NEVPT2)^[32] to account for dynamic correlation without using the frozen-core approximation (*nofrozencore*). Various active spaces were explored, namely CASSCF(7,10), CASSCF(7,11), and CASSCF(7,13), which included all five *d*-orbitals, two doubly occupied carbazolido-based orbitals and their antibonding combinations, as well as one (two, four, respectively) ligand-based unoccupied orbitals. We consider CASSCF(7,11) for [Cr(L^{MIC})₂]⁺, [Cr(L^{Py})₂]⁺ and [Mn(L^{MIC})₂]²⁺ and CASSCF(7,10) for [Cr(L^{NHC})₂]⁺ most reliable / comparable, the arguably more appropriate CASSCF(7,13) active space proved difficult to converge (and also computationally very demanding) for some of the compounds. State averaging was applied as given below. The Ab-Initio Ligand Field Theory (AILFT) analysis^[33] was conducted at the NEVPT2 level of theory as well with CASSCF(3,5) and 40 doublet roots as well as 10 quartet roots. Molecular orbitals and optimized geometries were visualized with Chemcraft,^[34] Avogadro,^[35] and IBOView.^[29]

Chromium MIC Complex $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$

Table S4: Energies of DFT-computed structures.

	E in [Eh]	G in [Eh]	E(SP) in [Eh]
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{r}^2\text{SCAN3c truncated}}$	-3665.890266	-3665.098647	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{r}^2\text{SCAN3c}}$	-4294.721925	-4293.504046	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{doublet r}^2\text{SCAN3c}}$	scf not converging		
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{camB3LYP}}$	-4304.131526	-4302.880943	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{PBE0}}$	-4301.879608	-4300.635713	-4305.226442
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{doublet PBE0}}$	-4301.843347	-4300.598725	-4305.190469
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{wB97XV}}$	-4304.759627	n.a.	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+_{\text{PBE}}$	-4301.635943	-4300.439543	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{sUKS r}^2\text{SCAN3c}}$	scf not converging		
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{sUKS PBE0}}$	-4301.964783	-4300.683215	-4305.272879
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{t r}^2\text{SCAN3c}}$	-4294.846135	-4293.631774	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{t PBE0}}$	-4301.994473	-4300.754611	-4305.341752
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{q r}^2\text{SCAN3c}}$	-4294.836153	-4293.624062	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]_{\text{q PBE0}}$	-4301.984829	-4300.747906	-4305.333074
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{sUKS r}^2\text{SCAN3c}}$	scf not converging		
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{sUKS PBE0}}$	-4301.555676	-4300.310070	-4304.904535
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{t r}^2\text{SCAN3c}}$	-4294.443915	-4293.224996	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{t PBE0}}$	-4301.586180	-4300.342281	-4304.934678
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{q r}^2\text{SCAN3c}}$	-4294.433199	-4293.215958	n.a.
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}_{\text{q PBE0}}$	-4301.577567	-4300.335327	-4304.925938

Table S5: Benchmark of computed structural parameters with values found in the solid state of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$. Note that the degeneracy of the four MIC ligands is lifted in the solid state through interaction with the counteranion BF_4^- . Bond lengths are given in [Å], angles in [°].

	SC-XRD	r ² SCAN-3c	PBE-D4/def2-SVP	PBE0-D4/def2-SVP	ωB97X-V/def2-SVP	cam-B3LYP-D4/def2-SVP
Cr-C2	2.144					
Cr-C1 (3×)	2.136	2.138	2.115	2.12	2.142	2.134
Cr-N2	2.025	2.019	2.004	2.005	2.017	2.012
N-Cr-C (between pincers)	91.9	91.9	91.2	91.3	91.5	91.5

Table S6: Löwdin's atomic spin densities on Cr in [a.u.].

	r ² SCAN-3c	PBE0
$[\text{Cr}(\text{L}^{\text{MIC}})_2]$	2.57	2.72
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$	2.83	2.87
$[\text{Cr}(\text{L}^{\text{MIC}})_2]^{2+}$	2.47	2.66

Table S7: Number of electrons in d -orbitals according to localized IBOs (cutoff: 0.7). All redox states (their ground states, respectively) are predicted to feature a d^3 electron configuration.

	r ² SCAN-3c	PBE0
[Cr(L ^{MIC}) ₂]	d^3	d^3
[Cr(L ^{MIC}) ₂] ⁺	d^3	d^3
[Cr(L ^{MIC}) ₂] ²⁺	d^3	d^3

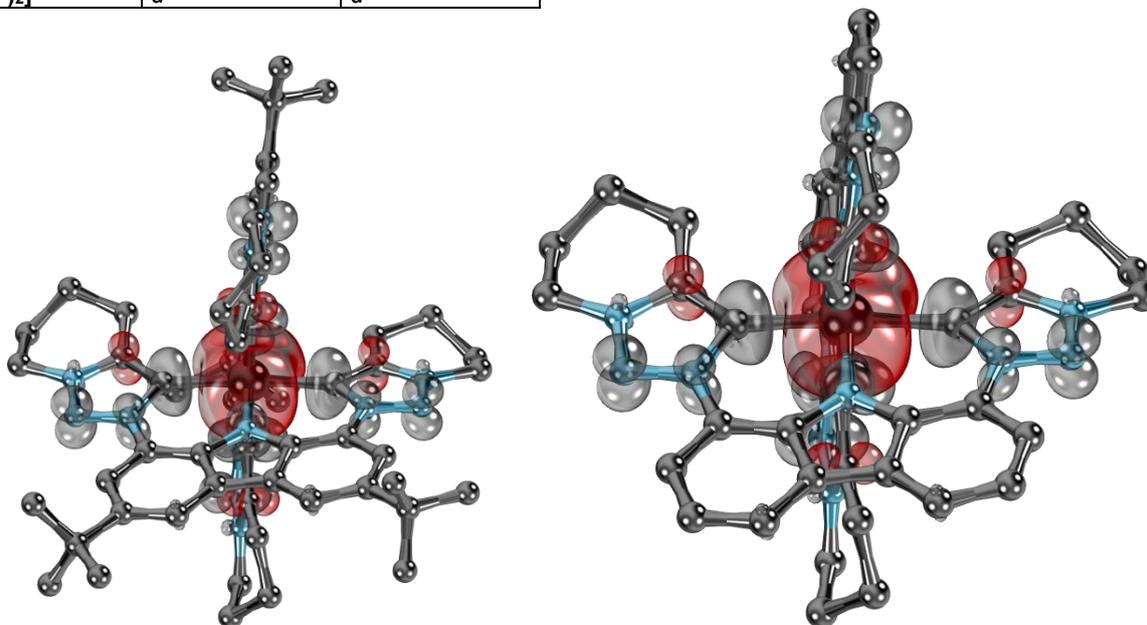


Figure S57: Spin density in [Cr(L^{MIC})₂] as obtained at the r²SCAN-3c level of theory ($S = 3/2$). Orbitals obtained with ZORA-PBE0-D4/def2-TZVPP//ZORA-PBE0-D4/def2-SVP are consistent. The spin density plot indicates anti-ferromagnetic coupling with a delocalized, ligand-centered radical. ^tBu in right structure truncated for clarity.

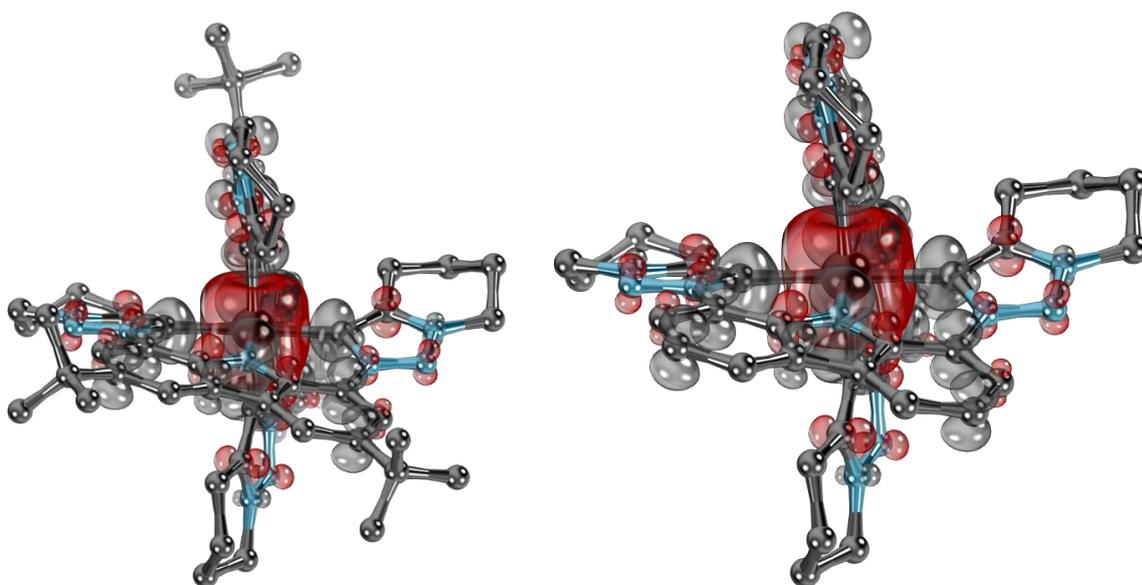


Figure S58: Spin density in [Cr(L^{MIC})₂]²⁺ as obtained at the r²SCAN-3c level of theory ($S = 3/2$). Orbitals obtained with ZORA-PBE0-D4/def2-TZVPP//ZORA-PBE0-D4/def2-SVP are consistent. The spin density plot indicates anti-ferromagnetic coupling with a delocalized, ligand-centered radical. ^tBu in right structure truncated for clarity.

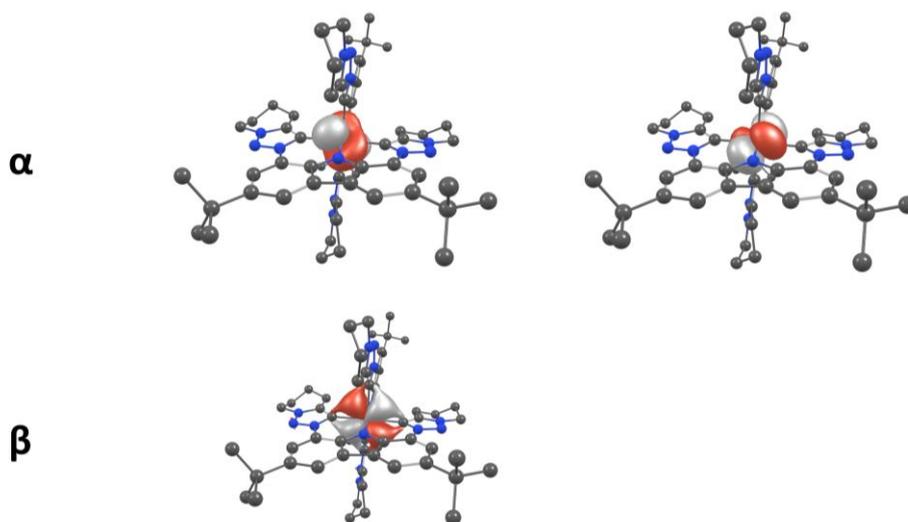


Figure S59: Metal-centered IBOs for the spin-flip (broken-symmetry, respectively) doublet excited state of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ as obtained at the ZORA-PBE0/def2-TZVPP//ZORA-PBE0-D4/def2-SVP level of theory. The computations with $r^2\text{SCAN-3c}$ did not converge.

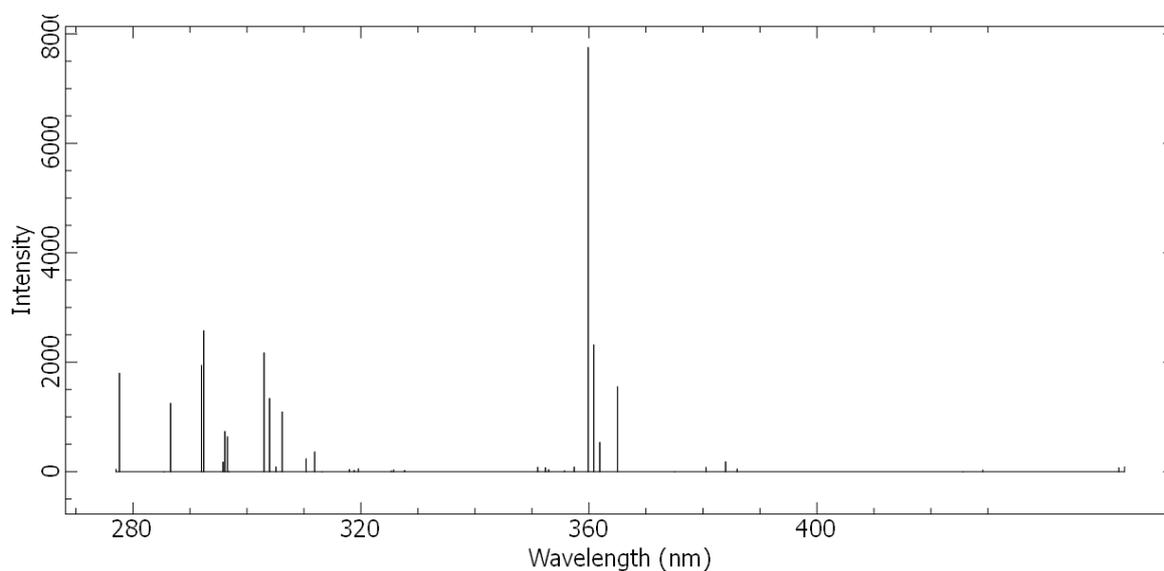


Figure S60: Absorption spectrum of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($S = 3/2$) as obtained by ZORA-cam-B3LYP/def2-TZVPP// $r^2\text{SCAN-3c}$.

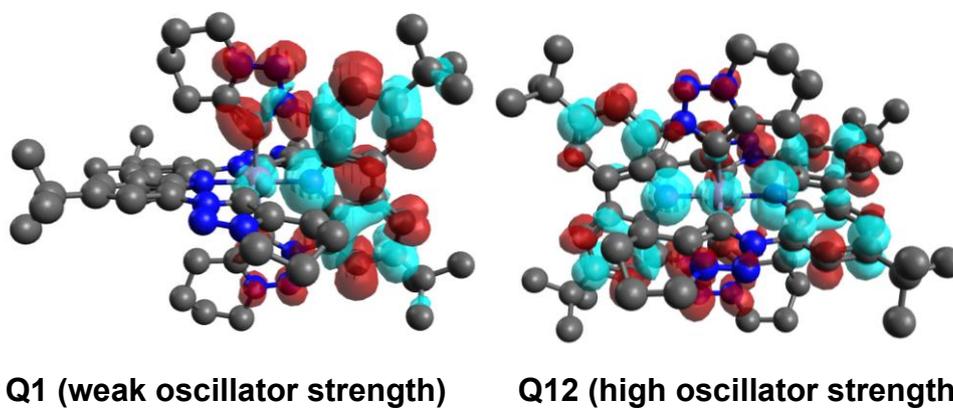


Figure S61: Transition difference densities for pertinent quartet excited state of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($S = 3/2$; cam-B3LYP).

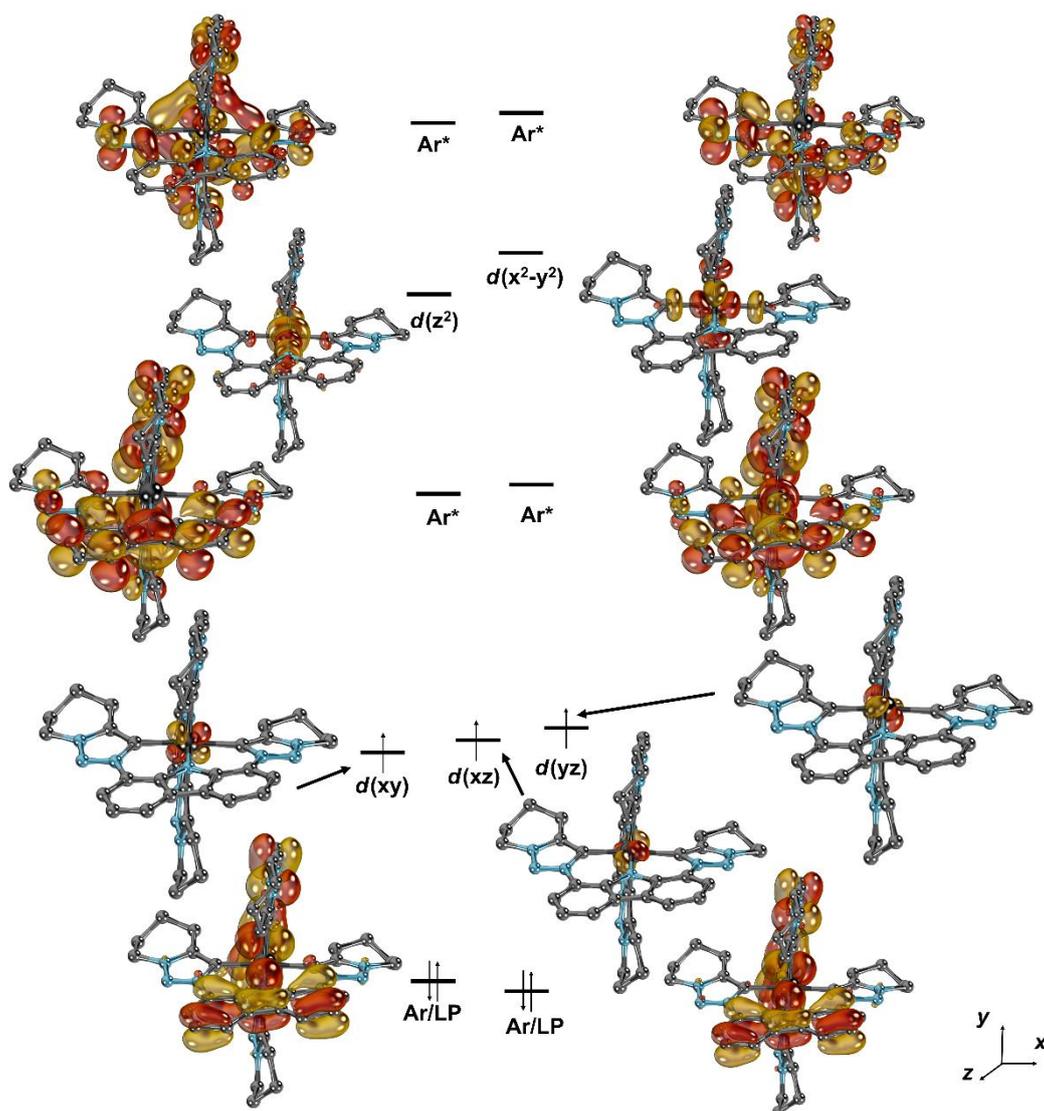


Figure S62: Molecular Orbital diagram ($c = 0.98$) of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($S = 3/2$) as obtained by state-averaged CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Isodensity values are adjusted for clarity.

Table S8: Configurations of pertinent roots (NEVPT2) for Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{MC}})_2]^+$ ($S = 3/2$) as obtained by CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Root 1 (LLCT) features low oscillator strength ($f_{\text{osc}} = 0.02$), roots 5 (ILCT; $f_{\text{osc}} = 0.07$) and 7 (LLCT; $f_{\text{osc}} = 0.14$) feature moderate oscillator strength, roots 6 (ILCT; $f_{\text{osc}} = 0.47$) and 8 (LLCT; $f_{\text{osc}} = 0.22$) feature high oscillator strengths.

ROOT 0: $E = 0$ eV	0.00545 [8]: 22101010000
0.98379 [0]: 22111000000	0.00463 [11]: 22101000010
0.00418 [1127]: 12112000000	0.00434 [6]: 22110000001
0.00301 [112]: 21121000000	
ROOT 1 (LLCT): $E = 2.36$ eV	ROOT 7 (ILCT/LLCT): $E = 2.87$ eV
0.62282 [124]: 21111000010	0.54593 [1132]: 12111000010
0.16427 [1133]: 21111000001	0.20963 [125]: 21111000001
0.13760 [84]: 21211000000	0.06544 [120]: 21111100000
0.01993 [1128]: 12111100000	0.04758 [1129]: 12111010000
0.01534 [121]: 21111010000	0.03743 [5]: 22110000010
0.00775 [11]: 22101000010	0.03324 [1092]: 12211000000
0.00556 [6]: 22110000001	0.01305 [1130]: 12111001000
0.00408 [125]: 21111000001	0.01076 [12]: 22101000001
0.00287 [1132]: 12111000010	0.00653 [124]: 21111000010
	0.00269 [3903]: 02112000010
	0.00255 [2]: 22110010000
ROOT 5 (ILCT/LLCT): $E = 2.71$ eV	ROOT 8 (ILCT/LLCT): $E = 2.91$ eV
0.48324 [120]: 21111100000	0.55798 [124]: 21111000010
0.27936 [1129]: 12111010000	0.22907 [1133]: 12111000001
0.08311 [1132]: 12111000010	0.05005 [1128]: 12111100000
0.05315 [125]: 21111000001	0.04426 [121]: 21111010000
0.03627 [1130]: 12111001000	0.02531 [84]: 21211000000
0.01066 [7]: 22101100000	0.02479 [11]: 22101000010
0.00892 [5]: 22110000010	0.02112 [6]: 22110000001
0.00864 [2]: 22110010000	0.01362 [122]: 21111001000
0.00530 [121]: 21111010000	0.00502 [125]: 21111000001
0.00309 [12]: 22101000001	0.00403 [1132]: 12111000010
	0.00317 [1614]: 11112000010
ROOT 6 (ILCT/LLCT): $E = 2.76$ eV	ROOT 9 ($d-d$ transition, ${}^4\text{T}_2$): $E = 3.03$ eV
0.45782 [1128]: 12111100000	0.68379 [3]: 22110001000
0.31975 [121]: 21111010000	0.19626 [10]: 22101000100
0.07223 [124]: 21111000010	0.10067 [2]: 22110010000
0.04294 [122]: 21111001000	0.00251 [1130]: 12111001000
0.04234 [1133]: 12111000001	
0.01770 [1]: 22110100000	
0.00725 [120]: 21111100000	

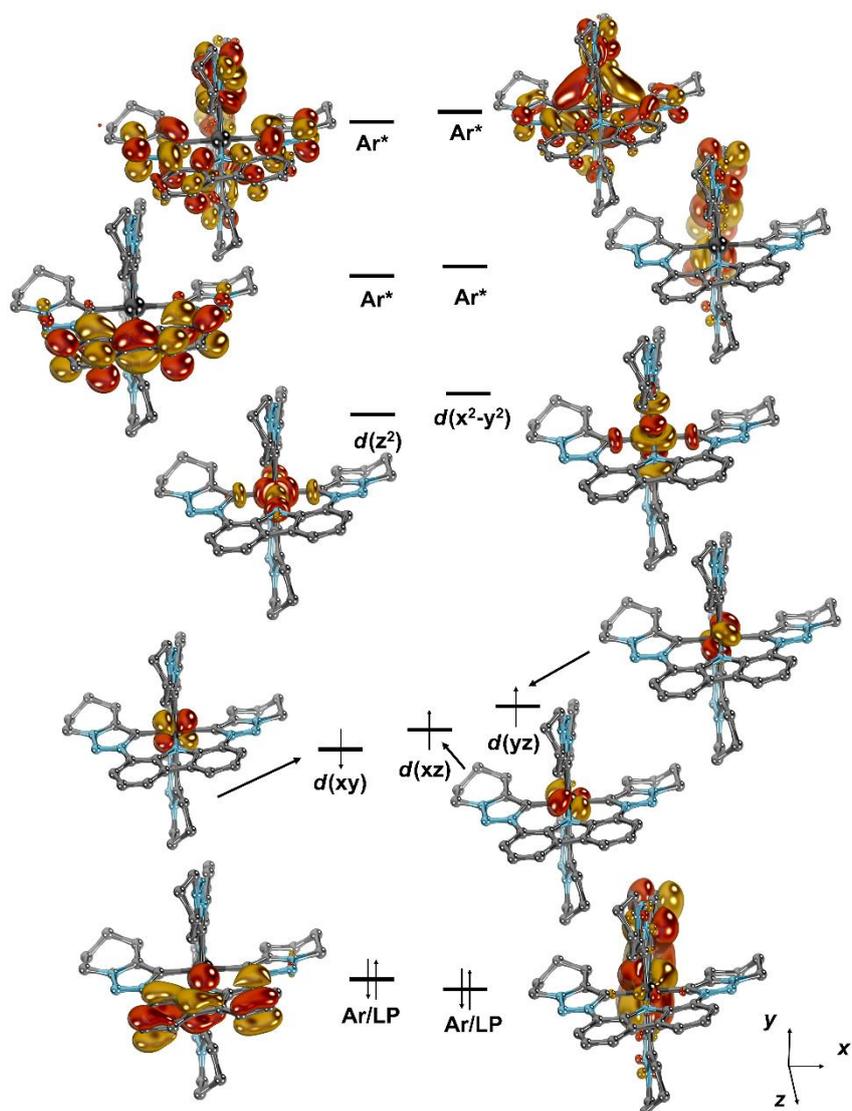


Figure S63: Molecular Orbital diagram ($c = 0.94$) of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ ($S = 1/2$) as obtained by state-averaged (40 roots) CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Isodensity values are adjusted for clarity.

Table S9: Configurations of pertinent roots (NEVPT2) for Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{MC}})_2]^+$ ($S = 1/2$) as obtained by CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals.

ROOT 0 (Spin-Flip State, ${}^2\text{E}$): $E = 1.70$ eV (vs. Q0)

0.94202 [9]: 22111000000
 0.01744 [3]: 22200010000
 0.00359 [8]: 22120000000
 0.00330 [52]: 22011100000
 0.00312 [46]: 22020010000
 0.00310 [2]: 22200100000
 0.00290 [727]: 20111002000
 0.00265 [4463]: 02111000200
 0.00261 [79]: 22002100000

ROOT 2 ($d-d$ transition, ${}^2\text{T}_1/{}^2\text{T}_2$): $E = 1.75$ eV (vs. Q0)

0.59177 [0]: 22210000000
 0.30435 [51]: 22012000000
 0.03554 [1]: 22201000000
 0.01780 [44]: 22021000000
 0.01376 [10]: 22110100000
 0.00642 [1501]: 12111000001
 0.00330 [9]: 22111000000
 0.00299 [18]: 22101010000
 0.00273 [205]: 21111000001

ROOT 3 ($d-d$ transition, ${}^2\text{T}_1/{}^2\text{T}_2$): $E = 1.80$ eV (vs. Q0)

0.50965 [1]: 22201000000
 0.39076 [44]: 22021000000
 0.03059 [0]: 22210000000
 0.02415 [51]: 22012000000
 0.01135 [17]: 22101100000
 0.00510 [11]: 22110010000
 0.00352 [205]: 21111000001

ROOT 4 ($d-d$ transition, ${}^2\text{T}_1/{}^2\text{T}_2$): $E = 1.81$ eV (vs. Q0)

0.29364 [16]: 22102000000
 0.22533 [9]: 22111000000
 0.01217 [45]: 22020100000
 0.00947 [79]: 22002100000
 0.00507 [46]: 22020010000

ROOT 5 (Spin-Flip State, ${}^2\text{E}$): $E = 1.92$ eV (vs. Q0)

0.73787 [9]: 22111000000
 0.11253 [16]: 22102000000
 0.11114 [8]: 22120000000
 0.00651 [52]: 22011100000
 0.00436 [46]: 22020010000
 0.00370 [80]: 22002010000
 0.00324 [53]: 22011010000

ROOT 6 (ILCT/LLCT): $E = 2.58$ eV (vs. Q0)

0.05035 [1498]: 12111001000
 0.04888 [13]: 22110000100
 0.02047 [203]: 21111000100
 0.00874 [20]: 22101000100
 0.00520 [4445]: 02112000100
 0.00361 [1651]: 12011000101
 0.00295 [3146]: 10111002100
 0.00294 [12]: 22110001000

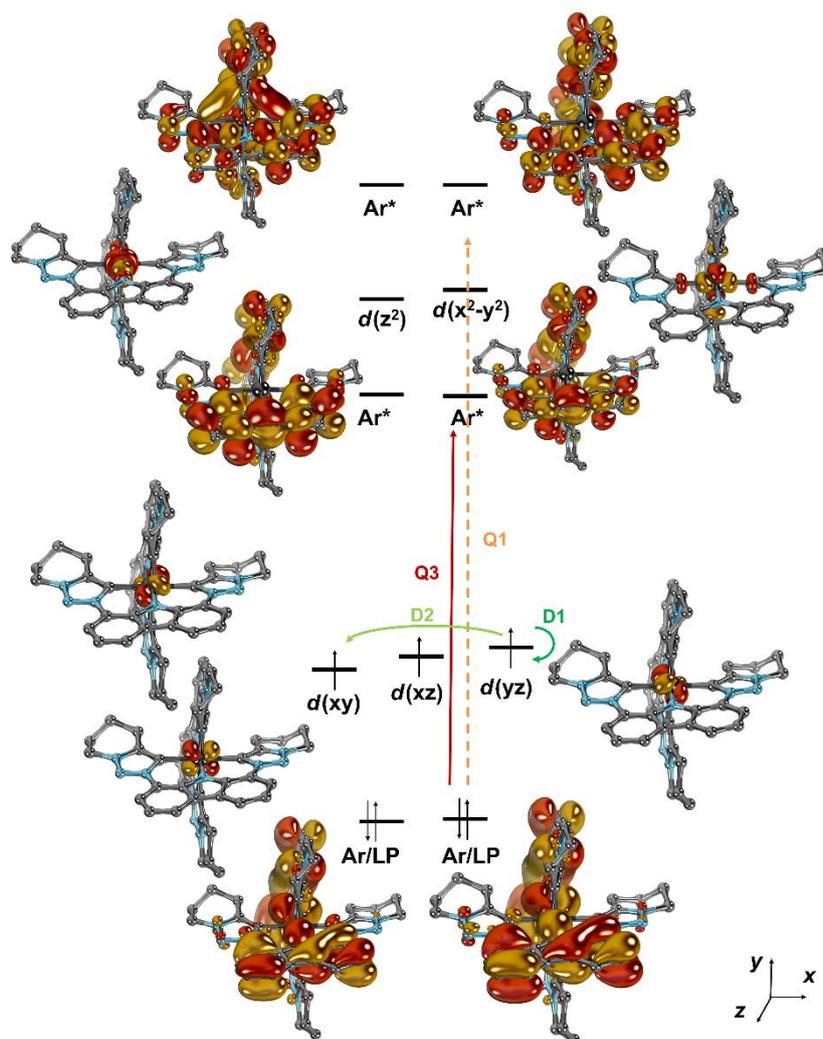


Figure S64: Idealized electronic nature of pertinent transitions (excited states, respectively) of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$. The D0 excited state is a spin-flip state; order of orbitals does not follow their energies, yet their occupations.

Table S10: Energies of vertical excited states by NEVPT2/CASSCF(7,11) of $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ (structural parameters of $S = 3/2$; separately state averaging for either quartets or doublets). Energies are given in [eV].

Quartet	Gasphase	CPCM(MeCN)	Doublet	Gasphase	CPCM(MeCN)
Q0	0.00	0.00	D1	1.70	1.73
Q1	2.36	2.50	D2	1.75	1.75
Q2	2.44	2.57	D3	1.80	1.82
Q3	2.66	2.68	D4	1.81	1.82
Q4	2.66	2.69	D5	1.92	1.92
Q5	2.71	2.73	D6	2.58	2.61
Q6	2.76	2.79	D7	2.59	2.62
Q7	2.87	2.96	D8	2.71	2.73
Q8	2.91	3.01	D9	2.79	2.75
Q9	3.03	3.04	D10	2.91	2.92
Q10	3.12	3.13	D11	2.92	3.21

Comparison of Ligands (NHC, py) and Metal (Mn)

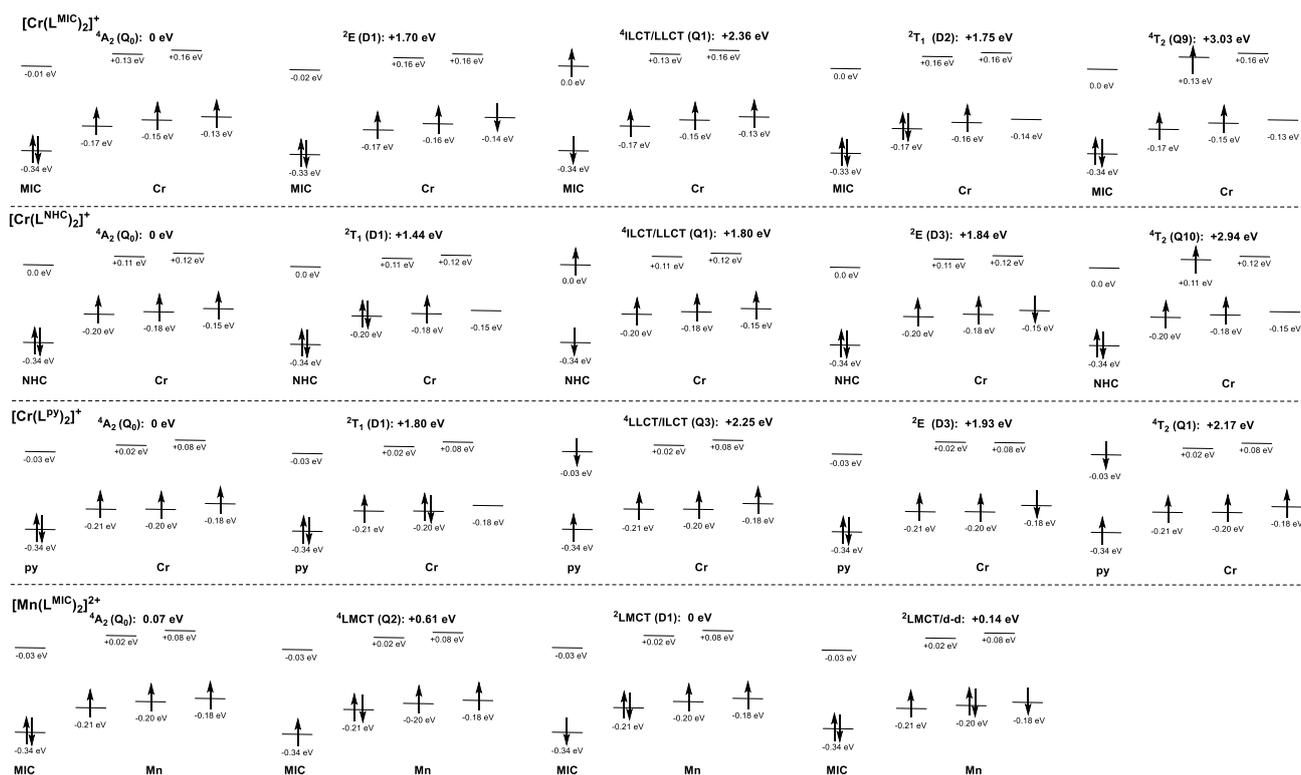


Figure S65: Idealized nature of pertinent transitions and their energies based on NEVPT2/CASSCF calculations (for all-state averaged calculations, in case of MIC-Cr additionally based on separate state-averaging for the quartet- and singlet states. Orbital energies are idealized, yet the order corresponds to their computed energies. Note that the orbital energies obtained by AILFT (vide infra) differ considerably, and further note that the states particularly for the Mn-complex are heavily multiconfigurational (vide infra).

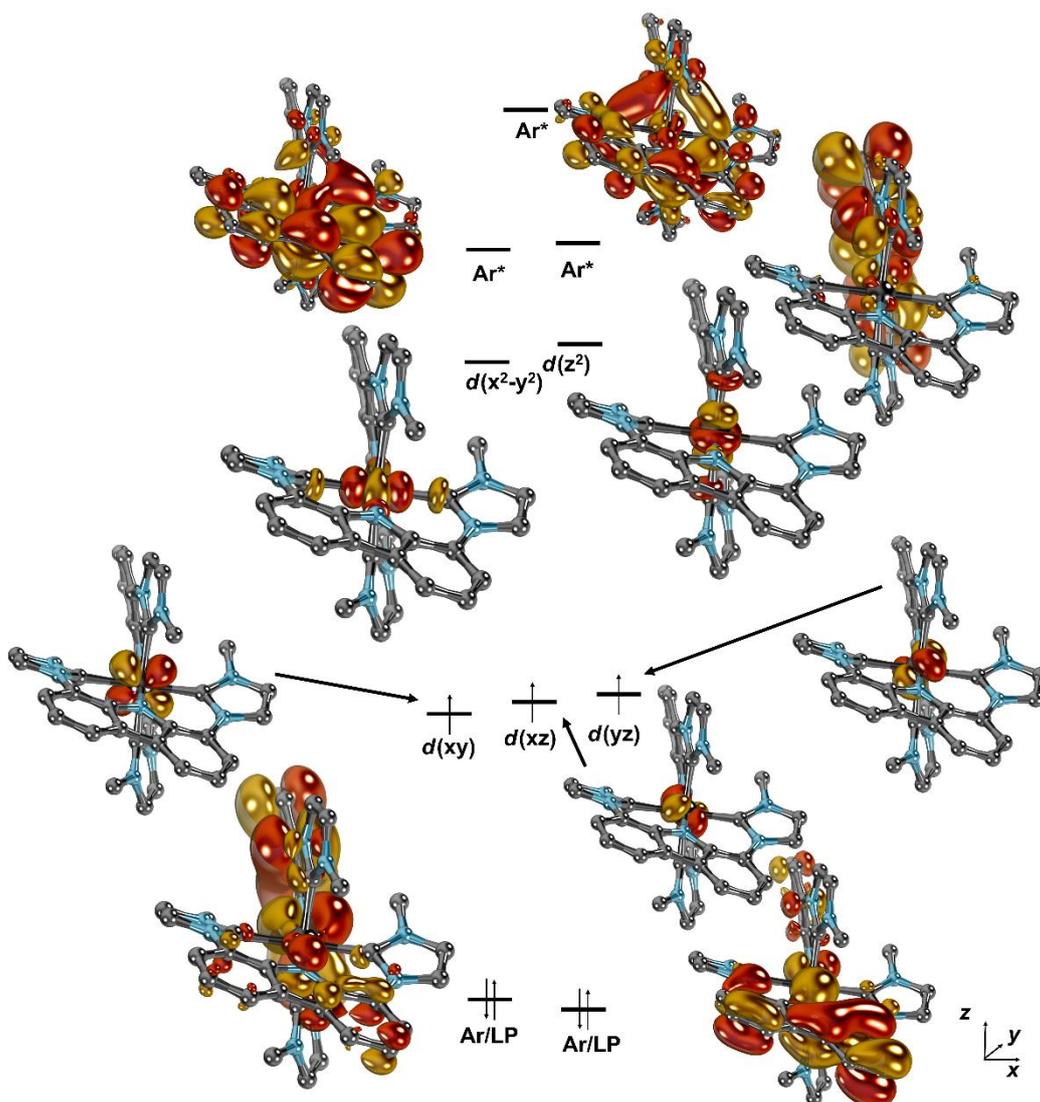


Figure S66: Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ ($S = 3/2$, 20 roots; $S = 1/2$, 40 roots) as obtained by state-averaged CASSCF(7,10) in order of decreasing occupation (and not energy) of natural orbitals. Isodensity values are adjusted for clarity.

Table S11: Configurations of pertinent roots (NEVPT2) for Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$ ($S = 3/2$, 20 roots; $S = 1/2$, 40 roots) as obtained by CASSCF(7,10) in order of decreasing occupation (and not energy) of natural orbitals.

DOUBLETS:	QUARTETS:
<p>ROOT 0 (<i>d-d</i> transition, ${}^2T_1/{}^2T_2$) E= 1.442 eV (vs. Q0)</p> <p>0.75464 [0]: 2221000000 0.15248 [41]: 2201200000 0.01187 [10]: 2211001000 0.01115 [921]: 1211100001 0.01002 [1]: 2220100000 0.00975 [9]: 2211010000 0.00518 [920]: 1211100010 0.00503 [883]: 1221100000 0.00270 [13]: 2211000001</p> <p>ROOT 1: (<i>d-d</i> transition, ${}^2T_1/{}^2T_2$) E= 1.803 eV (vs. Q0)</p> <p>0.61112 [7]: 2212000000 0.28321 [14]: 2210200000 0.03649 [8]: 2211100000 0.01178 [37]: 2202001000 0.00899 [36]: 2202010000 0.00369 [40]: 2202000001 0.00362 [66]: 2200200001 0.00334 [42]: 2201110000 0.00300 [62]: 2200210000</p> <p>ROOT 2: (<i>d-d</i> transition, ${}^2T_1/{}^2T_2$) E= 1.828 eV (vs. Q0)</p> <p>0.61912 [1]: 2220100000 0.28818 [35]: 2202100000 0.01076 [8]: 2211100000 0.00839 [0]: 2221000000 0.00760 [16]: 2210101000 0.00723 [15]: 2210110000 0.00698 [19]: 2210100001 0.00497 [151]: 2111100001 0.00369 [41]: 2201200000 0.00336 [18]: 2210100010</p> <p>ROOT 3: (Spin-Flip State, 2E) E= 1.844 eV (vs. Q0)</p> <p>0.91963 [8]: 2211100000 0.01319 [2]: 2220010000 0.01180 [3]: 2220001000 0.00699 [1]: 2220100000 0.00455 [46]: 2201100001 0.00288 [12]: 2211000010 0.00280 [35]: 2202100000 0.00263 [37]: 2202001000</p> <p>ROOT 4: (<i>d-d</i> transition, ${}^2T_1/{}^2T_2$) E= 2.017 eV (vs. Q0)</p> <p>0.61112 [7]: 2212000000 0.28321 [14]: 2210200000 0.03649 [8]: 2211100000 0.01178 [37]: 2202001000 0.00899 [36]: 2202010000 0.00369 [40]: 2202000001 0.00362 [66]: 2200200001 0.00334 [42]: 2201110000 0.00300 [62]: 2200210000</p> <p>ROOT 10: (<i>d-d</i> transition) 3.001 eV (vs. Q0)</p> <p>0.27471 [9]: 2211010000 0.16637 [113]: 2121100000 0.15282 [883]: 1221100000 0.08748 [151]: 2111100001 0.08538 [921]: 1211100001 0.04942 [15]: 2210110000</p>	<p>ROOT 0: (4A_2) E= 0 eV</p> <p>0.95330 [0]: 2211100000 0.01143 [25]: 2201100001 0.00568 [24]: 2201100010 0.00366 [4]: 2211000010 0.00345 [657]: 1211200000 0.00271 [23]: 2201100100 0.00259 [3]: 2211000100</p> <p>ROOT 1: (LMCT) E= 1.803 eV</p> <p>0.50260 [630]: 1221100000 0.23517 [662]: 1211100001 0.06759 [661]: 1211100010 0.05508 [56]: 2121100000 0.02251 [88]: 2111100001 0.02148 [660]: 1211100100 0.02058 [87]: 2111100010 0.00774 [762]: 1201100002 0.00688 [86]: 2111100100 0.00614 [761]: 1201100011 0.00510 [658]: 1211110000 0.00350 [659]: 1211101000 0.00338 [5]: 2211000001 0.00285 [651]: 1212100000 0.00258 [868]: 1122100000 0.00252 [759]: 1201100101</p> <p>ROOT 2: (LMCT) E= 1.907 eV</p> <p>0.41277 [56]: 2121100000 0.26089 [88]: 2111100001 0.05713 [662]: 1211100001 0.05107 [87]: 2111100010 0.04858 [630]: 1221100000 0.03435 [661]: 1211100010 0.02809 [86]: 2111100100 0.02402 [660]: 1211100100 0.00760 [188]: 2101100002 0.00703 [657]: 1211200000 0.00557 [187]: 2101100011 0.00529 [84]: 2111110000 0.00476 [77]: 2112100000 0.00404 [874]: 1121200000 0.00393 [4]: 2211000010 0.00319 [85]: 2111101000 0.00315 [3]: 2211000100</p> <p>ROOT 3: (<i>d-d</i> transition, 4T_2) E= 2.935 eV</p> <p>0.49448 [1]: 2211010000 0.24409 [2]: 2211001000 0.13834 [6]: 2210110000 0.07783 [7]: 2210101000 0.00517 [29]: 2201010001 0.00325 [5]: 2211000001 0.00303 [32]: 2201001001 0.00277 [28]: 2201010010</p> <p>ROOT 4: (LLCT/ILCT) E= 2.938 eV</p> <p>0.67384 [86]: 2111100100 0.11430 [660]: 1211100100 0.06988 [56]: 2121100000 0.02648 [3]: 2211000100 0.01961 [83]: 2111200000</p>

0.02856 [10]: 2211001000	0.01578 [8]: 2210100100
0.02152 [150]: 2111100010	0.01333 [88]: 2111100001
0.01610 [919]: 1211100100	0.01044 [185]: 2101100101
0.01526 [16]: 2210101000	0.00502 [184]: 2101100110
0.00969 [1]: 2220100000	0.00480 [657]: 1211200000
0.00762 [19]: 2210100001	0.00431 [661]: 1211100010
0.00681 [920]: 1211100010	0.00419 [662]: 1211100001
0.00548 [67]: 2200120000	0.00331 [87]: 2111100010
0.00289 [2442]: 0221200000	0.00286 [99]: 2111000110
0.00272 [1027]: 1201100002	
0.00261 [257]: 2101100002	

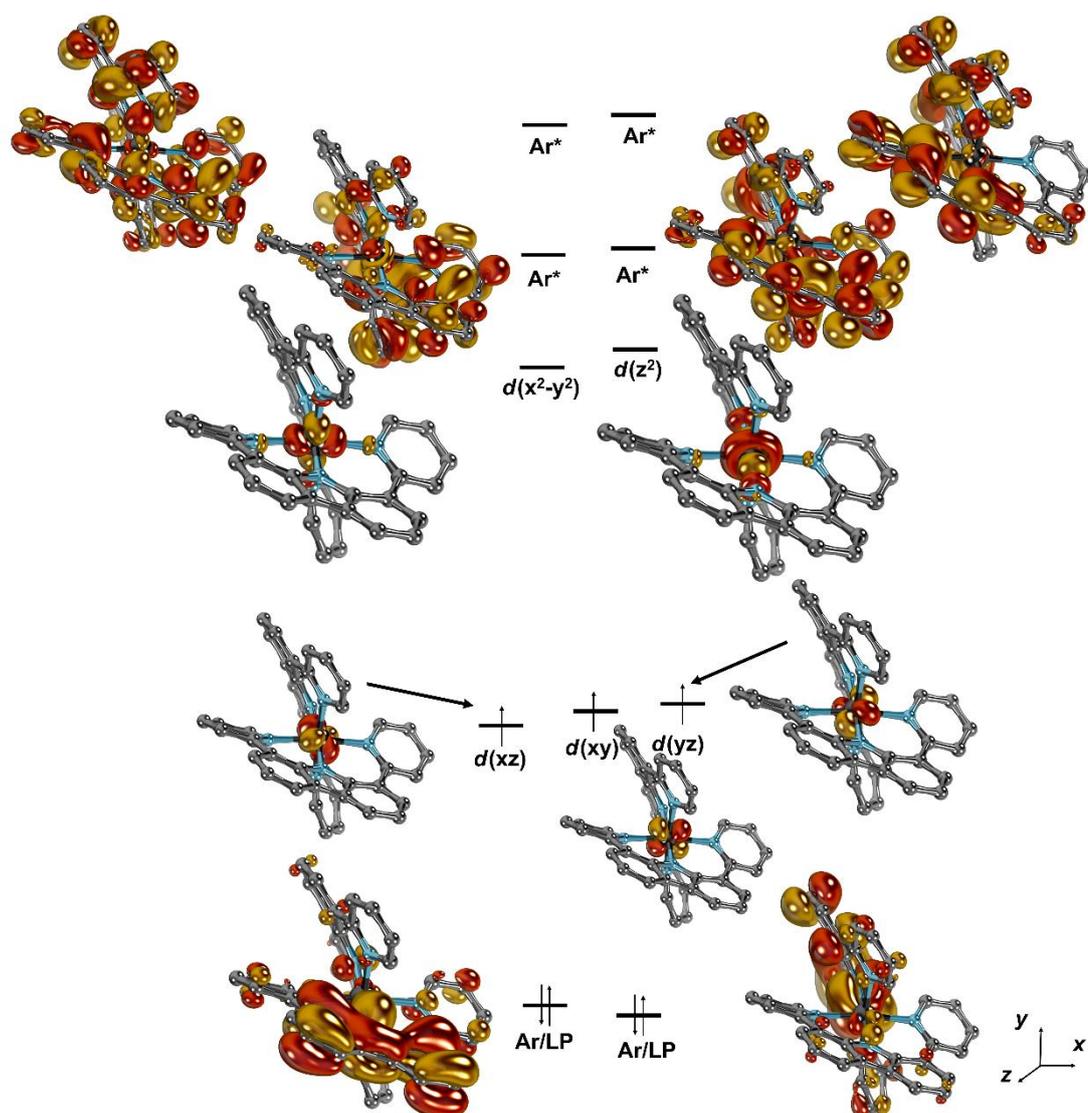


Figure S67: Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ ($S = 3/2$, 20 roots; $S = 1/2$, 40 roots) as obtained by state-averaged CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Isodensity values are adjusted for clarity.

Table S12: Configurations of pertinent roots (NEVPT2) for Molecular Orbital diagram of $[\text{Cr}(\text{L}^{\text{Py}})_2]^+$ ($S = 3/2$, 20 roots; $S = 1/2$, 40 roots) as obtained by CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals.

DOUBLETS:	QUARTETS:
<p>ROOT 0: (<i>d-d</i> transition, ${}^2\text{T}_1/{}^2\text{T}_2$) E= 1.803 eV (vs. Q0)</p> <p>0.54620 [8]: 22120000000 0.23308 [9]: 22111000000 0.12315 [16]: 22102000000 0.01744 [11]: 22110010000 0.01237 [0]: 22210000000 0.00929 [45]: 22020100000 0.00700 [51]: 22012000000 0.00670 [44]: 22021000000 0.00661 [1498]: 12111001000 0.00491 [1]: 22201000000 0.00269 [29]: 22100020000</p> <p>ROOT 1: (<i>d-d</i> transition, ${}^2\text{T}_1/{}^2\text{T}_2$) E= 1.824 eV (vs. Q0)</p> <p>0.66238 [0]: 22210000000 0.24090 [51]: 22012000000 0.02336 [3]: 22200010000 0.00995 [17]: 22101100000 0.00992 [1]: 22201000000 0.00940 [9]: 22111000000 0.00763 [8]: 22120000000 0.00344 [4]: 22200001000 0.00335 [81]: 22002001000 0.00334 [44]: 22021000000 0.00323 [1499]: 12111000100 0.00278 [80]: 22002010000</p> <p>ROOT 2: (Spin Flip, ${}^2\text{E}$) E= 1.938 eV (vs. Q0)</p> <p>0.63519 [9]: 22111000000 0.18782 [8]: 22120000000 0.06844 [16]: 22102000000 0.02388 [45]: 22020100000 0.01905 [1]: 22201000000 0.01712 [44]: 22021000000 0.00612 [11]: 22110010000 0.00402 [19]: 22101001000 0.00401 [1498]: 12111001000 0.00360 [2]: 22200100000 0.00308 [79]: 22002100000 0.00274 [18]: 22101010000</p> <p>ROOT 3: (Spin-Flip, ${}^2\text{E}$) E= 2.089 eV (vs. Q0)</p> <p>0.91394 [9]: 22111000000 0.01896 [2]: 22200100000 0.01078 [79]: 22002100000 0.01043 [1]: 22201000000 0.00951 [44]: 22021000000 0.00926 [19]: 22101001000 0.00536 [59]: 22010110000 0.00464 [18]: 22101010000 0.00264 [8]: 22120000000</p> <p>ROOT 4: (<i>d-d</i> transition; ${}^2\text{T}_1/{}^2\text{T}_2$) E= 2.098 eV (vs. Q0)</p> <p>0.48915 [44]: 22021000000 0.37243 [1]: 22201000000 0.07322 [9]: 22111000000 0.01493 [10]: 22110100000 0.01073 [53]: 22011010000 0.00873 [54]: 22011001000 0.00492 [51]: 22012000000 0.00304 [0]: 22210000000</p>	<p>ROOT 0: (${}^4\text{A}_2$) E= 0 eV</p> <p>0.97182 [0]: 22111000000 0.01137 [9]: 22101001000 0.00355 [1127]: 12112000000 0.00302 [31]: 22011000100</p> <p>ROOT 1: (<i>d-d</i> transition, ${}^4\text{T}_2$) E= 2.167 eV</p> <p>0.93162 [7]: 22101100000 0.02051 [1]: 22110100000 0.01957 [28]: 22011100000 0.00702 [11]: 22101000010 0.00331 [1155]: 12102100000 0.00312 [51]: 22001100100</p> <p>ROOT 2: (<i>d-d</i> transition, ${}^4\text{T}_2$) E= 2.226 eV</p> <p>0.73365 [1]: 22110100000 0.18382 [29]: 22011010000 0.02325 [13]: 22100110000 0.02300 [7]: 22101100000 0.00400 [5]: 22110000010 0.00372 [14]: 22100101000 0.00349 [8]: 22101010000</p> <p>ROOT 3: (LLCT/ILCT) E = 2.253 eV</p> <p>0.19784 [1133]: 12111000001 0.19009 [1130]: 12111001000 0.13683 [1132]: 12111000010 0.13163 [1120]: 12121000000 0.09854 [124]: 21111000010 0.08321 [1131]: 12111000100 0.02335 [122]: 21111001000 0.01967 [1092]: 12211000000 0.01706 [123]: 21111000100 0.01266 [1129]: 12111010000 0.01107 [6]: 22110000001 0.00908 [1128]: 12111100000 0.00611 [120]: 21111100000 0.00566 [112]: 21121000000 0.00465 [1172]: 12101002000 0.00440 [4]: 22110000100 0.00438 [84]: 21211000000 0.00361 [3]: 22110001000 0.00336 [1175]: 12101001001 0.00284 [32]: 22011000010</p> <p>ROOT 4: (LLCT/ILCT) E= 2.299 eV</p> <p>0.40286 [122]: 21111001000 0.19572 [123]: 21111000100 0.08957 [112]: 21121000000 0.08824 [124]: 21111000010 0.07166 [1131]: 12111000100 0.02714 [125]: 21111000001 0.02421 [84]: 21211000000 0.01461 [1132]: 12111000010 0.01459 [4]: 22110000100 0.00787 [121]: 21111010000 0.00670 [164]: 21101002000 0.00417 [3]: 22110001000 0.00405 [119]: 21112000000 0.00402 [30]: 22011001000 0.00373 [1130]: 12111001000 0.00363 [5]: 22110000010 0.00327 [1092]: 12211000000 0.00264 [165]: 21101001100</p>

ROOT 11: (*d-d* transition) E= 3.305 eV

0.37471	[17]:	22101100000
0.10986	[203]:	21111000100
0.09355	[1498]:	12111001000
0.04662	[202]:	21111001000
0.04040	[1501]:	12111000001
0.03733	[58]:	22010200000
0.03702	[51]:	22012000000
0.03612	[1499]:	12111000100
0.02925	[204]:	21111000010
0.02306	[80]:	22002010000
0.01903	[1488]:	12121000000
0.01741	[12]:	22110001000
0.01486	[0]:	22210000000
0.01295	[157]:	21211000000
0.01274	[192]:	21121000000
0.01038	[10]:	22110100000
0.00985	[11]:	22110010000
0.00823	[3]:	22200010000
0.00507	[52]:	22011100000
0.00375	[55]:	22011000100
0.00358	[1500]:	12111000010
0.00348	[15]:	22110000001
0.00312	[2]:	22200100000
0.00298	[1453]:	12211000000
0.00283	[14]:	22110000010

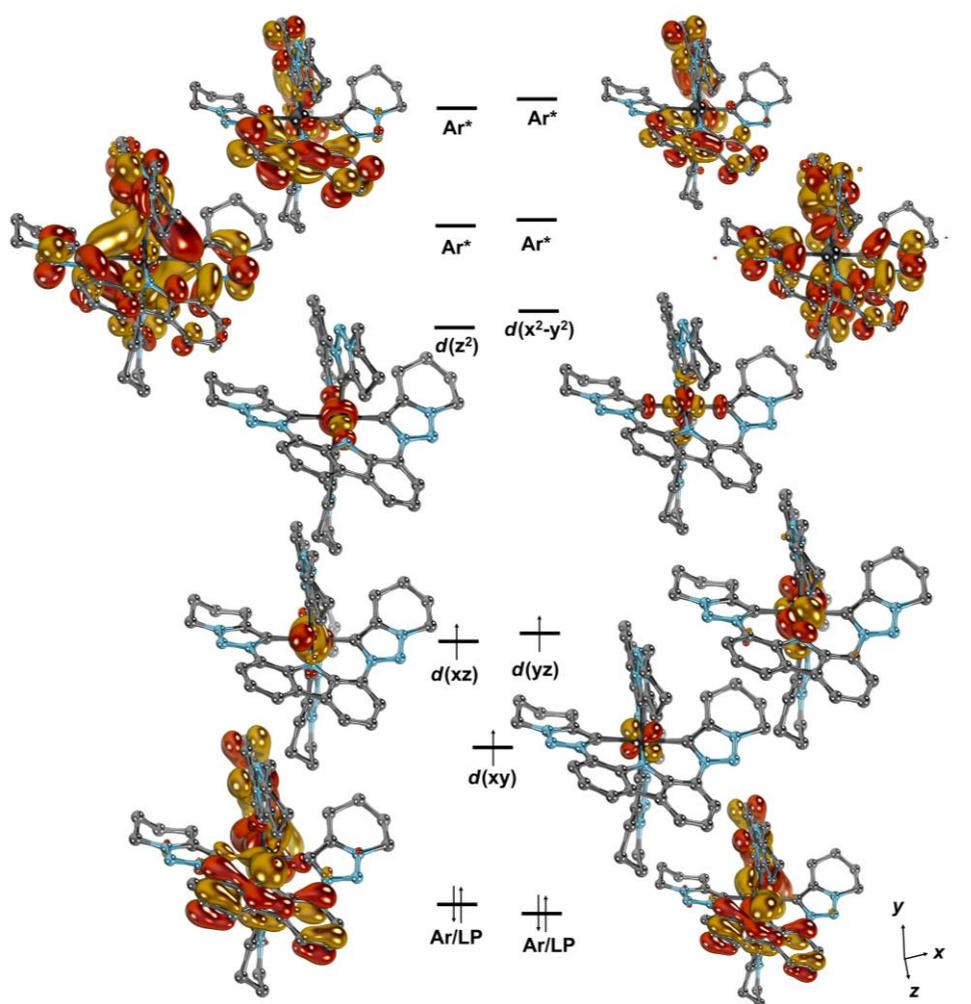


Figure S68: Molecular Orbital diagram of $[\text{Mn}(\text{L}^{\text{MIC}})_2]^{2+}$ ($S = 3/2$, 40 roots; $S = 1/2$, 80 roots) as obtained by state-averaged CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Isodensity values are adjusted for clarity.

Table S13: Configurations of pertinent roots (NEVPT2) for Molecular Orbital diagram of $[\text{Mn}(\text{L}^{\text{MIC}})_2]^{2+}$ ($S = 3/2$, 80 roots; $S = 1/2$, 40 roots) as obtained by CASSCF(7,11) in order of decreasing occupation (and not energy) of natural orbitals. Note that the non-truncated complex features experimentally in the solid-state an $S = 3/2$ ground state,^[3] which is calculated to be essentially isoergic ($\Delta E = +0.07$ eV).

DOUBLETS:	QUARTETS:
<p>ROOT 0: (MLCT) E= 0 eV</p> <p>0.33455 [1453]: 12211000000 0.27704 [0]: 22210000000 0.12101 [1488]: 12121000000 0.09446 [8]: 22120000000 0.05676 [4309]: 02212000000 0.04087 [1866]: 11221000000 0.02052 [4414]: 02122000000 0.00435 [1496]: 12111100000 0.00431 [1634]: 12011200000 0.00410 [5184]: 01222000000 0.00337 [58]: 22010200000 0.00261 [1490]: 12120010000 0.00254 [1498]: 12111001000 0.00252 [156]: 21220000000 0.00250 [199]: 21112000000</p> <p>ROOT 1: (LMCT/<i>d-d</i> transition) E= 0.138 eV (vs. ROOT0, doublet)</p> <p>0.35154 [1488]: 12121000000 0.24648 [8]: 22120000000 0.12409 [1453]: 12211000000 0.09243 [0]: 22210000000 0.06365 [4414]: 02122000000 0.04487 [199]: 21112000000 0.02234 [4309]: 02212000000 0.01532 [16]: 22102000000 0.00378 [1455]: 12210010000 0.00293 [1535]: 12101020000 0.00262 [51]: 22012000000</p> <p>ROOT 2: (LLCT/ILCT) E= 0.164 eV (vs. ROOT0, doublet)</p> <p>0.59447 [157]: 21211000000 0.19813 [1]: 22201000000 0.06575 [1873]: 11212000000 0.06039 [570]: 20221000000 0.02817 [9]: 22111000000 0.00674 [338]: 21011200000 0.00480 [200]: 21111100000 0.00422 [2748]: 10222000000 0.00371 [192]: 21121000000 0.00343 [1460]: 12202000000</p> <p>ROOT 3: (LLCT/ILCT) E= 0.339 eV (vs. ROOT0, doublet)</p> <p>0.67572 [192]: 21121000000 0.15280 [9]: 22111000000 0.08474 [1978]: 11122000000 0.02857 [44]: 22021000000 0.00972 [157]: 21211000000 0.00528 [239]: 21101020000 0.00439 [570]: 20221000000 0.00431 [1495]: 12112000000 0.00403 [233]: 21101200000 0.00397 [305]: 21021100000 0.00258 [1]: 22201000000</p> <p>ROOT 4: (LLCT/ILCT) E= 0.531 eV (vs. ROOT0, doublet)</p> <p>0.63887 [1495]: 12112000000 0.23932 [9]: 22111000000 0.03952 [1978]: 11122000000 0.03306 [192]: 21121000000 0.00605 [1508]: 12110020000 0.00592 [1873]: 11212000000 0.00454 [1628]: 12012100000 0.00448 [157]: 21211000000 0.00399 [1502]: 12110200000</p>	<p>ROOT 1: ($^4\text{A}_2$) E= 0.069 eV (vs. ROOT0, doublet)</p> <p>0.20448 [0]: 22111000000 0.15115 [1127]: 12112000000 0.07660 [1613]: 11112000100 0.06639 [112]: 21121000000 0.05075 [553]: 20111010100 0.04258 [1850]: 11022001000 0.04081 [3913]: 02111010100 0.02996 [123]: 21111000100 0.02944 [1612]: 11112001000 0.01827 [1586]: 11121000100 0.01616 [1623]: 11111011000 0.01456 [30]: 22011001000 0.01258 [1155]: 12102100000 0.01195 [1142]: 12110010100 0.01155 [1162]: 12101110000 0.01094 [84]: 21211000000 0.01044 [226]: 21021001000 0.01001 [1121]: 12120100000 0.00749 [122]: 21111001000 0.00710 [161]: 21101010100 0.00681 [1129]: 12111010000 0.00654 [1582]: 11122000000 0.00630 [1473]: 11220001000 0.00569 [541]: 20112001000 0.00546 [1255]: 12012001000 0.00521 [2675]: 10112010100 0.00490 [1253]: 12012100000 0.00484 [133]: 21110011000 0.00451 [1260]: 12011110000 0.00444 [1479]: 11211010000 0.00438 [252]: 21011110000 0.00432 [1131]: 12111000100 0.00389 [7]: 22101100000 0.00365 [3901]: 02112001000 0.00351 [1134]: 12110200000 0.00313 [124]: 21111000010 0.00291 [1588]: 11121000001 0.00258 [9]: 22101001000 0.00256 [4704]: 01121010100</p> <p>ROOT 2: ($^4\text{A}_2$ – mixes with LLCT/ILCT) E= 0.169 eV (vs. ROOT0, doublet)</p> <p>0.30202 [0]: 22111000000 0.25073 [112]: 21121000000 0.13489 [1128]: 12111100000 0.08292 [1127]: 12112000000 0.07013 [1]: 22110100000 0.05270 [1582]: 11122000000 0.03711 [84]: 21211000000 0.01996 [3899]: 02112100000 0.00980 [1583]: 11121100000 0.00796 [1477]: 11212000000 0.00265 [159]: 21101020000</p> <p>ROOT 3: (ILCT/LLCT) E= 0.605 eV (vs. ROOT0, doublet)</p> <p>0.55052 [1092]: 12211000000 0.34241 [1120]: 12121000000 0.03466 [1470]: 11221000000 0.01598 [1127]: 12112000000 0.00851 [112]: 21121000000 0.00764 [119]: 21112000000 0.00759 [1259]: 12011200000 0.00616 [1128]: 12111100000 0.00328 [1585]: 11121001000 0.00311 [1122]: 12120010000 0.00304 [1161]: 12101200000</p>

	<p>ROOT 4: (ILCT/LLCT) E= 0.690 eV (vs. ROOT0, doublet)</p> <p>0.44917 [1127]: 12112000000 0.28075 [112]: 21121000000 0.14177 [119]: 21112000000 0.04419 [0]: 22111000000 0.03263 [84]: 21211000000 0.01419 [1092]: 12211000000 0.00373 [1140]: 12110020000</p> <p>ROOT 5: (ILCT/LLCT) E= 0.719 eV (vs. ROOT0, doublet)</p> <p>0.52764 [1120]: 12121000000 0.35870 [1092]: 12211000000 0.07345 [119]: 21112000000 0.00438 [1094]: 12210010000 0.00402 [1167]: 12101020000 0.00395 [1470]: 11221000000 0.00350 [1232]: 12021100000 0.00264 [1259]: 12011200000</p>
--	--

Comparison of Ligands (NHC, py) and Metal (Mn): AILFT

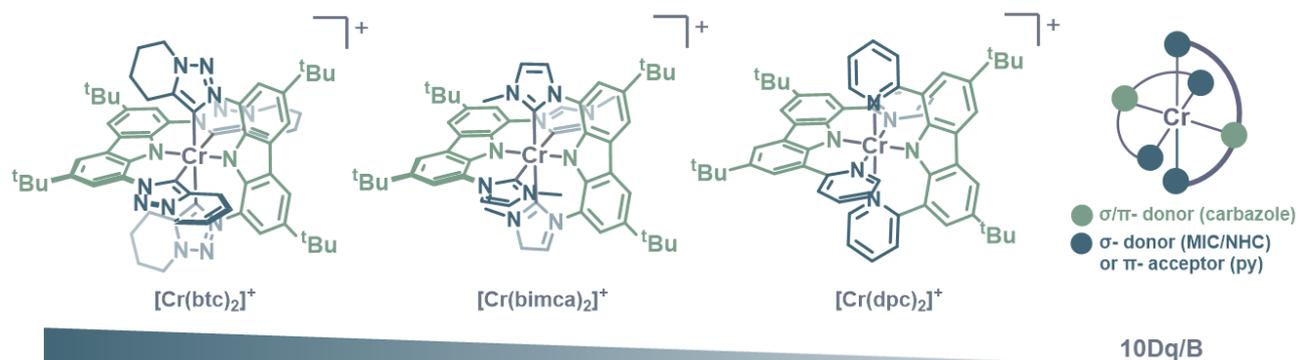


Table S14: Ab-Initio Ligand Field (AILFT) comparison of MIC, NHC and py ligands as well as comparison with MIC-Mn complex as obtained at the NEVPT2//CASSCF(3,5) level of theory. Energies are given in $[cm^{-1}]$.

$[Mn(L^{MIC})_2]^{2+}$	$d(xz)$	$d(yz)$	$d(xy)$	$d(x^2-y^2)$ C-C-C-C	$d(z^2)$ N-Mn-N	10 Dq (1st transition)
	0.0	281.0	2633.0	32798.4	35795.2	35155.4
$[Cr(L^{MIC})_2]^+$	$d(xy)$	$d(yz)$	$d(xz)$	$d(z^2)$ C-Cr-C	$d(x^2-y^2)$ N-C-N-C	10 Dq (1st transition)
	0.0	537.5	1317.6	23608.8	24154.8	25102.6
$[Cr(L^{NHC})_2]^+$	$d(xy)$	$d(yz)$	$d(xz)$	$d(x^2-y^2)$ C-C-C-C	$d(z^2)$ N-Cr-N	10 Dq (1st transition)
	0.0	1644.8	3479.4	23604.5	25586.4	24558.2
$[Cr(L^{Py})_2]^+$	$d(xy)$	$d(yz)$	$d(xz)$	$d(z^2)$ N-Cr-N	$d(x^2-y^2)$ py-py-py-py	10 Dq (1st transition)
	0.0	634.0	3217.5	15589.0	23413.9	17866.3

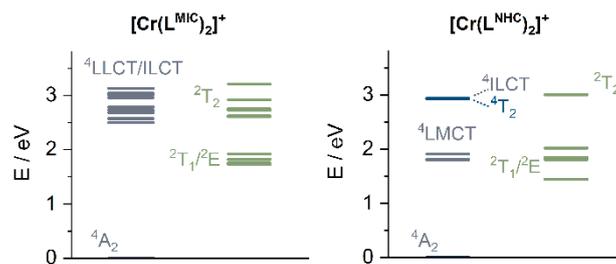


Figure S69: NEVPT2/CASSCF calculated quartet and doublet state energies with their character assignment for $[\text{Cr}(\text{L}^{\text{MIC}})_2]^+$ and $[\text{Cr}(\text{L}^{\text{NHC}})_2]^+$.

XYZ Coordinates

Truncated Systems used for CASSCF

107

[Cr(L^{MIC})₂]²⁺_r2SCAN3c_truncated.xyz

24	0.000000000	0.000000000	0.000000000
7	-0.092425272	-0.172861905	-4.329088293
7	-0.076112104	2.016066112	0.065631802
7	-0.239796928	1.289058681	-2.863888658
7	0.068852075	-2.017359992	-0.077715820
7	-0.299859625	1.115777376	-4.186416425
7	2.941299325	-1.113975125	0.138295535
7	0.149367902	1.111035910	2.940568903
7	-2.849684097	-1.290491715	-0.363729842
7	-4.317929514	0.173736559	-0.294417039
7	4.314154560	0.426788906	-0.078356191
6	0.106574634	-0.818518945	-3.144654293
7	0.104140514	-0.449753346	4.307325079
6	-0.234175107	4.237072774	-0.574304425
7	4.253838870	-0.874522562	0.084994734
7	0.218857063	0.856901095	4.249231683
6	-0.403298471	5.286584110	-1.474040488
1	-0.412490503	6.312229719	-1.113416949
6	-0.221453162	2.878477507	-0.994657847
6	-0.524427421	3.677724193	-3.251612432
1	-0.622348505	3.455586069	-4.307632193
6	-0.563825216	5.017487520	-2.830958221
7	-4.165715897	-1.113714068	-0.501771694
6	-0.346643117	2.619341695	-2.366849441
6	0.844736507	-4.198554382	0.028815777
6	-0.005914680	0.142746497	-2.133621386
6	0.018210239	2.813072943	1.182650341
6	-0.569188799	-4.240904030	-0.209976363
6	-2.132022586	-0.147029432	-0.081086799
6	-0.986327394	-2.881611867	-0.249923689
6	-0.061405830	4.197544346	0.849253300
6	-3.145984248	0.815456876	-0.021546193
6	1.803898570	-5.186222063	0.207735925
1	1.514872133	-6.233994918	0.175775977
6	1.178175108	-2.813140932	0.077538726
6	2.137909308	0.000000000	0.007727236
6	0.000000000	0.000000000	2.136149179
6	3.475274675	-3.476290492	0.427251894
1	4.510859721	-3.187196917	0.561768341
6	0.393273922	-2.285935541	-3.139887827
1	-0.495715167	-2.826193690	-2.789223755
1	1.183382320	-2.497328939	-2.415063306
6	-0.045433998	-1.029676141	3.082459569
6	2.525449634	-2.471883696	0.234555877
6	3.087301916	1.019166986	-0.130555953
6	-0.045743900	-0.744838346	-5.681873101
1	0.911594897	-0.455295582	-6.133403502
1	-0.851492613	-0.287846416	-6.263753191
6	0.162232583	2.474535367	2.532311976
6	-0.167237008	-2.259022063	-5.592808424
1	0.054969414	-2.679784335	-6.578500629
1	-1.199448647	-2.538701404	-5.344370884
6	3.137841089	-4.835189397	0.431008273
6	0.032463972	5.188654322	1.817270798
1	-0.029037049	6.235149268	1.528475034
6	0.788794877	-2.795867820	-4.529455894
1	1.814250820	-2.481601978	-4.767852397
1	0.783706125	-3.889956788	-4.524558896
6	-2.351637184	-2.622603411	-0.435216212
6	-5.668545223	0.751219751	-0.336917672
1	-6.185656397	0.460791109	0.586393814
1	-6.195913340	0.299066274	-1.181959302
6	-3.155588945	2.280313373	0.277144483
1	-2.745421319	2.826289859	-0.582126840
1	-2.484314561	2.483591818	1.115631083
6	2.983829446	2.492493203	-0.365950038
1	2.247304916	2.921944016	0.314991144
1	2.594009285	2.657226133	-1.379947847
6	-1.463327395	-5.292319016	-0.396270059
1	-1.106309198	-6.318765986	-0.364902580
6	0.207675052	4.842151682	3.159064189
6	-4.566719336	2.793364848	0.581201451
1	-4.876222423	2.476343174	1.586599098
1	-4.557248374	3.887472606	0.581192227
6	0.263046152	3.483358305	3.491432263
1	0.375843478	3.196829974	4.530110272
6	-5.563923627	2.265063161	-0.448047188
1	-5.241456528	2.545343375	-1.459416087
1	-6.560475627	2.690707999	-0.294258450
6	5.626509477	1.079015683	-0.170194170
1	6.292575549	0.402956645	-0.713703489
1	6.015760211	1.202050298	0.848624872

6	0.093355092	-1.109441707	5.620158511
1	0.864882502	-0.637582722	6.235614737
6	5.462733965	2.428110745	-0.854048537
1	6.411464998	2.969151270	-0.781722686
1	5.250585913	2.281848832	-1.921363025
6	4.328434721	3.207603763	-0.192695893
1	4.255331740	4.214594972	-0.614370005
1	4.547505475	3.326745509	0.877168047
6	-2.810257321	-5.023844600	-0.627151782
6	-3.229991832	-3.683138104	-0.631729941
1	-4.280789160	-3.462331758	-0.777442812
6	-0.595375113	-3.133754881	4.331648357
6	-0.229023699	-2.509494356	2.981337146
1	0.696543759	-2.964514821	2.605844658
1	-0.999553459	-2.726452659	2.237344073
1	-0.882534149	-0.914701120	6.082687954
1	-1.640845233	-2.905582772	4.580836462
1	-0.515739030	-4.222422632	4.256673851
6	0.1317693286	-2.603096097	5.435166262
1	1.367431500	-2.795694844	5.177559747
1	0.120830389	-3.100497244	6.390065700
1	-0.703661658	5.811225377	-3.554806065
1	0.289151239	5.597179353	3.931580956
1	3.901871435	-5.587544230	0.585037779
1	-3.529072172	-5.819071414	-0.783370424

107

[Mn(L^{MIC})₂]²⁺_r2SCAN3c_truncated.xyz

25	0.000000000	0.000000000	0.000000000
7	0.029464360	0.022286650	-1.938212250
7	2.868009713	0.300195034	-1.098857644
7	0.000000000	0.000000000	1.939091684
7	-0.429461302	-2.818459467	-1.143365752
7	-2.830018636	-0.218837776	-1.185709937
7	0.430460903	2.825067858	1.129799151
7	4.260275944	0.018500940	0.398927223
7	-4.239635909	0.017970638	0.308490884
7	0.060750810	4.240785773	-0.328811638
7	-0.523785455	-4.124954250	0.926737289
7	-0.287258951	-4.224357823	-0.359617849
7	0.458438083	4.138237889	0.922352191
7	-4.151295196	-0.220483266	-0.978132232
7	4.181610334	0.303115896	-0.884378623
6	2.093027675	0.000000000	-0.007430677
6	0.026672521	2.078735522	0.052454400
6	-0.120255128	-2.068771009	0.036981979
6	1.109848213	0.292663464	-2.762217459
6	0.344370630	1.057022404	2.178312598
6	-2.074635417	0.018441990	-0.066495478
6	1.289154364	3.165460343	3.396892700
1	1.610051984	4.169530016	3.098536023
6	0.752852424	0.309093532	-4.128915272
6	-1.037952200	-0.152727766	-2.806901428
6	-0.266442072	-0.625683943	-3.558979005
1	-4.316386543	-0.808215468	-3.307278752
6	1.670336513	0.710389976	-5.096869680
1	1.367165058	0.735413720	-6.151513670
6	-3.047676355	0.177129415	0.923091530
6	-0.022947412	-3.034345347	-0.959244616
6	1.409393642	2.763571436	4.732678127
6	-2.381058346	-0.369554551	-2.526237334
6	3.313625990	1.011521281	-3.390015990
1	4.337320986	1.249925666	-3.083799075
6	-0.235576152	3.045954092	-0.905707166
6	0.716399073	2.350025639	5.2439665874
6	0.875874842	1.522946394	5.104741804
1	0.906454597	1.200884447	6.152937741
6	-0.254210767	-1.053749061	2.796607977
6	2.429441501	0.556830921	-2.425344542
6	3.051605384	-0.188514545	0.986343177
6	-0.580322423	-2.368817348	2.482665386
6	-0.986521935	-2.835430895	4.839202513
6	0.346206961	0.679638468	4.128708483
6	-1.535556733	-0.278753326	-5.195148966
1	-1.202942854	-0.206197440	-6.238013738
6	-0.132147454	-0.687756163	4.149571676
6	-0.985772909	-3.233887251	3.487793119
1	-1.273677625	-4.254975559	3.218312992
6	-0.495825742	-1.569062392	5.165379326
1	-0.423702036	-1.259083960	6.215221614
6	2.939387915	1.128106644	-4.731375252
6	-2.867654484	-0.604915977	-4.901399726
6	-0.638400735	-0.055721074	-4.160306141
6	5.592403434	-0.032907037	1.019474450
1	6.178590841	0.800272846	0.598205315
1	6.070912924	-0.978201336	0.702123265
6	-0.468771765	-5.393186474	-2.479472682
1	-1.490037528	-5.048334261	-2.734243687

1	-0.346249934	-6.382922575	-2.952514235	1	-4.116339892	-1.598691954	-3.331587657
6	-0.786605908	3.017268757	-2.289010099	6	-2.691568299	-1.320552706	-4.910596319
1	-0.024221284	2.531161284	-2.930798283	6	0.411016302	2.428070227	2.510651261
1	-1.650647327	2.332658975	-2.316999607	6	2.950515517	0.741276263	-4.916627199
6	3.003415699	-0.544856490	2.432458895	6	-0.237978602	-2.977689925	4.961512796
1	2.259958863	-1.343357009	2.593107808	6	3.266981684	0.965642562	-3.563239652
1	2.637139105	0.329285777	3.000839055	1	4.282499703	1.264113184	-3.332531671
6	4.372331254	-0.948899962	2.974144548	6	-4.217194894	-0.551822233	-0.980409121
1	4.325636998	-0.994036348	4.075444609	1	-4.964469591	-0.777578568	-1.719894324
1	4.636738389	-1.969620443	2.633617016	6	-4.357537112	-0.163665456	0.292315423
6	5.441500992	0.034830926	2.518762159	1	-5.249364790	-0.025162052	0.883951525
1	5.171679799	1.062854721	2.830646441	6	-0.353166679	-3.353023785	3.612154504
1	6.417785337	-0.187627261	2.982843592	1	-0.475958131	-4.407386659	3.401101744
6	-0.333281659	-5.556421906	-0.982030001	6	4.197975809	1.013276122	0.474469234
1	-1.174205213	-6.100660404	-0.521996145	1	5.037615833	1.165523686	1.136066656
1	0.601274284	-6.083589638	-0.714109589	6	4.041278364	1.344719620	-0.800182255
6	-5.582098800	0.106664864	0.911581379	1	4.709509129	1.861460686	-1.466680025
1	-6.210269591	-0.648395011	0.411536380	6	-0.353529744	-4.247465798	0.876260756
1	-5.990488613	1.105673589	0.670317038	1	-0.635579421	-5.019172893	1.569737243
6	-3.005828219	0.459348504	2.395592556	6	-0.024422025	-4.349118112	-0.414456763
1	-2.267846666	1.254094448	2.597335848	1	0.035538847	-5.214450111	-1.056540548
1	-2.625424321	-0.442106220	2.911048987	6	-0.533869431	4.321072627	-0.340740089
6	0.292826006	-3.008127271	-2.423528973	1	-0.814429290	5.174414975	-0.938764100
1	1.143749351	-2.328685170	-2.601720465	6	-0.093322697	4.255050007	0.918884472
1	-0.564820400	-2.559476886	-2.958747695	1	0.046054031	5.040332249	1.640416222
6	-5.455361660	-0.099284819	2.399656839	6	-1.095145362	2.763890417	-2.166160621
1	-5.212422427	-1.157445545	2.619205655	1	-0.286457351	2.488135106	-2.846774979
1	-6.433761955	0.100801970	2.869803355	1	-1.578240123	3.671453638	-2.534664881
6	-4.378687585	0.820593933	2.955989490	1	-1.831928869	1.961393190	-2.140156541
1	-4.345216814	0.763866899	4.057249998	6	-2.927677887	0.552870456	2.162095612
1	-4.629815935	1.871286492	2.709801472	1	-2.508130160	-0.219555528	2.810892533
6	0.566436933	-4.401544033	-2.991101455	1	-3.907839369	0.847081699	2.542068731
1	0.553266800	-4.351965606	-4.092920426	1	-2.269799029	1.422619204	2.172739381
1	1.581412917	-4.742400213	-2.706809825	6	0.764713644	-2.877651278	-2.205172470
6	0.007911639	5.571859476	-0.951030827	1	-0.045761453	-2.696300929	-2.915671128
1	-0.739359027	6.145259818	-0.369156526	1	1.308058369	-3.777574517	-2.503388561
1	0.983776162	6.056771575	-0.785639563	1	1.452125357	-2.033831109	-2.216905033
6	-0.341919087	5.452427199	-2.369595459	6	3.002811197	-0.290637479	2.170668549
1	-0.790219664	6.410237281	-2.691965156	1	2.698450823	0.393405330	2.968029492
1	0.620916237	5.431386692	-2.928483001	1	3.998036743	-0.683843254	2.393531729
6	-1.134067770	4.352058900	-2.826221217	1	2.300345282	-1.120377823	2.121519043
1	-1.133557178	4.318312434	-3.929362533	1	3.702491771	0.900174335	-5.680280334
1	-2.200444983	4.542761589	-2.570222930	1	-3.360437538	-1.710727601	-5.668146416
1	1.868127404	3.428063664	5.471351714	1	-0.304491248	-3.728838660	5.739455025
1	-1.314419290	-3.533351989	5.615890282	1	1.217221399	3.655598579	5.597770453
1	3.655785252	1.490125170	-5.475343067	79			
1	-3.591844578	-0.808291010	-5.696175127				

[Cr(L ^{NHC}) ₂] ⁺ _r2SCAN3c_truncated.xyz			
24	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.002286901
7	0.008843982	0.038965427	-2.003956850
7	-2.851249469	-0.551845245	-1.235855337
7	-0.256408966	-2.907661969	1.210600102
7	-0.591682590	3.037007530	-0.824228789
7	0.111171407	2.911399095	1.197530608
7	-3.101278137	0.061687025	0.798414161
7	2.778223589	0.902008173	-1.170168297
7	0.254311773	-3.085567869	-0.855732063
7	3.058194941	0.382647583	0.880914256
6	-0.105761922	-1.089848629	2.857337974
6	0.755652101	0.096684803	-4.197837194
6	-0.201619528	2.114176510	0.115046280
6	-0.589615982	-0.394166678	-4.196391794
6	-2.303443391	-0.762531523	-2.547379437
6	0.062898829	-0.708051065	4.223822775
6	1.071824479	0.339740960	-2.844094810
6	0.242191844	1.076877216	2.838975872
6	-0.273858771	-2.438999400	2.573287108
6	0.096817859	-2.153074919	0.123632211
6	0.783526092	3.305980667	3.506189336
1	0.979367890	4.344178547	3.263675003
6	-1.007050496	-0.380860636	-2.852472990
6	2.354156564	0.777958870	-2.535491420
6	0.317125456	0.701309019	4.196948602
6	-1.431195129	-0.860219557	-5.217780939
1	-1.077598756	-0.866470004	-6.245740321
6	0.646774899	1.621349584	5.200678244
1	0.706711250	1.293820513	6.235285552
6	2.132507051	0.320951275	-0.109500094
6	0.924080888	2.919538065	4.858554026
6	-0.013540084	-1.646179837	5.258398676
1	0.112600096	-1.325271220	6.289201372
6	1.684819079	0.290459922	-5.225748126
1	1.405318426	0.082358568	-6.255080113
6	-2.130133172	-0.172219052	-0.126510192
6	-3.116766269	-1.249377140	-3.561675597

[Cr(L ^{Py}) ₂] ⁺ _r2SCAN3c_truncated.xyz			
24	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.962526678
7	2.121013865	0.094510486	-0.207941071
7	-0.160514812	-0.145487300	-1.957420150
7	0.216329633	2.121548044	0.043350604
7	-0.032008348	-2.105315401	0.130911644
7	-2.114168796	0.069534504	0.038812824
6	0.200279726	1.086420207	2.798798327
6	-1.740900825	-2.974262590	3.332031522
1	-2.144536806	-3.946588695	3.074978989
6	0.874059113	-0.108141988	-2.879416176
6	-1.962682340	-2.532171055	4.641273586
6	-0.771657862	-0.518198567	4.076989255
6	-0.670510922	-2.852357281	1.069898719
6	2.801488784	0.466700240	-1.329776217
6	-0.600186447	-0.968587858	2.739751655
6	-1.042943773	-2.244773782	2.361526705
6	0.671065024	2.368310313	2.452147067
6	0.803104992	2.825636292	1.055007329
6	-1.448147316	-1.291995740	5.009468162
6	-1.583968739	-0.923602628	6.023754845
6	-0.187198915	0.804074992	4.121470800
6	0.576180566	2.958517013	4.855386942
6	-1.232518919	-0.723090080	-2.612907300
6	2.212370905	0.238077456	-2.663527248
6	0.846562936	3.265106764	3.510290840
1	1.168265330	4.278479239	3.298716311
6	0.119669011	2.714528515	-1.174940896
1	-0.411055162	2.146811568	-1.930054460
6	1.456877064	4.030266401	0.776817838
1	2.013689810	4.530076513	1.558166562
6	0.020105904	1.719314510	5.150231668
1	-0.259756355	1.467650399	6.169995771
6	0.493550763	-2.751979575	-0.942398790
1	1.062836789	-2.146457026	-1.636271903
6	0.337417006	-4.092028094	-1.179785573
1	0.873603998	-4.528459172	-2.066660492
6	2.793670872	0.086823627	0.975007298
1	2.228151441	-0.262861109	1.829624073
6	3.062111212	0.171163129	-3.791271671

1	4.117696528	0.383559834	-3.673428185	C	2.75405801253853	13.41852436775872	14.97249387607928
6	-0.924911676	-0.997519451	-3.966883347	C	1.10760574074534	10.25881878109140	12.90165859894888
6	2.639731920	-0.238200466	-5.058524309	C	4.56318082652215	9.45845944388967	12.74728034314423
6	-2.945121727	-0.640887908	-0.766953733	C	2.73719152746445	11.04308823426787	6.55993677598187
6	0.444439980	-0.582158452	-4.1451866540	H	2.90503119356510	9.97177062415641	6.39680978210698
6	-2.493117359	-1.075058537	-2.092779090	H	3.26557929731917	11.59169431423060	5.77563127046377
6	4.105115619	0.476628535	1.118830386	C	6.22707753984355	12.93547683504080	14.41979300103506
1	4.578215187	0.426918125	2.092876172	C	1.25165942324485	11.36178019613876	6.60342454103801
6	-0.874628123	-4.221951957	0.849043558	H	0.77582054417807	10.92300317487246	5.71995570640212
1	-1.385491600	-4.814380421	1.594576582	H	1.10195738006831	12.44828607232377	6.54102653654142
6	4.106808422	0.956441702	-1.210681466	C	-1.27908470809945	9.82335460020794	13.23734713417406
1	4.611761957	1.340083743	-2.086960675	C	8.91157315425832	12.65164731707268	13.66709986342617
6	1.313070854	-0.638446540	-5.221379983	H	9.94686510516355	12.53889140063957	13.35147395294985
1	0.967970272	-1.008436121	-6.183738176	C	0.63664391423915	10.82552415662737	7.89283160291400
6	-2.640492171	0.698916001	1.116728141	H	0.80288473894888	9.74026758148497	7.95089710725780
1	-1.966787791	1.329116971	1.684375940	H	-0.44789152486804	10.97489402934127	10.97489402934127
6	-1.846046111	-1.606983567	-4.811018351	C	1.19230809539475	14.83340858342343	11.09468501493486
1	-1.587716585	-1.795180981	-5.850359003	C	4.71908726979218	17.81217488758816	10.16438138281182
6	0.671277973	3.936341760	-1.470682327	H	4.56008585721602	18.53980495010011	10.96927145223801
1	0.555747172	4.349876581	-2.466391167	H	4.19481018686345	18.17159896286051	9.27488617311930
6	-0.393069503	-4.841471026	-0.283032025	C	6.18189274794785	15.40023651007593	11.17882868675216
1	-0.563258045	-5.902090289	-0.440989940	H	6.58422585087318	14.76032304715158	10.38434446031226
6	4.761939300	0.962567923	-0.003077945	H	6.45812709070981	14.92221283936602	12.11993434628323
1	5.778046996	1.340063816	0.063761965	C	6.04022115703170	9.41282449123328	12.50107110486677
6	-3.365344067	-1.738140635	-2.973246571	H	6.51333134925683	10.28735526276897	12.94641112633696
1	-4.338174877	-2.053287176	-2.616663098	H	6.21524082903643	9.49146079554315	11.42054389646478
6	1.410791382	4.583390463	-0.487459134	C	-1.51338008489449	14.15244194112829	11.39999935264957
1	1.926957835	5.515096044	-0.698070840	H	-2.55154526717571	13.86464655198085	11.53706524825445
6	-3.079517444	-2.012085415	-4.308545035	C	8.60544985266041	12.90230737303536	15.00446344118481
6	-4.270704813	-0.856776263	-0.365618558	C	8.60600333019500	16.79265218031303	11.08085433140621
1	-4.927983223	-1.463832943	-0.970665476	H	6.64743491142496	17.34332700609607	10.41898612280380
6	-3.948500646	0.563946720	1.501844025	H	7.88918598750858	16.69459002153128	10.95592867089365
1	-4.302269081	1.092906876	2.379989638	C	7.25472383624311	13.04968787392361	15.35049281886255
6	-4.762340302	-0.284347098	0.782146407	H	6.97564183361756	13.26408347005999	16.373944775500317
1	-5.788812141	-0.466294159	1.086229127	C	6.20224792221828	17.58272617146275	9.92349180779616
1	0.743226691	3.701387397	5.626146377	H	6.34708305315578	17.03593568197493	8.98186308847269
1	-2.515762895	-3.145877010	5.341876094	H	6.69019175961434	18.55611833786440	9.80548840420443
1	-3.806732673	-2.515138056	-4.934370917	C	4.49109270959673	7.02346001314325	13.43289482645279
1	3.344704219	-0.283171977	-5.880184304	H	3.77439402090041	6.26672093400191	13.10362342954709

Non-truncated Systems used in DFT

155

[Cr(L^M)₂]⁺_camB3LYP.xyz

Cr	3.68797615124547	12.49707214494685	12.00045020964063	C	6.68733383507430	8.13797677293522	13.04557822819674
N	3.35455227230508	11.40107245282449	7.83638637949063	H	7.68926118123845	8.03185569622053	12.61712641227082
N	5.69943632329704	12.46029766695154	12.00630749291406	H	6.821599565647186	8.22507381942998	14.3303557897787
N	4.86493136948479	11.80413247270911	9.17831557368000	C	-1.18383793870674	15.39535694660347	10.87036897212299
N	1.67522354776978	12.53423958046204	11.99561168888056	C	0.17998100686193	15.71116135724094	10.73528208658190
N	4.64430771313951	11.50963857448974	7.91638915028785	H	0.47196295565322	16.67987070677083	10.3449745799195
N	2.44768672591939	9.76931656977123	12.93150357138250	C	-2.42116394266190	8.91007483900280	13.69802243466679
N	4.87630737748131	13.13587119259586	14.83288569704790	C	0.69050893006867	14.29859068455311	16.09987027108902
N	2.55520352395722	15.24104313535482	10.98095706994937	C	1.260832102638846	13.57959270639072	14.88056874642766
N	4.08492668808784	16.55791996838647	10.56913634466553	H	0.80761095744357	12.58922647684766	14.78458608378026
N	3.90850320622329	8.33109009709285	13.13699723928896	H	1.01753309439089	14.11941242188893	13.96620150638424
C	2.73311293408357	11.61273124241932	9.02836557367958	C	10.44863431689851	11.63228676154637	16.11738008878337
N	3.37806218012072	13.60185857582125	16.16785917341211	H	10.89283115567852	11.35717416063703	15.15449245943201
N	7.89357918445794	12.26445774916382	11.30885517385783	H	9.75184986455032	10.83586990054805	16.40423205390022
N	2.62918375513618	8.50787852656918	13.25331537959313	H	11.25498570004430	11.66271182904149	16.0015231326818
N	4.66211050537175	13.43813932678503	16.09356798340390	C	10.73205988425282	14.08043672985507	15.63481360138157
C	8.91476621805835	12.07614788927668	10.37827967009267	H	10.24648635959485	15.06199936119586	15.58505865919452
H	9.94781086873189	12.12758939611117	10.70951076150381	H	11.17969691512619	13.87824427024717	14.65595568189178
C	6.52576872064297	12.21910331894848	10.94202285574448	H	11.54841622229935	14.14280697430863	16.36439271842776
C	7.24804381555170	11.76167026084252	8.68654730992145	C	-2.23242847314030	16.42425886157610	10.43602921090660
H	6.97188348187199	11.55059000091652	7.65935783457919	C	-2.04430505792414	17.72338195842570	11.23765169685470
C	8.60642554555346	11.83025385569057	9.04463102488950	H	-2.16254404515570	17.54011437670304	12.31201807971134
N	2.79393155634129	16.44896733906381	10.52110871745347	H	-2.78901566514032	18.47011013056372	10.93704398481884
C	6.22120562849422	11.94091098307611	9.60136173021445	H	-1.05336194425752	18.16279594012012	10.07954707099074
C	-0.53260018044288	11.92912353761242	12.31770867654329	C	-3.65946355180612	15.91906781708840	10.67133071565408
C	3.73778656510843	11.90324933333113	9.95332213976591	H	-3.86931309764677	15.00659517733662	10.10138642766517
C	6.52618983235897	12.65298346991545	13.08226025740088	H	-4.37960636753199	16.67981862475769	10.5035317083245
C	-0.50751293584695	13.25663052697584	11.75945535961948	H	-3.84880638581977	15.71409140399518	11.73130780521904
C	3.67153664068808	14.52694352708782	11.33642505055583	C	9.19802334564584	13.33007529492764	17.44198398217459
C	0.86621315805957	13.56630004601837	11.600141714652985	H	8.50680289004867	12.56613079215025	17.81463382156583
C	7.89606544613627	12.53201032778355	12.72447886569768	H	8.68360907916144	14.29791954499868	17.45883193044216
C	4.68974088309034	15.44174107276415	11.05947219253043	H	10.03291284005530	13.38855440428649	18.14914460839504
C	9.67017368014634	11.62816003668390	7.96074619692944	H	2.98835743546633	15.04707776946498	17.60853726540144
C	-1.56292083088515	11.08824254826121	12.72167994845934	H	0.90642782786610	15.37493511180055	16.04114295525994
H	-2.59303226936153	11.42786757631862	12.63354680440257	H	-0.40019532713069	14.19893602441208	16.09371730727329
C	0.83085844008723	11.54336495998004	12.42022287526901	C	-1.91224763622255	7.55208962688660	14.19237657060933
C	3.59143473258655	10.45079873534782	12.60005003682159	H	-1.38126084766655	7.00470342090206	13.40485851691159
C	3.74927961063397	13.08605423526868	14.05120154787991	H	-2.75903928762899	6.93325815147180	14.50923387486595
C	0.06501095169669	9.43174054080685	13.30819612071330	H	-1.24085131703274	7.65517110069339	15.05265993894114
H	0.32605562040376	8.44791263043318	13.67617147010452	C	-3.38603628246357	8.664249306444751	12.52579287277037
C	1.24127969670684	11.51474416136293	9.11671873932492	H	-3.82266664058877	9.59703783454150	12.15325870868461
H	0.82295447637643	12.52348738235781	9.21744067365535	H	-4.21185267399778	8.01432683575142	12.8392373135459
H	0.96627542066669	10.98264260766006	10.02904179702826	H	-2.87038480406097	8.17812615743046	11.68933905990052

C	-3.17883863585329	9.59257652885145	14.84982446619573	H	4.26700766420974	18.09394632788606	9.23151322170076
H	-2.51434147027470	9.76979364938634	15.70364997628389	C	6.17858991132802	15.38976189936035	11.28984281166131
H	-4.00979077569575	8.96316471590743	15.19079590643393	H	6.62956371019822	14.73533527913898	10.53149752623519
H	-3.59647212136574	10.55824210783860	14.54488566803383	H	6.40896853549549	14.93045536825661	12.25551674606146
C	-2.06313568187084	16.71778480326803	8.93564796317668	C	6.04319141574639	9.4222890837030	12.42910257724712
H	-1.06904742621607	17.11860813360614	8.70894851429302	H	6.53141965519250	10.29757349585485	12.86231774510925
H	-2.80299209866857	17.45533417819951	8.60229258693181	H	6.18757004388519	9.504342222617592	11.3424222617592
H	-2.20086101771807	15.80662070413067	8.34160360564923	C	-1.49798602942279	14.12128273726684	11.34845577143408
C	1.27332307792622	13.73598410173248	17.39261055461977	H	-2.53855179858286	13.83986508257058	11.49101922017283
H	1.07232086834071	12.65780720435863	17.45517618408497	C	8.57768449962808	12.79613126519967	15.02475742591863
H	0.81471344510202	14.19765389530852	18.27354110415103	C	6.79384993969317	16.78319305286449	11.19428505936867
C	9.49851870161117	10.23861961450273	7.32340498502559	H	6.58512333087230	17.35370179194889	11.121184032590402
H	9.61185807653803	9.44731388274580	8.07366133018805	H	7.88365646360122	16.69235574912922	11.12632419013579
H	10.25310909025928	10.07782491253506	6.54403916846903	C	7.22604994719079	12.93868400061781	15.37079638067795
H	8.51349808346171	10.12131361400407	6.85867472867027	H	6.94347412958744	13.12899735589519	16.40018534306248
C	9.50418210790072	12.71175288490556	6.88156572539380	C	6.242317036438685	17.53817733148120	9.99195722201083
H	8.52057005760467	12.66039629852531	6.40186674784164	H	6.43726163010167	16.96929459337943	9.07139729445832
H	10.26233988582098	12.59479427652828	6.09787183166092	H	6.72777228791119	18.51354957907601	9.87219618477095
H	9.61420443927587	13.71299600453863	7.314493580752929	C	4.52066447572929	7.05172543197071	13.42696543948092
C	11.08951707639627	11.72464948664808	8.52855457455738	H	3.79046163389417	6.29294196398564	13.12949423401269
H	11.28589299349787	12.70782634257785	8.97169485188637	H	4.66327473717431	6.97687840595898	14.51335241964460
H	11.82063999397766	11.57332793840367	7.72664145382282	C	9.69480420656527	12.86107963140355	16.06858720446550
H	11.27598827159145	10.96006749064664	9.29151603274859	C	2.74280520270970	13.97850163257905	17.40621187994977

155

[Cr(L^{MIC})₂]⁺_d_PBE0.xyz

Cr	3.68878834243712	12.49238709911110	12.00385778182834	H	5.66329919439468	6.80604868435187	11.61751941195584
N	3.32798694842098	11.47062295822204	7.84836053523041	C	6.70310777858116	8.15066143274644	12.95777829146557
N	5.67982855140526	12.45410010275927	12.00650300078664	H	7.69061644939700	8.03853043663443	12.49635282729291
N	4.84780406397732	11.87587979474778	9.17538819436650	H	6.87603823694451	8.24661449847388	14.04011534906521
N	1.69468403365146	12.53011962909466	12.00269236989853	C	-1.16476126520534	15.34607329239985	10.77231641916008
N	4.61707408569819	11.60406900791141	7.908394240509555	C	0.19969630024947	15.66139990629314	10.63524466225165
N	2.46917355087488	9.78952206877540	12.96518026504079	H	0.49378255782535	16.61951051650041	10.21607199554679
N	4.85715331101997	13.07473729593430	14.83227420194467	C	-2.38074914611385	8.95334916984349	13.83791440063042
N	2.56906025737701	15.20207771803562	10.93662203713065	C	0.70368121175274	14.39066194738428	16.03367597243470
N	4.10682360370441	16.51641829894738	10.55987625587807	C	1.27328679354361	13.65949649295018	14.82109131994041
N	3.93318421600640	8.35333840657444	13.13920871312251	H	0.764369832842600	6.92114627535774	12.69618343656550
C	2.71796621624274	11.64259426171754	9.05194524534828	H	6.34204080775068	6.00576273435397	13.03559347405098
N	3.35510702057326	13.58191590101785	16.14463951527557	H	5.66329919439468	6.80604868435187	11.61751941195584
C	7.87721320555576	12.27656492225925	11.30689457151696	C	6.70310777858116	8.15066143274644	12.95777829146557
N	2.65739193079432	8.52946820310731	13.29490326196204	H	7.69061644939700	8.03853043663443	12.49635282729291
N	4.63487887308164	13.37491023225086	16.09392137114534	H	6.87603823694451	8.24661449847388	14.04011534906521
C	8.89769105948189	12.11557786878879	10.36863919303731	C	-1.16476126520534	15.34607329239985	10.77231641916008
H	9.93335817175480	12.15145703238092	10.69802469651834	C	0.19969630024947	15.66139990629314	10.63524466225165
C	6.50633274422575	12.24633038381585	10.93670805913708	H	0.49378255782535	16.61951051650041	10.21607199554679
C	7.22564270443520	11.85968035807297	8.66558103798672	C	-2.38074914611385	8.95334916984349	13.83791440063042
H	6.94607656210295	11.67907076696291	7.63152212168371	C	0.70368121175274	14.39066194738428	16.03367597243470
H	8.58491683488502	11.91471141641685	9.02520693111954	C	1.27328679354361	13.65949649295018	14.82109131994041
N	2.81814683722116	16.40466766774491	10.46369869265074	H	0.764369832842600	6.92114627535774	12.69618343656550
C	6.19750319614717	12.01038386857510	9.58876967231330	H	6.34204080775068	6.00576273435397	13.03559347405098
C	-0.51426956535134	11.93242144798633	12.344671107229622	H	5.66329919439468	6.80604868435187	11.61751941195584
C	3.73201357545546	11.93932846204056	9.97159259330780	C	6.70310777858116	8.15066143274644	12.95777829146557
C	6.50444667074192	12.60992427799923	13.08803495838028	H	7.69061644939700	8.03853043663443	12.49635282729291
C	-0.49221242070028	13.23914698943178	11.74484184913674	H	6.87603823694451	8.24661449847388	14.04011534906521
C	3.67237203972108	14.49370773554799	11.34242208547785	C	-1.16476126520534	15.34607329239985	10.77231641916008
C	0.88445876206298	13.54691061858446	11.57675021762118	C	0.19969630024947	15.66139990629314	10.63524466225165
C	7.7813753948116	12.49708509268529	12.72824138379066	H	0.49378255782535	16.61951051650041	10.21607199554679
C	4.69900091844231	15.41345624581292	11.09250061221546	H	-2.1011642896598	16.35614535310176	10.29742427292863
C	9.65444860300741	11.73931781670195	7.9374168957981	C	-2.03381420873960	17.67485621802162	11.06579051940845
C	-1.54084882758309	11.10070439692595	12.78077215196448	H	-2.16172562503756	15.1969614119226	12.14422774372653
H	-2.57392889741448	11.43429020013074	12.68976879049200	H	-2.77829467650873	18.41167932921962	10.73805730090266
C	0.85347576095074	11.55095820217246	12.45419331623494	C	-1.04174294082899	18.11344698774263	10.90568314260008
C	3.60169925348486	10.47006411763925	12.58936822334582	C	-3.63576734070834	15.822920434369419	10.52916018756294
C	3.74291004862234	13.06565377522078	14.02878917740003	H	-3.83452710743252	14.92052588769224	9.98483104899571
C	0.09741431624190	9.45901082439815	13.39887102844606	H	-4.35552505684368	16.59961637971924	10.17447731464971
H	0.36266944234007	8.48145960818648	13.78609929544371	H	-3.83912996656273	15.68070599391706	11.59356939880288
C	1.23678385699493	11.49169868530622	9.16223242195241	C	9.15626655019610	13.12868933098103	17.47558506847381
H	0.78428551902073	12.48396808097962	9.29395922887276	H	8.47566806769307	12.33613335046111	17.81100456792513
H	0.99819108017280	10.07164318908929	10.07164318908929	H	8.62622375341863	14.08756925131141	17.53485351622710
C	2.74316318349780	13.43076277518292	14.93970085739336	H	9.98881304190419	13.16905261637823	18.18809688541606
C	1.13822050361196	10.27668588130478	12.95942530386225	H	3.00101396238768	15.03050378213607	17.58569117917150
C	4.57859743854073	9.4731578378824	12.71641020842944	H	0.96495534999973	15.45872120758417	15.98868777198345
C	2.70098320084557	11.12447650507168	6.57904897498487	H	-0.39040337322816	14.33685916980243	16.00627450087523
H	2.90110110119933	10.06206993593820	6.38696287139321	C	-1.86768911120441	7.60299007715945	14.34211928010443
H	3.19850146022569	11.7070932847752	5.79735628446160	H	-1.35825368488335	7.03898935687164	7.05062294733426
C	6.19880573701196	12.85785609187646	14.43153112526289	H	-2.71057338413411	6.99376681895315	14.68977078422185
C	1.20906298885769	11.39214637211410	6.65264075011997	H	-1.17563540888682	7.71611759002688	15.85986632020706
H	0.73400881463417	10.95657344661354	5.76605348374220	C	-3.37672578548584	8.69449574057579	12.69742254074080
H	1.02109458291577	12.47493274261807	6.61558869886519	H	-3.81979638295770	9.62364502963020	12.32063161790328
C	-1.24789364618171	9.84980270132007	13.33310235572056	H	-4.19782897975457	8.05481268196884	13.04530250945131
C	8.89114935049315	12.58607697441222	13.67862892566792	H	-2.88669848887878	8.19050585722035	11.85513477034892
H	9.92930668879394	12.48455799699670	13.36434701014600	C	-3.10003443139393	9.66317118744911	14.99579176582375
C	0.63491717558189	10.80867295163380	7.93714571371533	H	-2.41015014775106	9.84978528513422	15.82819926835697
H	0.83748016702937	9.72751336727715	7.96937935232492	H	-3.92720545627890	9.04679961292523	15.37083122904049
H	-0.45472701173055	10.92156585409407	7.95969877376864	H	-3.51776211238564	10.62778457567948	14.68378614597566
C	1.21371252136607	14.79773604617972	11.03358331687804	C	-2.02204916653816	16.60823502544347	8.79368308954533
C	4.75013874875644	17.76015347489797	10.15518995936803	H	-1.02559285388182	17.00663824709744	8.56841254923130
H	4.54597541400321	10.93192050330471	9.29151603274859	H	-2.76022200169023	17.334707	

C	11.06332693640136	11.82890489766253	8.50390163102390	H	3.78575198708781	6.27285050498322	13.08225120512582
H	11.25632634027632	12.80342347240965	8.96980439398264	H	4.60216500373619	6.94183440738425	14.50701123394367
H	11.79416143989144	11.70041541188680	7.69658170527878	C	9.71205933253717	12.96731844197525	16.04680554813430
H	11.25594413694805	11.04598301219861	9.24805615219907	C	2.75625092241798	13.97924528207337	17.41896178430017

[Cr(L^{MCC})₂]⁺_PBE0.xyz

Cr	3.68713299155759	12.48950766703299	12.00058586283287	H	6.34157677401549	6.81238092001456	11.64858555603968
N	3.33818284686227	11.42358242841120	7.84252001638252	C	6.99133833782751	8.15029290441776	13.03797663629295
N	5.68993370631717	12.45340205454244	12.00425543972216	H	7.69587506259683	8.04743924971740	12.61255750324397
N	4.85340882629391	11.82578217014013	9.17667028269877	H	6.82361458616836	8.23881526022519	14.12669334456513
N	1.68281691699469	12.52431601937424	11.99299946310612	C	-1.16813940205058	15.38135330205166	10.83310243817603
N	4.62859190330525	11.54094300270710	7.91229732720321	H	0.49264905535616	16.66072127476736	10.30068479600128
N	2.45330694426313	9.76908159570860	12.92867302227938	C	-2.40465538412040	8.92281483811946	13.744429714381143
N	4.86682640385037	13.10944000890945	14.8295093286921	C	0.68891625216942	14.31455262342695	16.06650509458913
N	2.56707596883648	15.22288743495056	10.97081196551562	C	1.26761744535119	13.59222200609694	14.85282148278571
N	4.10298661859798	16.53666322528285	10.58125425033702	H	0.79340261503255	12.60697202097509	14.74596015070441
N	3.91612232889713	8.33421205361592	13.12665421831074	H	1.0342634469434	14.13760030277926	13.93417262958358
C	2.72118147659055	11.61942450364937	9.03900607162554	C	10.46376162897750	11.62746712521736	16.09292733788162
C	3.36586115350321	13.58840150213531	16.15435305114899	H	10.91298137502197	11.37956507126705	15.12394984779289
C	7.88513840704917	12.26431601937424	11.30571908615585	H	9.78677492056027	10.80892124038008	16.36756582512345
N	2.63600965926162	8.50648370225230	13.24913397912252	H	11.27171300495645	11.66487876251011	16.83486318464059
N	4.64992851351112	13.41381022941991	16.09039942210298	C	10.68423963290758	14.08840466830749	15.65062325811378
C	8.90501098755733	12.08514291720306	10.37014065422332	H	10.17079719797437	15.057127979172858	15.61251152873876
H	9.94086988634145	12.13030847600506	10.69791623656554	H	11.13625348379072	13.91019062633887	14.66787737934437
C	6.51269725418809	12.22378164475355	10.93844676612650	H	11.50040655796213	14.16500283890504	16.38049203223280
C	7.23216025343589	11.79180150360074	8.67466499903027	C	-2.21113349332972	16.40555902481384	10.38390962919103
H	6.95291961722714	11.59182392819782	7.64411275533281	C	-2.02192735249068	17.71054001787972	11.17230499644196
C	8.59174506121875	11.85489064134362	9.03175842657060	H	-2.14285460436561	17.53857179743381	12.24900697963959
N	2.81227814139589	16.42897347112559	10.50689287940682	H	-2.764718332894035	18.45651548427810	10.86187190431859
C	6.20359036120036	11.96090223384012	9.59436035972191	H	-1.02880302908964	18.14663274354106	11.01200645643246
C	-0.52663236597785	11.92868861195633	12.31994917323554	C	-3.63778359111458	15.90589903697125	10.61849470378995
C	3.73149517788290	11.91165403725813	9.96182758352521	H	-3.84718332894039	14.98612371764180	10.05803550011496
C	6.51370786984603	12.63449604056447	13.08056312119286	H	-4.35614661092972	16.66414159486291	10.28473758158471
C	-0.50048020599530	13.24862564012880	11.75105404631411	H	-3.83244754126138	15.71469775468817	11.68120981065927
C	3.67580010066329	14.50909945480201	11.35118258727403	C	9.17652673873707	13.268446724788668	17.44812461713363
C	0.87813747412259	13.55597039514616	11.58981550425840	H	8.49924768741037	12.48252889781741	17.80516727165859
C	7.88788536755361	12.5174370222472	12.72099411585188	H	8.64380251343457	14.22698741511370	17.48519136693879
C	4.70057532072988	15.42571674065663	11.09111024067663	H	10.10896048246612	13.3286891555907	18.15709414394564
C	9.65164337278112	11.66114702301986	7.94637259780836	H	2.98341314385915	15.04058846306939	17.5803552697275
C	-1.55652690620119	11.09019558019389	12.73556933462455	H	0.91514867516192	15.38996270751016	16.00913944975561
H	-2.88474994508002	11.4287405271653	12.64953221164309	H	-0.40310433631804	14.22552649627605	16.05254136545459
C	0.84069589680225	11.54176110915014	12.42333404262503	C	-1.89529994066734	7.56223476304092	14.22420737021402
C	3.39382725904493	10.45426417464821	12.59147685847234	H	-1.38425285018741	7.01265618164915	14.32362405595106
C	7.44471914257972	13.06745689092398	14.03972511097810	H	-2.74001532221406	6.94770004884691	15.5776191475296
C	0.07640924279635	9.43386547624422	13.32659338056715	H	-1.20557222833200	7.65848471145248	15.07205620556549
H	0.33805040615679	8.44975867783695	13.69933783500671	H	-3.39656308946830	8.68815186017818	12.59531461954874
C	1.23609429521916	11.50136472028687	9.13830473290519	H	-3.8362713517848	9.62553284107553	12.23588646503724
H	0.80631465593690	12.50492734166356	9.26190753696452	H	-4.21990280016514	8.04269263303162	12.92691995743276
H	0.97722933279351	10.95269736081328	10.048499737070565	H	-2.90390902760413	8.20079297416739	11.74481685492284
C	2.74543148877000	13.41059582396371	14.95686565069771	C	-3.12746015962054	9.61072887182634	14.91317287848247
C	1.12088106540946	10.25760690325812	12.90862965227911	H	-2.44061173090172	9.77980261311776	15.75183237411848
C	4.65959143124311	9.46133533661816	12.73524910938232	H	-3.95729151728390	8.98876749996116	15.27289561962554
C	2.71579376227847	11.07321163364465	6.57222597337724	H	-3.54217592737969	10.58208700599566	14.61859933000509
H	2.89090728642495	10.00336613164329	6.39776398882613	C	-2.03285010013160	16.68152593223596	8.88310164596732
H	3.23505960693857	11.63174135019708	5.78714349450076	H	-1.03544903199756	17.07739584296676	8.65734782639979
C	6.21061940654332	12.90678384512277	14.42103238439467	H	-2.76911553406333	17.41841491790160	8.53747156199646
C	1.23042908716958	11.37930718536196	6.62788818433480	H	-2.17000527839531	15.76382037259162	8.29761959358610
H	0.75297478390465	10.94638383761896	5.74129510684343	C	1.25766016791381	13.74687401599325	17.36050981364138
H	1.07106259578377	12.46611730539022	6.57727567884499	H	1.04368006290672	12.67014511114157	17.42376485420531
C	-1.26843550536640	9.82749728385099	13.26184488999618	H	0.79924921537562	14.21425779179073	18.23963781923554
C	8.90301364860176	12.63234505471009	13.66662507919500	C	9.47661420323392	10.27694397620908	7.30280728468409
H	9.94070018619952	12.52646808227953	13.35206348840628	H	9.59050059932196	9.48082659726630	8.04900857028784
C	0.62875948466610	10.82420916082225	7.91247066791201	H	10.22962361052790	10.11937931755997	6.51997040822802
H	0.80223781718278	9.73842816262236	7.95665244948044	H	8.48938723115655	10.16367416039518	6.83940463824300
H	-0.45771200352449	10.96564400662231	7.92305077767946	C	9.48199677074970	12.75040260848424	6.87599644649679
C	1.21016791041594	14.81867826481180	11.07358044680177	H	8.49538753776597	12.70291684352924	6.39979951906918
C	4.74393919002633	17.78178388562076	10.17738114557852	H	10.23713768076919	12.63653577208553	6.08770524099119
H	4.56549405762477	18.52104935926363	10.96943431234379	H	9.59545879438734	13.74976661283580	7.31428323676607
H	4.23965273161747	18.13145611059561	9.27108905738551	C	11.06971042869995	11.75413408824102	8.51184306716205
C	6.18436906909065	15.39001981936896	11.25254199312194	H	11.26656927693246	12.73511621870958	8.96227243078716
H	6.61072024067683	14.73650846716326	10.47909312174042	H	11.80032023405079	11.61001437564791	7.70694877208995
H	6.43486639587772	14.92272114133307	12.20911113967994	H	11.25875839787797	10.98237844537381	9.26850799054293
C	6.04271546616378	9.42071908599446	12.49311013491271	155			
H	6.51133789269389	10.29958408795499	12.94137186197187				
H	6.22039038213563	9.50488962009037	11.41150752563266				
C	-1.50407905422175	14.14349076222218	11.37828555288347				
H	-2.54529534948817	13.86164828217473	11.51542517289394	[Cr(L ^{MCC}) ₂] ⁺ _PBE.xyz			
C	8.59245361417875	12.87306946475183	15.00778198436441	Cr	3.68582302676768	12.47479919812851	12.00811568063571
C	6.80733312418803	16.77980822482884	11.15248716172386	N	3.30140756946004	11.43849410519622	7.82665665534188
H	6.62674647692185	17.342493565574029	12.08072990334586	N	5.68850077696204	12.43074714580619	10.00725702396761
H	7.89425934961696	16.68188121376967	11.05501476238127	N	4.84363305761294	11.85438618783455	9.12193388443520
C	7.24051394571291	13.01472728321637	15.35432255051419	N	1.68161792992311	12.52245037493308	11.99989748849801
H	6.96030423792179	13.22308162819386	16.38083878947326	N	4.60933199417989	11.57765404440518	7.87488886416801
C	6.22993461752389	17.55153114252279	9.97303038889309	N	2.44121866818124	9.75569104858571	12.94650248367036
H	6.39656556953591	16.99180027966661	9.04139729423511	H	4.86933418722080	13.04761723681254	14.85210741614259
H	6.71902046088455	18.52485747184433	9.85148752798062	N	2.58092735608085	15.21426592429313	10.95908246259175
C	4.49964449347777	7.03150410069398	13.41725855244894	N	4.14651248439750	16.54236884744865	10.61515406053757
				N	3.91851874710854	8.29961622310970	13.12495389431381

C	2.69288513620252	11.61000877666202	9.04581056029443	C	10.57400815441847	11.65024502417228	16.07636120898514
N	3.34849685279994	13.54368843245108	16.18467183094905	H	11.02641262527262	11.44091154624773	15.09108010375497
C	7.90208300828985	12.26183204301114	11.29593311924326	H	9.94154556790117	10.78593312799325	16.34796487187666
N	2.62198256939866	8.471130435862684	13.27156286788127	H	11.39498322317665	11.71882662840775	16.81317653255402
N	4.64854977181248	13.34418614649945	16.13696403583090	C	10.66238236826237	14.14329055974791	15.67585691041922
C	8.92380503021251	12.10377563420210	10.34679812795195	H	10.09355814270252	15.09019807852841	15.65321750120322
H	9.96832585221334	12.14258511192809	10.67348638634193	H	11.11895940584187	14.00061602872046	14.68063644549493
C	6.51715726922027	12.22478443259436	10.92669813661146	H	11.484166601389987	14.25481875437879	16.40671031533596
C	7.23471381125933	11.84334742114711	8.63566949782514	C	-2.21736706161876	16.39201495237096	10.25661216587965
H	6.94836900040256	11.66342964389530	7.59534721363111	C	-2.03215214620691	17.72942298325828	11.01142176422485
C	8.60325072398158	11.90142281371871	8.99324794747140	H	-2.16533662659671	17.59073758386468	12.09937856378554
N	2.84056740759047	16.43887603886030	10.48960903075653	H	-2.77490564683993	18.47242594652782	10.66793481444744
C	6.20040510142724	11.99028777865684	9.57071311601554	H	-1.02917229288854	18.16082484725296	10.84683084467668
C	-0.55019633330744	11.93252606734092	12.32896058984024	C	-3.65681741530250	15.89926145491646	10.49061932629151
C	3.71642890391662	11.91551683026931	9.96888920403309	H	-3.86394842925609	14.95650846742429	9.95267026564305
C	6.52300210895724	12.537654394040634	13.092240536454898	H	-4.37508661824631	16.65325037994597	16.31376503355371
C	-0.51801973044594	13.24752412805997	11.73337541328400	H	-3.86650196560129	15.73862949839675	11.56354815303063
C	3.68973786026658	14.49515696698293	11.38257709740879	C	9.20985594825955	13.20508605124887	17.48590042468064
C	3.87386208925488	13.55398592325844	11.57447877458435	H	-1.93859661963727	12.37782130991716	17.8316058118750
C	7.90797692831801	12.48901184803373	12.72180470405416	H	8.63376455497148	14.14564678639120	17.55210968389681
C	4.72927849243323	15.42341661743926	11.15848108182882	H	10.05294185632187	13.28417708738767	18.19467585520468
C	9.66848091152580	11.72825974317636	7.89697054951432	H	2.98817035083494	15.001020585658834	17.63649543161497
C	-1.58764231456798	11.09788014688536	12.76178279260323	H	0.93210987608759	15.42545896108297	16.02840392571435
H	-2.62632114453057	11.43963963647312	12.67118724649442	H	-0.42515982300060	14.28675244858836	16.04375969156460
C	0.82671049577382	11.5376588985686	12.44197138944241	C	-1.93856633404227	7.569425647632080	14.3137674861585
C	3.59233351302565	10.44218466024770	12.58559151277082	H	-1.44564615592500	7.00266743435643	13.50326545557053
C	3.73962465197164	13.03258588429799	14.04566742574375	H	-2.78993186846300	6.96379511271782	14.67140982070019
C	0.05178240025359	9.429429007963994	13.37762489018826	H	-1.22635511994818	7.66365319924808	15.15325272503345
H	0.31338748766378	8.44156527628330	13.76233414139447	C	-3.47058900888274	8.70872483416996	12.69745703774759
C	1.20667447115650	11.45096736603709	9.16164634231733	H	-3.90861253499479	9.65527346573593	12.33572320450549
H	0.74720397798932	12.44765743827778	9.30493976982781	H	-4.30155030764566	8.07523206598961	13.05757200189293
H	0.97206362651826	10.88429224429386	10.07728145387041	H	-3.00254169535472	8.20127570830841	11.83482764884826
C	2.73217622549619	13.39199135879032	14.96705349361927	C	-3.13414185349538	9.65509699344492	15.01518054591536
C	1.10664781039366	10.24929007963994	12.94058418987596	H	-2.42113399157258	9.82416227384196	15.82422659125885
C	4.57382500427650	9.43586035537769	12.71825440634324	H	-3.96932926163442	9.04318016635475	15.40232719792923
C	2.66460260519064	11.084233470452439	6.55337125260267	H	-3.54526514958499	10.63611952009240	14.71822772559420
H	2.66821141226546	10.01359530160332	6.36186388362774	C	-2.01893627584292	16.623988485051050	8.74004178636215
H	3.16200299272378	11.66811269353604	5.76088850707652	H	-1.01122171883662	17.01515636383154	8.51389657063054
C	6.21773978796754	12.84739516419015	14.44481341758379	H	-2.75529125085175	17.35556430808973	8.36010315790177
C	1.16272117773394	11.34915853128003	6.6332593629120	H	-2.150111332689364	15.68272039113174	8.17629107607829
H	0.68167131735869	10.90457267249838	5.74455594960600	C	1.21693767200415	13.75129231435529	17.37667366502328
H	0.96972913651591	12.43893275220683	6.59087645294880	H	0.96907377241282	12.67317420283955	17.43062337710146
C	-1.29932949188990	9.83300672509810	13.31354418158749	H	0.75919613790549	14.22924635291754	18.26034782823816
C	8.93010143840014	12.60555579658825	13.67183680567751	C	9.49617585195907	10.34251762204099	7.23134083035057
H	9.97583409868217	12.51855835085571	13.35108567452466	H	9.61810110798326	9.53110993655268	7.97127866492224
C	0.59252802859030	10.766583452672	7.930954444060752	H	10.25147841170079	10.197794841700718	6.43734753785260
H	0.79450536224003	9.67674487070932	7.96269406213180	H	8.50003370330216	10.23015490606128	6.76827666109860
H	-0.50458226229641	10.88137024258510	7.96053708196324	C	9.48976037093448	12.83711180370031	6.83309838016539
C	1.21735731777725	14.81348686529293	11.03605210931537	H	8.493766512537290	12.79346545424637	6.35808961005604
C	4.80715962405391	17.79219068533241	10.22293729451731	H	10.24623193622899	12.73201805591810	6.03411233629562
H	4.59235155685780	18.54615028010156	11.00386794602911	H	9.60540936356758	13.83906677669634	7.28431259383630
H	4.33641988113835	18.13520745971793	9.28638094258376	C	11.09697536748366	11.82177823498381	8.46257600282529
C	6.21054775351517	15.39752344683572	11.38785062006863	H	11.29098846985458	12.80316316397771	8.93188899139735
H	6.67889884943641	14.73016700877525	10.63923612927447	H	11.83119356447776	11.69489898325665	7.64756644462975
H	6.42286786494438	14.93786983234756	12.36671097874128	H	11.29597694299141	11.03411378579054	9.21147935526057
C	6.04935248286724	9.38792775619140	12.45450239556888				
H	6.53285333758860	10.26632016703363	12.90785712191898				
H	6.21476517583772	9.48702848219616	11.36382014313928				
C	-1.52102401618272	14.14160054429028	11.32790365959246				
H	-2.57175002807954	13.86373984741489	11.46202829376482				
C	8.61803396502679	12.83334577412263	15.02720030604815				
C	6.84192581017907	16.79539873389926	11.29863235846554				
H	6.62459956403080	17.37187622870569	12.22004645247581				
H	7.93964964270805	16.69489136402685	11.24534123065850				
C	7.25800912003120	12.95492769695161	15.38389057830396				
H	6.67573183833073	13.15386592312904	16.41966175801818				
C	6.31016169144905	17.56176836552586	10.08268482493454				
H	6.51865845883400	16.99145038413547	9.15643471484784				
H	6.80553916359586	18.54231046147400	9.97360440453318				
C	4.50590195116959	6.98563960614403	13.40460135811314				
H	3.77646899790210	6.22516474127153	13.07995970003851				
H	4.62800683184548	6.89170014636301	14.50059871096088				
C	9.4768325062609	12.95809136405995	16.06465095270926				
C	2.73042128221322	13.94042774132893	17.45451286512816				
H	3.19763039912037	13.33921393488519	18.25240992689217				
C	5.85148367347428	6.86594920108908	12.69312369119142				
H	6.34949161833328	5.94219024725265	13.03589269281532				
H	5.68969561576839	6.7589499462355	11.60266634219247				
C	6.70841644099782	8.10307442829952	12.98176186924100				
H	7.71039024712275	7.99733371131062	12.53141136037179				
H	6.86627299299840	8.18815860993470	14.07540449843699				
C	-1.17371011814730	15.37507930730697	10.74993753350218				
C	0.20133739447530	15.68817264788277	10.62566272118636				
H	0.50616890036161	16.65232058582369	10.20832403342430				
C	-2.44257937641401	8.94104481809574	13.82905369257139				
C	0.67635868898060	14.34789213274311	16.07241187842694				
C	1.25546665121087	13.61867066737024	14.85026048188523				
H	0.74763586888245	12.64374232216385	14.72191633546103				
H	1.04789763636989	14.18396540224661	13.92738600934712				
C	10.57400815441847	11.65024502417228	16.07636120898514				
H	11.02641262527262	11.44091154624773	15.09108010375497				
H	9.94154556790117	10.78593312799325	16.34796487187666				
H	11.39498322317665	11.71882662840775	16.81317653255402				
C	10.66238236826237	14.14329055974791	15.67585691041922				
H	10.09355814270252	15.09019807852841	15.65321750120322				
H	11.11895940584187	14.00061602872046	14.68063644549493				
H	11.484166601389987	14.25481875437879	16.40671031533596				
C	-2.21736706161876	16.39201495237096	10.25661216587965				
C	-2.03215214620691	17.72942298325828	11.01142176422485				
H	-2.16533662659671	17.59073758386468	12.09937856378554				
H	-2.77490564683993	18.47242594652782	10.66793481444744				
H	-1.02917229288854	18.16082484725296	10.84683084467668				
C	-3.65681741530250	15.89926145491646	10.49061932629151				
H	-3.86394842925609	14.95650846742					

C	7.88748371737378	12.46593161713116	12.71254312950543	H	8.64974465989699	13.74142315096493	17.62033553150261
C	4.69615436007220	15.45651139050790	11.16377066413865	H	10.00413607143816	12.76619182143900	18.19542661159525
C	9.59531901200605	11.96515684899333	7.86257150795932	H	3.14220943190133	15.01050141032543	17.62936068608697
C	-1.53780691258058	11.13662620577885	12.83623316980169	H	1.13746945350902	15.57957004671317	16.01634123463115
H	-2.57492571074351	11.44607375062737	12.71838927093583	H	-0.29223814925089	14.55573743815257	16.04176266726879
C	0.84871166828652	11.57782273688210	12.51325984928369	C	-1.84794814589224	7.74106934578653	14.62235765692674
C	3.61047304319944	10.47343655405861	12.62582895274828	H	-1.29171414609663	7.11473028060223	13.91379949399196
C	3.75008861769444	13.05205665700392	14.05042927239262	H	-2.69414982411814	7.14612425436621	14.98425526254181
C	0.11052608616812	9.52825516062557	13.55073614891499	H	-1.20340015579497	7.94902210310861	15.48573293274952
H	0.37292320625698	8.56883528469885	13.98245290436985	C	-3.27149377989797	8.64083766397846	12.78767395075393
C	1.22773799398524	11.39134348021776	9.17201681154459	H	-3.71778448007562	9.51866901539705	12.30567375399952
H	0.72041841557408	12.35954868292632	9.28144955973078	H	-4.09379714267019	8.00399878193011	13.13570284632671
H	1.02495717340479	10.83345185927014	10.09125581291580	H	-2.17185297601523	8.08394504467930	12.02633028926571
C	2.77408068992113	13.45007045652781	14.96777474259495	C	-3.18087434692871	9.80862142911403	15.01155127366623
C	1.15066246113157	10.32884336601668	13.07319225769785	H	-2.55764100529145	10.09850616230721	15.86645480808655
C	4.56924645303207	9.46313408317101	12.75194376932233	H	-4.00349943982860	9.18901770941452	15.38860589055312
C	2.68722166179474	11.12533622935483	6.57090916723295	H	-3.62359761458328	10.71911137133610	14.59070208590545
H	2.96543240391114	10.08389375373217	6.36417686679317	H	-1.94274354501758	16.46219152181941	8.55762856622307
H	3.13144632410432	11.75370656871968	5.79271692713962	H	-0.94824624229077	16.87328089604636	8.34789130195499
C	6.20307782853380	12.75208915779176	14.43866981200684	H	-2.68120138655425	17.16396075125854	8.15153178585122
C	1.18098541912780	11.28157155231850	6.66613599890866	H	-2.04115284405892	15.51590802297193	8.01148374343758
H	0.72965473233565	10.80982347554615	5.78615786442636	C	1.29737608481496	13.89945123561104	17.35911598064107
H	0.91061766898392	12.34659539405437	6.62762663201854	H	0.97530016471068	12.84963066255489	17.41287756400796
C	-1.23538428155699	9.90843981928316	13.45681319043637	H	0.87703148358768	14.40364167908777	18.23645506961075
C	8.89660418170545	12.49357654192808	13.65877459642988	C	9.42735774409594	10.61122759320302	17.152867599320584
H	9.93581653905539	12.40765278003085	13.34591912823031	H	9.56432417360972	9.77832003867559	7.85330704740843
C	0.66497726878949	10.65826094512806	7.95667445099646	H	10.17420041531279	10.50798012862437	6.35624784064207
H	0.94618906277564	9.59529193154257	7.99110196186978	H	8.43826158644697	10.50722371105342	6.69157122636556
H	-0.42953300708688	10.69074473372205	7.98889940190326	C	9.38833598815565	13.10650029718210	6.85325625859565
C	1.23302538475379	14.75918577673579	10.94079580720267	H	8.39978651725601	13.06511779252273	6.38096348242379
C	4.73743347792217	17.79012075686422	10.18513760459977	H	10.13752547348044	13.04238523252030	6.05497798576649
H	4.44584726749911	18.54659203413999	10.92502385427400	H	9.49324751769066	14.08554758786514	7.33679375936131
H	4.31626745543757	18.08378023368523	9.21861751604035	C	11.01932849890986	12.05312303669638	8.41396683756044
C	6.15737071194360	15.48634082400785	11.47060787481422	H	11.09247744765000	13.01028795600003	8.91645127103203
H	6.68689915305029	14.84235408508889	10.75528789044919	H	11.73802058468703	11.97232802083610	7.59067502867760
H	6.32715221600448	15.04804819484995	12.45904898067297	H	11.23979183308050	11.23981315394080	9.11651553499097
C	6.01387416267587	9.35981079054826	12.38451387429187				
H	6.54644584398018	10.24709609520990	12.73120393668268				
H	6.08982133496414	9.36439657470641	11.28730727464297				
C	-1.48920005058779	14.8232775446775	11.24493890537731				
H	-2.53403925533856	13.81715605807443	11.38414800919098				
C	8.57905327386161	12.62354590172340	15.02523726864275				
C	6.72620644362545	16.90175039956768	11.40084264465211				
H	6.42419613433260	17.47626803528135	12.28895715203399				
H	7.82034804410017	16.85340707518777	11.42052145019078				
C	7.23269607203342	12.76404598395182	15.38197853898959				
H	6.95864147313888	12.90420952207866	16.42166506071720				
C	6.34289796432189	17.61523735443881	10.14424916812302				
H	6.53152698820291	17.0419408550108	9.25121825536044				
H	6.70362116990439	18.60490854784863	10.04519069481381				
C	4.49598447433138	7.07450042722158	13.57906813291142				
H	3.73878847307336	6.31909426668466	13.34898124862632				
H	4.68176840469115	7.05178888747648	14.66091975953440				
C	9.69760770184859	12.61130597912865	16.06334629653140				
C	2.81028781971672	13.98133592078309	17.44130218003821				
H	3.22893557420093	13.34328555487553	18.22574987418325				
C	5.78300695400434	6.88310258006843	12.79956196143696				
H	6.28038583279577	5.978853741133784	13.16778810614690				
H	5.55482700712829	6.70996190462813	11.73814243483754				
C	6.67524535656039	8.10704612382446	12.9556333468308				
H	7.63836587360605	7.94796180534792	12.45848063115367				
H	6.89869355313255	8.26104699414746	14.02162786161579				
C	-1.14083878864752	15.59017966174536	10.602478896657110				
C	-2.32398400069879	15.28575306197279	10.47642366960624				
H	0.51871445176152	16.53672117465104	10.02130449920130				
C	-2.36566327653212	9.02401829517964	13.97057950363475				
C	0.80272356128963	14.53280220638018	16.06501233425961				
C	1.31811494247210	13.75981948593939	14.85311521348268				
H	0.75831081712024	12.82009814372053	14.75098161578808				
H	1.14342296363258	14.32213953400241	13.93068871228864				
C	10.43421726254419	11.26404627535019	15.97282414698350				
H	10.88314487376886	11.10470742437178	14.98532260884346				
H	9.75306885409017	10.42809456718417	16.17462286233772				
H	11.24379092800904	11.22590177514076	16.71185896494301				
C	10.67657667456437	13.75817646889071	15.76357670657829				
H	10.17321465745841	14.73131588318507	15.81484491266595				
H	11.13437410736994	13.66519146105468	14.77181473502296				
H	11.48963496025546	13.75978744192085	16.49960687483827				
C	-2.18024074647072	16.25879322001855	10.06277344779050				
C	-2.03303472860723	17.60188168416234	10.79692519226970				
H	-2.19135026677796	17.48150627375019	11.87555694480278				
H	-2.77667911148018	18.31723521491100	10.4520895643628				
H	-1.04303083699542	18.04880028893089	10.64784378259218				
C	-3.60792055305457	15.74804739320681	10.26607055442182				
C	-3.78248686242036	14.9479190444475	9.75135108871206				
H	-4.31921565134112	16.47336090208480	9.85523675005086				
C	-3.85301206400028	15.62234380985077	11.32804971872519				
C	9.16757081409091	12.78322085880280	17.48775816961761				
H	8.84404486718615	11.973728281296795	17.77307484881171				
H	8.64974465989699	13.74142315096493	17.62033553150261				
H	10.00413607143816	12.76619182143900	18.19542661159525				
H	3.14220943190133	15.01050141032543	17.62936068608697				
H	1.13746945350902	15.57957004671317	16.01634123463115				
H	-0.29223814925089	14.55573743815257	16.04176266726879				
C	-1.84794814589224	7.74106934578653	14.62235765692674				
H	-1.29171414609663	7.11473028060223	13.91379949399196				
H	-2.69414982411814	7.14612425436621	14.98425526254181				
H	-1.20340015579497	7.94902210310861	15.48573293274952				
C	-3.27149377989797	8.64083766397846	12.78767395075393				
H	-3.71778448007562	9.51866901539705	12.30567375399952				
H	-4.09379714267019	8.00399878193011	13.13570284632671				
H	-2.17185297601523	8.08394504467930	12.02633028926571				
C	-3.18087434692871	9.80862142911403	15.01155127366623				
H	-2.55764100529145	10.09850616230721	15.86645480808655				
H	-4.00349943982860	9.18901770941452	15.38860589055312				
H	-3.62359761458328	10.71911137133610	14.59070208590545				
H	-1.94274354501758	16.46219152181941	8.55762856622307				
H	-0.94824624229077	16.87328089604636	8.34789130195499				
H	-2.68120138655425	17.16396075125854	8.15153178585122				
H	-2.04115284405892	15.51590802297193	8.01148374343758				
C	1.29737608481496	13.89945123561104	17.35911598064107				
H	0.97530016471068	12.84963066255489	17.41287756400796				
H	0.87703148358768	14.40364167908777	18.23645506961075				
C	9.42735774409594	10.61122759320302	17.152867599320584				
H	9.56432417360972	9.77832003867559	7.85330704740843				

H 5.96659675067743 9.26287351173809 11.16771346628377
C -1.50840037273821 14.05062397825553 11.18777608219277
H -2.54988227000515 13.79190982325371 11.34277418151068
C 8.58924594021117 12.50980892906752 15.03429837682559
C 6.65970413609187 16.94636236736588 11.50090827876618
H 6.28035126904339 17.51610414361101 12.35979836884656
H 7.74959917118347 16.92179012511874 11.59006330812286
C 7.24503753094753 12.63263996981307 15.39805922871843
H 6.97851490863401 12.73732163451127 16.44017122429915
C 6.24339437703900 17.63716476031314 10.20357838381336
H 6.58343934950035 17.05038679387162 9.34017317185696
H 6.69581969857568 18.62971429953013 10.11826051341087
C 4.41890471447836 6.98921852773034 13.50823450347965
H 3.64031795862655 6.24993463091109 13.30183338892781
H 4.65257646225550 6.95803440495784 14.57977182708527
C 9.70932531549733 12.47572538122518 16.071821144560942
C 2.81021842092343 13.93421557926267 17.47021974703818
H 3.17684591786275 13.25908449875722 18.24868569435134
C 5.67233607604640 6.78547643845336 12.67102932692207
H 6.16517978334075 5.86907071255044 13.00940142112000
H 5.39898478438717 6.63728261381783 11.61823159079400
C 6.59524749959913 7.99347643845336 12.81437220523049
H 7.53778553709626 7.82105843872594 12.28660116366549
H 6.84632722359423 8.13576756722292 13.87413503076814
C -1.15912481747957 15.22240563062618 10.50254680683659
C 0.20302860510421 15.53851654620825 10.36481359288512
H 0.48619307391639 16.46490521069207 9.88194236694398
C -2.39839875874167 9.17605850868550 14.17978252350053
C 0.86802215544222 14.62177130450033 16.05426413684121
C 1.35727965405791 13.82807583677382 14.83784347884651
H 0.74728182364840 12.92233064801010 14.72517763549045
H 1.22744740875628 14.40496952741019 13.91734280768393
C 10.48229477053231 11.14929345286735 15.92422365993260
H 10.93706978296724 11.04676479364364 14.93414075149139
H 9.82090194045418 10.29170196198297 16.08742015151902
H 11.28789816193491 11.10477849098473 16.66436173154962
C 10.66659544057354 13.65863607807506 15.82137077006367
H 10.13779748650295 14.61383596900829 15.90518370109923
H 11.13197282053073 13.61087013970830 14.83213272726528
H 11.47032351235304 13.646620547982683 16.56467026014308
C -2.19931731703736 16.18076107855626 9.92582160342756
C -2.04704848994443 17.55995504606357 10.59872641096380
H -2.19466887467346 17.48405561013914 11.68107319422588
H -2.79630636479592 18.25136966985196 10.19949083050705
H -1.06112528460532 17.99904389453356 10.41783067780699
C -3.63246330207454 15.68705369255823 10.15399085925754
H -3.81284300207791 14.71620832705428 9.67924455088999
H -4.33415104719341 16.40095299308711 9.71309610805712
H -3.87452379464962 15.6101526576849 11.21967619942067
C 9.18351953864621 12.57348418871837 17.50793994963920
H 8.51374957963509 11.74267844993286 17.75602616667839
H 8.65758647985794 13.51756270838070 17.68811436728372
H 10.02623296655603 12.53256455488955 18.20415050383872
H 3.18496521077067 14.94275014180934 17.68375337514349
H 1.27757031836129 15.6405298536938 16.03062985963030
H -0.22099035899606 14.71431221778355 16.00959515333257
C -1.89653120779808 7.90696434954618 14.89316287215449
H -1.38226308564124 7.22494606361904 14.20714500407919
H -2.75004094471296 7.36503687920377 15.31078737347512
H -1.22293924428997 8.14697901761382 15.72336631404007
C -3.35829229987141 8.738114684180581 13.05111653138960
H -3.80186506484060 9.59716764550288 12.53841829178261
H -4.17770916942355 8.14395585910408 13.46859284090123
H -2.83734013202812 8.12721145615846 12.30655845094357
C -3.16330698912704 10.03290946973594 15.20132770001943
H -2.501113074816462 10.36342995547563 16.00876060573222
H -3.97656624207880 9.44921808053756 15.64464495430262
H -3.60815811252035 10.91966302597715 14.73933092437334
H -1.96812369914841 16.32096185431561 8.40778172027167
H -0.98137942717322 16.7358388417245 8.17903345719462
H -2.71773920324912 16.99419617641756 7.97936517131981
H -2.05587594044900 15.35033168501113 7.90804380392964
C 1.29369009111108 13.92824861600299 17.34745579256299
H 0.91975530836111 12.89624001179644 17.36035815950701
H 0.87892135585222 14.43341662684186 18.22488568543889
C 9.51405766154248 10.87145870903441 7.08416707189848
H 9.64941825690769 10.00661950399545 7.74212866057644
H 10.27920681974146 10.82812880593952 6.30223370529103
H 8.53778710533288 10.78179392807410 6.59781843815868
C 9.43294686951564 13.38281336099051 6.92127313140530
H 8.45244016207749 13.34949481308790 6.43628453298474
H 10.19297087809230 13.36938405307182 6.13339891951184
H 9.51731135227208 14.33268408478942 7.45994706804918
C 11.07238272237058 12.27237277853516 8.43764464418136
H 11.23814197272124 13.20141540890276 8.99414667706058
H 11.78992992286936 12.25381559906163 7.61229297147717
H 11.30468129852086 11.42330630284648 9.08965982479380

[Cr(L^{MIC})₂]_q_r2SCAN3c.xyz

Cr 3.67808074288023 12.49162745940842 12.00714101388243
N 3.36514505988863 11.35313054639976 7.83218149467213
N 5.69988432289137 12.42912870092021 12.01223321637767
N 4.86674247308446 11.46979528610819 9.27530934116882
N 1.65917820876966 12.54057874869013 11.99881115975321
N 4.66142820410418 11.13103757691768 7.98919081326100
N 2.40176830521961 9.67268033613241 12.57263742549357
N 4.91350710997732 13.41719656727391 14.75156977941559
N 2.54011434427649 15.34243378016446 11.30996460101288
N 4.07028558282273 16.58196727949029 10.62409449092070
N 3.89558523107425 8.29366943681367 13.03702085883600
C 2.75630117761237 11.80830645288192 8.96932706995542
N 3.42017109253273 13.57903449634579 16.9668353536096
C 7.89526303857042 12.09496303858182 11.35561983901855
N 2.58781392249486 8.36883158643227 12.84261937664278
N 4.72598285358332 13.72962019991321 10.46562454750753
C 8.91459727942248 11.66445807522103 16.9886628324758
H 9.94782324339605 11.77284641082215 10.81068394261341
C 6.52094722120014 11.97567814703608 11.00814288593768
C 7.22898892578709 11.01714246693693 8.90753709357326
H 6.95527920673847 10.61427511864295 7.94118176056587
C 5.85528215087331 11.10230575853254 9.26993139303993
N 2.76702959655029 16.58931230678738 10.85795200305030
C 6.20117651986357 11.46392928211797 9.74175728126473
C -0.56159417403363 11.89801464253154 12.14199814247490
C 3.73865361138047 11.90030840907462 9.95476335308599
C 6.53968274153668 12.85765770243797 13.01238905160829
C -0.52389387016094 13.31003842881195 11.92470004445472
C 3.66003749294555 14.53037406802130 11.37624271712412
C 0.85598786702287 13.64352287300456 11.82886861149510
C 7.91057040670685 12.69126025401516 12.65413624899422
C 4.66176235336067 15.38475458983185 10.91634845168103
C 9.63846405949022 10.58064375584582 8.28791072627694
H -1.60883241117097 10.98768426287531 12.28924144115960
H -2.63458217823367 11.34403600432795 12.24410344678115
C 0.80211190962009 11.48255067751089 12.18897229154771
C 3.55327004795932 10.44195246464033 12.58033530150288
C 3.76492139780330 13.06864739667152 10.6090190986437
C 0.00875272288022 9.22514736192778 12.55019204090891
H 0.25359926355731 8.18751705850741 12.2726232359512
C 1.30434958233076 12.167409758262346 8.93062851585173
H 1.21074756948217 13.26256277167908 8.94982327711200
H 0.80846215981932 11.80646301528776 9.83245438877974
C 2.78790378616957 13.19012478029144 10.54920231078586
C 1.07247120457683 10.12696239205336 12.41435811580966
C 4.52525669919683 9.50118734434424 12.91588465607533
C 2.74357877546991 11.04886310371679 6.64721516038549
H 2.56130991754693 9.96590376082244 6.49255751609698
H 3.45735614931472 11.31306107531419 5.76013609672019
C 6.24645216951069 13.37423112703522 14.2803048732064
C 1.43381271885852 11.81629250505259 6.43191330950764
H 0.90343969379676 11.46947053515568 5.53839446252043
H 1.64185406380660 12.8861996357920 6.29669572213222
C -1.32977507552183 9.63463331101188 12.48582167014439
C 8.94132897567479 13.08105388786741 13.50944010889065
H 9.97327993822365 12.93971196400853 13.1991247728294
C 0.59895640923365 11.60298932815555 7.69293927692453
H 0.42137687800689 10.52709726669919 7.83020534766278
H -0.38294958529456 12.07657102785627 12.07536838797876
C 1.19703927296781 14.97726235070346 11.55949450398458
C 4.71470436781975 17.80113952037298 10.14445355120433
H 4.8867679080490 18.46812882100555 11.00127308579003
H 4.01964059160827 18.29842123532500 9.46023812812637
C 6.12077743944971 15.19805040478287 10.64603512782135
H 6.23794596900137 14.53970257543884 9.77359576522433
H 6.58797865759763 14.67466715816032 11.48159114356896
C 5.99694375042456 9.59333743029538 13.16307980788141
H 6.12525852717007 10.49787862332352 13.7378662219743
H 6.52507324015846 9.71099658368607 12.20760857694304
C -1.52757519332066 14.27877901318784 11.80834440972299
H -2.56569408909036 13.97612171077254 11.89317278688184
C 8.63866383287930 13.64792561406263 14.74831520608248
C 6.84284051966531 16.52722574721976 10.40059172138218
H 7.00742051144591 17.03980027486532 11.35880812263664
H 7.83125358803994 16.32459450110283 9.97573355905780
C 7.29377907832050 13.77756703607808 15.11909900524546
H 7.03205159525385 14.18243279625429 16.08568550999286
C 6.03429109208247 17.43692877999286 9.47818380757591
H 5.83935394402290 16.92677074918202 8.52533093022498
H 6.57792559568977 18.36045901270749 9.25131155383726
C 4.48377487290202 7.00989418857812 13.41043334421685
H 4.02995944434771 6.23459212361271 12.78396382277195
H 4.21844632675662 6.79941845585472 14.65621266323179
H 9.77627062178372 14.08978896399415 15.6575325820860
C 2.81672538779846 13.86683074542209 17.49476871925554
H 3.51705708351729 13.53597897265706 18.26843866894799
C 5.99606454855633 7.07983412531040 13.24643776299905

H	6.43577842636837	6.18530951995826	13.70062135370454	H	9.96263672826728	12.17077841289824	10.71495437205018
H	6.25718645913920	7.06910506564825	12.17981368190298	C	6.5358882103835	12.23843896371466	10.93537257040327
C	6.52934931809478	8.35661992431980	13.89378182408930	C	7.27056328203565	11.87946627332303	8.66472865402009
H	7.62382544300159	8.37158239882209	13.87474902045694	H	7.00851526004229	11.70813073877578	7.62842757011067
H	6.22543411801948	8.38263069044508	14.94992900519425	C	8.62446858552936	11.94242797162423	9.03411216772747
C	-1.17723508728082	15.60665313566529	11.58924528074193	N	2.79589384001835	16.42145518578205	10.43282272894609
C	0.18475094239122	15.93429282509932	11.46124571571782	C	6.23580809139213	12.01154765127869	9.58474089663744
H	0.47588924715791	16.95708840906657	11.26067907926505	C	-0.54976484499938	11.94146679031049	12.34035203108687
C	-2.48424781834687	8.63756339849553	12.63398042054025	C	3.75361503490215	11.90562780929750	9.94738893482989
C	0.64473209098439	13.47108908688815	16.33567736947942	C	6.53418601968150	12.58978108031464	13.09845903714903
C	1.31711672695691	12.92013174767266	15.07363722673576	C	-0.51960231681283	13.24103704697061	11.73355114452805
H	1.15577785677908	11.83533009015351	15.00236849306259	C	3.65896738065004	14.51422056562657	11.36283543323692
H	0.84681755482813	13.35222842095135	14.18906784096077	C	0.85905274735319	13.54391773454533	11.55971210932898
C	10.64083746951206	12.86789383956319	16.04087008107755	C	7.90824020103345	12.48848355359405	12.72972161659316
H	11.08378737062715	12.40785671311524	15.15226420101536	C	4.67939126205105	15.44327040225525	11.13122211458006
H	10.03487292233559	12.10749079056951	16.54535067937866	C	9.69295102684320	11.78699286700731	7.94911882248793
H	11.45667875053133	13.16227641471525	16.71232206081602	C	-1.58371576742129	11.13002773876518	12.78756996742659
C	10.64947741235761	15.13395106763045	14.95438804488380	H	-2.60987239766071	11.47652611442060	12.69847840436750
H	10.05126443362762	16.0077943397243	14.67395322605771	C	0.81515868235846	11.54413382403479	12.45006040064241
H	11.09485946308740	14.72669755667588	14.04157925824474	C	3.56453417778733	10.42063155009189	12.58571535461317
H	11.46533499954207	15.46814027769760	15.60693120583895	C	3.76237317757821	13.04199260574723	14.06563499003493
C	-2.21335193419684	16.72836899530170	11.46965113512368	C	0.03450770254192	9.46995605400209	13.41292261804066
C	-1.96795713890685	17.77468808698050	12.57363236529517	H	0.27932152571753	8.49481727469853	13.80968346839118
H	-2.04649587109243	17.31277341361050	13.56387846666584	C	1.27189665877983	11.41151816744436	9.13047420081707
H	-2.70908400334118	18.58046490183233	12.50750293853165	H	0.79624188300604	12.39468104943321	9.24235900525235
H	-0.97318153684947	18.22314787327264	12.49059040949725	H	1.04156466317857	10.85848224469905	10.04461332259747
C	-3.64876724987525	16.20980438073626	11.61614669367187	C	2.77121353930762	13.40328407619947	14.98480396478626
H	-3.89475343451955	15.47817690444827	10.83882999841611	C	1.08413675956703	10.26767667735642	12.95460719553309
H	-4.35108623560355	17.04523201226969	11.52228124249623	C	4.52216750901144	9.40479651702282	12.68664847580457
H	-3.81242854327388	15.74475830389809	12.59443652338986	C	2.74440746243904	11.05987460053689	6.53481145858865
C	9.26543070028815	14.71704992011756	16.97818280854382	H	2.96213459089994	10.00037948118784	6.34929114456458
H	8.67187475102332	14.00722842779044	17.56448635117552	H	3.22546560351596	11.65125174597336	5.75019390689510
H	8.65253751505861	15.60458738085675	16.78644558746777	C	6.23607178226207	12.83118606083433	14.44374272045563
H	10.11776269763765	15.02563090262832	17.59342592174436	C	1.24377010616291	11.29819224208191	6.61689459522532
H	2.69176116119705	14.95482567939524	17.59052567079167	H	0.77614579207694	10.85069353059296	5.73414335629671
H	0.52306012193238	14.55944615613519	16.24277197253027	H	1.03303896271202	12.37531748233386	6.58680717088579
H	-0.36047989553696	13.04587638137108	16.420844716704390	C	-1.30187059082561	9.88334296312514	13.5220916413063
C	-1.99776540101301	7.20113485009006	12.86105477968959	C	8.92608295059615	12.59098801033482	13.66868773290375
H	-1.39345329517182	6.84095362601149	12.02139913868880	H	9.96023589815722	12.50471453624904	13.34599869458069
H	-2.86199439973819	6.53526974510213	12.9600455195031	C	0.69118280220635	10.69529577534237	7.90688763848711
H	-1.40337426838514	7.11484318955071	13.77718474189780	H	0.93785752086667	9.62523943367763	7.94472824255913
C	-3.34174056251573	8.65409826674794	11.35390084020069	H	-0.40003546918533	10.77198266762169	7.93101138741305
H	-3.76658350093004	9.64511306645253	11.16702008296468	C	1.18900693183310	14.79144751915867	11.00992562049509
H	-4.17090458206617	7.94126921303632	11.43971552686829	C	4.74842296293826	17.79043935458668	10.15503975963810
H	-2.73702986263649	8.37842241116147	10.48308722071220	H	4.52142110937260	18.55211184693736	9.01183070000017
C	-3.35950870018130	9.03993518308563	13.83627634087432	H	4.29780751583509	18.10284660623144	10.2841176241837
H	-2.76692827892713	9.04720143550288	14.75758553881075	C	6.15207342831956	15.43713189887535	11.38867597434311
H	-4.18668561709049	8.33066234782974	13.96193422949976	H	6.64285407915563	14.77831995269558	10.66060317166192
H	-3.78910591275926	10.03773847858633	13.70591124579000	H	6.34610844653939	14.99954203562032	13.27156114586609
C	-2.08873463953749	17.40429646947838	10.09080239918224	C	5.98971751711401	9.34671062820035	12.40428332811175
H	-1.09728983639192	17.84325154647526	9.94402621367583	H	6.48395253164745	10.20905896176691	12.85489286590445
H	-2.83063284331227	18.20576675817793	9.98917482547587	H	6.140829751577507	9.44252950097558	11.32016555707191
H	-2.25550315729433	16.67574504706513	9.28983158509553	C	-1.52408963606151	14.11968602036268	11.33524993288096
C	1.46901023019972	13.16456937195858	17.58422938547713	H	-2.56178416275766	13.84120664264546	11.48458826815825
H	1.62112864132509	12.08078803200513	17.67669401916388	C	8.61795822371114	12.80081652359089	15.01486886770192
H	0.95882602403314	13.50308965662181	18.49254061489133	C	6.75548096593463	16.84216219216032	11.29513107981589
C	9.41594293373683	9.074409358215	8.05197720487052	H	7.49228330986476	17.42744094254166	12.18701871365914
H	9.49992434482860	8.52319435268373	8.99499795266731	H	6.84663881288166	16.76244744280713	11.27711452198208
H	10.16416199208931	8.68085665667448	7.35318736758103	C	7.27087433828892	12.92350587619591	15.37565448405266
H	8.42432290741023	8.87449580104607	6.63431563577261	H	7.00444434122550	13.10863176900851	16.40638729264062
C	9.51802306677298	11.32932626956074	6.94698040991729	C	6.24890299526298	17.562519874887826	10.04719863034858
H	8.53637016115996	11.18290871476197	6.48636914045009	H	6.47372164615834	16.96503375031921	9.15390306497469
H	10.27766660022591	10.97208984075665	6.24105521896914	H	6.73618582666492	18.53443691714097	9.92053265276150
H	9.66218611338775	12.40533513684860	7.09366372900632	C	4.43520694993129	6.947707747332596	13.32530387652690
C	11.06646127951765	10.77546737531575	8.81145710241519	H	3.70354223732087	6.20623039248323	12.99200478013000
H	11.29459140252807	11.83447990919163	8.97448334878590	H	4.57208688820177	6.83471169299275	14.04849570035783
H	11.78156705904933	10.38925620339197	8.07700627296956	C	9.74523244549013	12.90353561075779	16.04637126861634
H	11.23060590827190	10.23714211466449	9.75128194750360	C	2.77374290458756	13.94821152373638	17.46846830786493
155				H	3.2220235631692	13.33882265625603	18.25872370845453
				C	5.76634326906278	6.83667487405733	12.59709751874357
				H	6.25441082246769	5.90789390062507	12.90916348841621
				H	5.59440186227542	6.76794693531328	11.51480586003420
				C	6.63242967062875	8.05297941641859	12.91667390196916
				H	7.62656831320622	7.94638686221672	12.47209326011443
				H	8.7763749725229	8.11827042746844	14.00386780017442
				C	-1.1873680305629407	15.33682750324227	10.74806591048790
				C	0.17415490890285	15.65278996407983	10.60616462634206
				H	0.45727738227582	16.60732029047357	10.18095986264398
				C	-2.44528726196178	9.01237036169816	13.88101810001176
				C	0.74769948299372	14.39967036800929	16.08146272286287
				C	1.30166715966167	13.64865898389490	14.86640855152270
				H	0.78127141356614	12.68806235327425	14.75935373037830
				H	1.10269471617933	14.20547165475750	13.94724461327003
				C	10.55362708869932	11.59173235343363	16.04785989225618
				H	11.00815574721600	11.39391190373860	15.0721905232320
				H	9.91113209221566	10.741320642899111	16.30057903066617
				H	11.36023350030842	11.64505914948478	16.78755584568558
				C	10.67233545380228	14.0751706431218	15.67092945022120
				H	10.11550922360352	15.01816801930187	15.64932369937934

[Cr(L^M)₂]⁺_r2SCAN3c.xyz

Cr	3.68656874240847	12.47524042271146	12.00743699854634
N	3.36576247014123	11.42674788771057	7.81492273483248
N	5.70474441939503	12.43564130085534	12.01212825820103
N	4.88479227147666	11.86282924162205	9.15989098625111
N	1.66708865041337	12.51870117005608	11.98918874939174
N	4.66840838018664	11.58090959913986	7.87257052594169
N	2.41175816236196	9.75437511519338	12.94714860275341

H	11.13128251267994	13.93135456858484	14.68790372464760	C	3.57582562705481	10.48054296051905	12.53639104014791
H	11.48064933649054	14.17004681663000	16.40479262580820	C	3.77534227851685	13.09835419718018	13.98139124858943
C	-2.23246121766028	16.34553312951825	10.26481484495854	C	0.13728228355495	9.15301245346687	12.00598116160325
C	-2.04815547431277	17.67981358019783	11.01305574505549	H	0.39342022166947	8.10022458463735	12.06281949769670
H	-2.15848602194009	17.53661057472422	12.09330254950881	C	1.35920333882035	12.42158392318944	8.87165962650766
H	-2.80120325345117	18.40466597945736	10.68409556397884	H	1.47802557667481	13.50386599260116	8.71067148772453
H	-1.06234337961560	18.11798394296150	10.82902265348882	H	0.80806771542730	12.31256805391998	9.80479971052334
C	-3.66380781389704	15.85431427715299	10.50957714966978	C	2.80246799458922	13.20471937218212	14.98035301645635
H	-3.87057145903473	14.91907284511466	9.97774187453806	C	1.17971872623393	10.07797053046131	12.07282074229876
H	-4.37341609957857	16.60418052456383	10.14597020289588	C	4.54403855951678	9.59030586419986	13.00611654225160
H	-3.86303549469638	15.70126807714201	11.57591701456806	C	2.60635025869273	10.77056402784052	6.71198395149648
C	9.22060413073416	13.14442203415905	17.46664436060484	H	2.28719221378146	9.72441308166686	6.80745253295100
H	8.57630545490549	12.32624741757183	17.80709350114636	H	3.359125662524681	10.82369886089168	5.91970439054576
H	8.66193083893220	14.08393622713814	17.54094201621330	C	6.18513978800450	13.66489247463468	14.09196918407524
H	10.06586127066174	13.28030048509160	18.15918177987644	C	1.42122598408283	11.68487670550870	6.46493256956423
H	3.03977333504457	14.99723636996161	17.65057753827255	H	0.84158545982144	11.28041547639900	5.62765970966028
H	1.04427027492911	15.45680036020617	16.03849897410221	H	1.77542556419411	12.67783691582561	6.15343873320911
H	-0.34579805672878	14.37354005571500	16.05113796005208	C	-1.20191737254605	9.55100120237681	11.91083962204941
C	-1.95582923210741	7.65882953208637	14.40882618651206	C	8.85424737987094	13.26641625802478	13.34065470396883
H	-1.46550099753523	7.07043389797394	13.62539282451491	H	9.88601402451810	13.07490467870061	13.05065290493996
H	-2.81126986527198	7.07958985987374	14.77074237581752	C	0.56861165271367	11.80258147237473	7.72165968863807
H	-1.25953387137067	7.77493214536464	15.24666661512672	H	0.20511874454299	10.807537548648376	8.01843951185345
C	-3.45895573336672	8.74839365504083	12.75156150590417	H	-0.32106777041347	12.41095073604311	7.52580039637942
C	-3.89722005864195	9.67589196579702	12.37107525584559	C	1.28715553683389	14.99677953284080	11.92487398360433
H	-4.27847888703294	8.12144542814379	13.12020847534834	C	4.77154289607995	17.84650018498446	10.56391573796592
H	-2.98076123341488	8.23072270169860	11.91312170488504	H	5.09678326373367	18.34409693897661	11.48688256455504
C	-3.14809113115332	9.75460620246981	15.03435465244089	H	4.01706071905316	18.47815183413660	10.08559190653997
H	-2.44569690005667	9.95123643287834	15.85163225347396	C	6.03219002699863	15.13654989243692	10.86012915599022
H	-3.97311515272220	9.15012156283814	15.42778013315929	H	5.93267042851348	14.64520369091041	9.42646752984851
H	-3.56146120819910	10.71323889425442	14.70534059509393	H	6.58168744278658	14.44106505757178	11.04102809844947
C	-2.05365975448972	16.57836597448529	8.75238590262933	C	5.94838695481661	9.75233552864836	13.48155737688067
H	-1.06308337981424	16.98125469881204	8.51811880239238	H	6.02504181170281	10.67741530996721	14.06247953461226
H	-2.79988607640152	17.29359524168121	8.38818507121624	H	6.60794401404350	9.88054904007207	12.61266843862951
H	-2.17744620827751	15.64145039541774	8.19892661816633	C	-1.41761697995389	14.26696425528460	14.07268203080486
C	1.26407813684942	13.77980351602346	17.37844482958320	H	-2.46052393894690	13.96170343181865	12.09583979438828
H	1.00317884114553	12.71385493490766	17.41321908269338	C	8.57271661571644	14.01290071649899	14.49504949178979
H	0.81265541512637	14.25396833763721	18.25568831940678	C	6.81231324404151	16.44170966099918	10.26596752677953
C	9.53796401668017	10.41327207495338	7.26889117914326	H	7.1765803386993	16.76019274482369	11.25387469930301
H	9.64820617713823	9.60478343013788	7.99962226279483	H	7.70149507942922	16.26686253108723	9.65052342658968
H	10.30400333568779	10.28436430365372	6.49593948290660	C	7.23119125144971	14.180738624979189	14.85921144444150
H	8.56007869179530	10.30469906452889	6.78941862796026	H	6.97469178099489	14.69457019779200	15.77957681665403
C	9.52061771879946	12.90038292933140	6.898056113524823	C	5.95183443292195	17.54312821682688	9.66039493345892
H	8.54215985102007	12.8505398021897	6.410011632688781	H	5.59291536453068	17.24291231025384	8.66548492493748
H	10.28673851168786	12.80849500675473	6.12002897889172	H	6.52736707216223	18.46523248076533	9.52209814656523
H	9.61839180956393	13.88821745710490	7.36123762043371	C	5.49834440362064	7.10100373434362	13.44990557901881
C	11.11226378955825	11.88178086720902	8.52027506713700	H	4.25554539859572	6.33109365415952	6.33109365415952
H	11.29572958674954	12.85207813102025	8.99478056881104	H	4.09936250789440	6.84829929888279	14.41821412193779
H	11.83913847314705	11.76856349490917	7.70973703567537	C	9.71941666476157	14.58209379955814	15.32906811796142
H	11.30956758734122	11.09137531206534	9.25271650811120	C	2.77658829124758	14.26545085991532	17.27497923244572

155

[Cr(L^{MIC})₂]²⁺_sUKS_PBE0.xyz

Cr	3.68291669359470	12.48545547630001	11.98907754622213	C	6.40859597873172	8.54428298403832	14.29373645541844
N	3.26545722080356	11.14270382830519	7.96185379223634	H	7.48932445607647	8.60866248301310	14.46002731799249
N	5.59884058249561	12.42872835235302	11.97966798445142	H	5.93812199668892	8.55127850417140	15.28798800334868
N	4.75161750621516	11.22731570121278	9.38084468685051	C	-1.07443310703997	15.62210117409846	12.08723073031283
N	1.76794501491942	12.52509359839462	12.00011935309610	C	0.28614136925094	15.96005455036934	11.98948403915584
N	4.49185662569630	10.77969338615567	8.17552880571189	H	0.58278076800158	17.00328997748966	11.92504803044066
N	2.49788197152496	9.65695660080117	12.35433073492212	C	-2.34610292792182	8.54282880531470	11.81628429501800
N	8.85940741439943	13.68009052700388	14.58000543275186	C	0.67204478504221	13.34694604151960	16.29304773452986
N	2.62096621588512	15.36237044240548	11.63327335524873	C	1.41138781941613	12.68468952983257	15.13325593270716
N	4.11333406294202	16.59884801067929	10.94477078321393	H	1.47295223465403	11.59754810248529	15.29304437342775
N	3.95579950713223	8.36314988521669	13.01259124021333	H	8.85514287656042	12.54210267124731	14.20696795401370
C	2.72111132173742	11.82522518726476	9.00654653635831	C	10.62248040803434	13.42873563640526	15.79571312037694
C	3.39728185248858	13.85771079938339	16.01642980149905	H	11.06290930373452	12.88106645819127	14.95426770714192
C	7.78511756798699	11.95868184989876	11.36350855810820	H	10.06285160929829	12.71304214337067	16.41042378093618
N	2.71706887072671	8.39213673777560	12.62699656021381	H	11.44985968303213	13.81901837356333	16.40049319424885
N	4.63966790633159	14.15032053314629	15.78715450093026	C	10.53128290965368	15.55454222520213	14.45863980824572
N	8.82255979631190	11.38677358154841	10.57839645539451	H	9.90878034162291	16.38800526525181	14.11010244986522
H	9.82468632567794	11.51327306474189	10.86019670527095	H	10.95871270540030	15.06039892243113	13.57807195745621
C	6.41681134187050	11.81608396022377	11.04389485627960	H	11.36349144299521	15.97434888109209	15.03657601395767
C	7.08176062515643	10.58165486132353	9.08379403651104	C	-2.11297449582004	16.73994303145022	12.16417449677430
H	6.78591486606798	10.08503918623516	8.16383984226035	C	-1.82742043524426	17.59737795324781	13.40685846823426
C	8.44030467834539	10.65980008153697	9.43371573650479	H	-1.89282265408231	16.99720901422825	14.32299140926472
N	2.88180484433366	16.61672124143417	11.35027566038963	H	-2.55970018527781	18.41028567486509	13.48414725381241
C	6.08134873083173	11.16391615839730	9.85551220524568	H	-0.83134288305442	18.05459778567027	13.37138432972740
C	-0.45224984093311	11.85105608050231	11.98250778322253	C	-3.53679710087748	16.19042125953942	12.26794216476240
C	3.71089705304362	11.87409305359439	9.99360777376136	H	-3.81574278879157	15.59935641097581	11.38664690367437
C	6.46369568037873	12.99184642736927	12.90396989296607	H	-4.24768606743212	17.02156014142460	12.33713857473272
C	-0.41951560146889	13.29683672012314	12.02521526780312	H	-3.67334487835806	15.57014558958520	13.16270197813257
C	3.66571778993197	14.49776308418782	11.43928347514622	C	9.21771378265932	15.33418714620134	16.5292121868843
C	0.9494555923743	12.64380764056410	12.00157037477010	H	8.66139287010422	14.67925594341612	17.24528418561962
C	7.81917052098895	12.76149904400743	12.56592508429187	H	8.57801969424963	16.18494468310714	16.29612582074398
C	4.66038091646448	15.35233154560928	10.95389730393469	H	10.07164464351735	15.73333395872534	17.12196258347926
C	4.97901497423272	9.99372178005572	8.53287125467928	H	2.51387659384985	15.3275482691134	17.18369414062101
C	-1.48543685047638	10.92494399604623	11.93243335490689	H	0.36150151395684	14.36094364314515	16.00021904841514
H	-2.51762892646273	11.27016542011366	11.91095663492343	H	-0.24765379696859	12.78958713442837	16.50173867926537
C	0.90296174954931	11.44210400408333	12.00163828150021				

H	-1.17501354967455	6.89019816176600	10.98048519101347	H	9.95526044067312	12.53165139212312	13.35758388599705
H	-2.69551471163765	6.41284264151213	11.74055191570719	C	0.61443246282466	10.87201472558960	7.95843328342449
H	-1.31976614446817	6.84955682353418	12.75598762002531	H	0.79579848855045	9.78615933305471	7.96970732682280
C	-3.10994544270489	8.78882579538624	10.50541946669717	H	-0.47309573983404	11.00740326625364	7.98673273602044
H	-3.53272143549327	9.79939464184412	10.45952265112647	C	1.21589273735822	14.80795340305882	11.06657581306035
H	-2.94119824190327	8.07951592563674	10.41116957377424	C	4.77096854310453	17.71394150791424	10.14901873699664
H	-2.45375940834095	8.65962636751957	9.63598840005472	H	4.58969429097271	18.4749178958705	10.92041785120718
C	-3.29117203038109	8.74017089941948	13.01203407245432	H	4.28015306960728	18.04748778697103	9.22887325019529
H	-2.76493780629483	8.58274164986979	13.96148398983546	C	6.17758697545321	15.35183807660558	11.30488490424053
H	-4.11891355247865	8.02263750322910	12.96111744131846	H	6.62812634998371	14.67054672107122	10.56985134527290
H	-3.72945202434546	9.74479798160898	13.03134770851056	H	6.40145875259030	14.91684841951452	12.28358112613287
C	-2.01398317793417	17.60818047335658	10.89961659483632	C	6.04028588501128	9.46800883044280	12.50106062901613
H	-1.02937355983055	18.07983516597464	10.79826684578348	H	6.51387915059199	10.34128071163371	12.95502367860955
H	-2.76084779824340	18.41050975500679	10.93328402295905	H	6.21134181071048	9.56759443100110	11.41932938876049
H	-2.19870006303810	17.01233986279173	9.99736538644423	C	-1.51216411842530	14.14446336429027	11.36660252686485
C	1.54663034627572	13.41741438478782	17.53822697740805	H	-2.55542426055288	13.86687746700821	11.49937261211468
H	1.84959631971174	12.40650537701719	17.84608339402413	C	8.59613776506092	12.87471351703124	15.00866555276935
H	1.00134124699476	13.85348474206366	18.38270145304677	C	6.81196794062472	16.73351247438144	11.17751674272497
C	1.6585493366771	8.49299874696955	8.42957089180283	H	6.61579916506544	17.32536726307858	12.08485770394812
H	9.20339553471329	8.01317191459197	9.41548275055663	H	7.90052383093815	16.62708388442401	11.10304959152324
H	9.90177405059721	7.9966684621370	7.78545058274366	H	6.724225901635877	13.00854395742720	15.35409159235924
H	8.17450068605140	8.30640365361702	7.99961045328529	H	6.954186339790059	13.21354536105654	16.37901949652900
C	9.41600508321508	10.63409661884679	7.13689524288566	C	6.25806461688283	17.47348869834437	9.96736561437861
H	8.43267005485759	10.50870492925019	6.66804110480809	H	6.43107662593691	16.87986583883827	9.05788833322968
H	10.15771111984812	10.17116169374220	6.47476323962478	H	6.75495354834674	18.44015307778773	9.82026157849259
H	9.63217455018894	11.70827590029366	7.18642115222172	C	4.52281489412460	7.08825009501895	13.45685762951025
C	10.89784108764516	10.15918303277027	9.08031848134479	H	3.80321433250434	6.3217746280455	13.15226859883478
H	11.19907696990487	11.21290222195710	9.13102605542878	H	4.65417282776949	7.01387646685112	14.54532329369288
H	11.60905947288520	9.65218924995791	8.41843819686483	C	9.71272618678688	12.9769111272973	16.05125613433336
H	11.00830520876408	9.71580990766738	10.07793739734478	C	2.73960581817300	13.91258478798409	17.39517677293622

155

[Cr(L^M)₂]₂sUKS_PBE0.xyz

Cr	3.68738861108582	12.49064533211046	12.00802451469015	H	5.69132471893231	6.85920316265993	11.66316720059632
N	3.31892676109819	11.48727596047965	7.87519485786315	C	6.70377355331695	8.19780945635128	13.02736315414649
N	5.70129528520874	12.45384727501396	12.00787064236385	H	7.69928534483869	8.09730726692153	12.57924562409032
N	4.85030619712426	11.86253465109131	9.20028810712164	H	6.859171117793052	8.284628821249498	14.11359968948349
N	1.67152976353564	12.52968086494954	12.00203515855997	C	-1.16335247290295	15.37521954795963	10.81222302433794
N	4.61168267606491	11.60054762982782	7.91851290203261	C	0.20449733567638	15.68220511000875	10.68026398311204
N	2.45132592853417	9.79823290694811	12.94290428222185	H	0.509583202194713	16.64169905194737	12.7188277999720
N	4.87332980630536	13.08291859700323	14.81548390783392	C	-2.40010442622647	8.91573734821665	13.74925067871908
N	2.56655444400548	15.18964355236609	10.96344549326266	C	0.68359908536495	14.27058950348685	16.04031528516745
N	4.11761377886877	16.48565716984239	10.56895454350741	C	1.27767939669666	15.8730842888229	14.81737794016696
N	3.92856302758712	8.37909956575570	13.15702714974427	H	0.79068705808465	12.60448261757850	14.66940650736220
C	2.711712429934449	11.65801677691167	9.07806614453032	H	1.06348406606005	14.15390896833359	13.91195826454911
N	3.35953377751266	13.54103248570723	16.13468767432044	C	10.47600571933814	11.6439759826952	16.10352094506051
C	7.89757065914243	12.26452577892071	11.30595823501655	H	10.92417927240837	11.39742095505824	15.13376393301784
N	2.64450407686558	8.52672192975115	13.27978902292725	H	9.80221446076068	10.82234127459758	16.37699119071241
N	4.64618839730730	13.37158153589351	16.09317674383602	H	11.28395812327486	11.68741041514616	16.84652799892454
C	8.91142417296635	12.08341047393328	10.36359713561259	C	10.67963678748621	14.10426195831464	15.66010755413686
H	9.94965099280806	12.1234345306100	10.68561194325090	H	10.15693013388331	15.06804253130888	15.62000695396365
C	6.52014487805038	12.22923096498796	10.94460044814300	H	11.13041351509862	13.9295769883507	14.67618129812791
C	7.22134299468459	11.80615302030573	8.67616992634701	H	11.49541796685286	14.18738352467545	16.39111802702419
H	6.93143413118472	11.613744179691616	7.64694102334489	C	-2.19783220043694	16.40177168084575	10.34701308258303
C	8.58399103495337	11.85833718398959	9.02732569086008	C	-2.00842679140117	17.71371132838997	11.12375073456804
N	2.82568883132658	16.39880741440398	10.47444561459085	H	-2.14009784559409	17.55011140304474	12.20060647009023
C	6.19518445912351	11.97682648038136	9.59990987525539	H	-2.74120854945661	18.46492042407577	10.79921106776313
C	-0.54095888018193	11.93046219272476	12.32297023265104	H	-1.00792116296726	18.13494392970442	10.97130475649174
C	3.73515841571955	11.94375014964525	10.01504558638255	C	-3.62994346290525	15.91477215740842	10.57528008361948
C	6.52528229951949	12.63070604963939	13.07889509453728	H	-3.83839849067052	14.98995467217005	10.20206653111057
C	-0.51372601386801	13.24853118726104	11.75189767120181	H	-4.34214427596778	16.67492567637691	10.2334738242733
C	3.66759219282507	14.456424719632714	11.36943906614905	H	-3.83005004208967	15.73093907067722	11.63828732974016
C	0.86939180373503	13.55159927509281	11.59461742317667	C	9.17337646273336	13.27523264230868	17.45182916486194
C	7.90305073014545	12.51663175174612	12.72055291315401	H	8.497486606718885	12.48617660142601	17.80400881368676
C	4.69934653710269	15.38481075628518	11.10581906283895	H	8.63159055905989	14.22869422714919	17.48442211068710
C	9.63421901899307	11.65748037367299	7.93307144467215	H	10.00591067953282	13.34110240434074	18.16368965002808
C	-1.56737403171294	11.08670171164779	12.73807873150269	H	2.95826738634943	14.97314704218801	17.58054671306347
H	-2.60164643733478	11.41967875822443	12.65143499615090	H	0.91021367393218	15.34759271298894	16.01211474700979
C	0.83065580245805	11.54849591717862	12.43012135106587	H	-0.80866201300706	14.18029344524215	16.01313097862235
C	3.58758034166139	10.50638273850319	12.59333750675252	C	-1.88523313860185	7.55804923417719	14.23177196420023
C	3.75564307493044	13.04089819914758	14.00084337927237	H	-1.36674624152613	7.01381321536826	13.43250959434983
C	0.07898983336405	9.43883910583877	13.3364947770913	H	-2.27272146749792	6.93827427657568	14.56503465299659
H	0.34946792396019	8.45783586717984	13.70797613011265	H	-1.19475347979836	7.66148018372498	15.07795114001535
C	1.23586007632671	11.51973421326663	9.19221059088895	C	-3.39224926798460	8.67097249019765	12.60253253771382
H	0.78963996910123	12.51041322834028	9.35585128958647	H	-3.83177095125262	9.60676293952685	12.23828834230418
H	0.99733658816313	10.93982263856717	10.08897314835342	H	-4.21465546120098	8.02320925966462	12.93506472853642
C	2.75135097491407	13.38095198243816	14.93370982655764	H	-2.89457685813952	8.18428794170149	11.75447967496920
C	1.12336536785206	10.26539807497414	12.91700565984998	C	-3.12914761733537	9.59810759050080	14.91730631126140
C	4.57007623474367	9.50434564787874	12.75659590833127	H	-2.44105285932250	9.77284282708558	15.75383755698855
C	2.68413887099642	11.16148898308490	6.60930528557905	H	-3.95692876464655	8.97273220207350	15.27877192570467
H	2.85625066682683	10.09521166920451	6.40825169110316	H	-3.54494243669821	10.56829684914249	14.62054206984586
H	3.19500470169674	11.73556727762192	5.82940313928789	C	-2.01087638186583	16.66602222621542	8.84523657455246
C	6.21132159180353	12.89708863159172	14.42033123831616	H	-1.00691583352075	17.04733078400674	8.624593247505778
C	1.19892865223948	11.46326567440999	6.6825123752593	H	-2.73845232583752	17.40717347953423	8.48754768989898
H	0.71333714090206	11.05535408372371	5.78758903623109	H	-2.15047423368594	15.74310384444775	8.26837508089485
H	-1.03868839161873	12.55121289549218	6.66846428592420	C	1.24238423468463	13.67554162187406	13.6200930346301
C	-1.26843911789902	9.82649617808574	13.26517703515757	H	1.03378405370518	12.59618581937521	17.35834130659802
C	8.91576715949907	12.6344377198059	13.66911371895420	H	0.77559426388		

H	9.56459883822418	9.47969838856584	8.03891186041391	H	7.84981104805724	16.32349861456713	9.95089203252854
H	10.19148792558599	10.11072967240222	6.49883359937425	C	7.23808485229164	13.82756161180054	15.08846024206598
H	8.45319967073400	10.16641444500319	6.84345518767326	H	6.97292296346609	14.244414726821876	16.05389999215312
C	9.46544157897367	12.74475199356083	6.860711107170703	C	6.04673370129421	17.45188497601741	9.53904922394138
H	8.47163444832285	12.70565664739333	6.39943815734554	H	5.83560565190676	16.97906793944702	8.56918364430309
H	10.211101246560821	12.623481164246647	6.06316890674459	H	6.58451108178668	18.38269634749724	9.32687288771825
H	9.59028189626813	13.74325113753713	7.29806810022442	C	4.51376624209924	7.043910476864009	13.47004723111254
C	11.05843246953144	11.74207420843425	8.48440669304127	H	4.03526419465473	6.26774182838342	12.86491157920816
H	11.26200328546911	12.72173537668320	8.93473155198599	H	4.24340099801306	6.86953467450965	14.51946551432339
H	11.78207328472544	11.59272127124058	7.67316257851900	C	9.71993927527311	14.15105141164145	15.64007375721105
H	11.24634868435678	10.97121047463532	9.24227470215726	C	2.78857545274893	13.96729690835021	17.43572227516746

155

[Cr(L^{MIC})₂]²⁺_t_PBE0.xyz

Cr	3.67745827514905	12.48548592274240	12.00554289142522	H	6.27410629939972	7.01729979900802	12.22474741865310
N	3.31327189107698	11.32586956312788	7.87411015101820	H	6.58445782100516	8.37143643977500	13.88224392862255
N	5.49498558512251	12.43534908507272	12.00328241573701	H	7.67883032365318	8.36948930574603	13.83356012247913
N	4.80203567007059	11.45580253736011	9.28762041401373	H	6.32038488537555	8.43523543130691	14.94824772342869
N	1.70647394249731	12.53200605078562	12.00766752350887	C	-1.11719006608026	15.61417568690277	11.63085157323622
N	4.58028434189834	11.11554739380505	8.03743736268766	C	0.24607830897107	15.93088217343551	11.50497939147486
N	2.45855187432403	9.67811897463392	12.59107228608072	H	0.54588988085648	16.95673035883723	11.31232613809663
N	4.86211443668629	13.46079919975196	14.71876230623777	C	-2.41427090410516	8.59722867025044	15.63085157323622
N	2.59522948844500	15.33129783900366	11.35001236652041	C	0.61544051501910	13.47024224917566	16.33055200529336
N	4.10769826402958	16.56906143484940	10.70925360325127	C	1.28479061317530	12.92692044496741	15.06890190200704
N	3.92999774509020	8.32569961030153	13.07840329904338	H	1.14835146789430	11.83794360088061	16.00395871716851
C	2.70186884492452	11.79815210778616	8.99510163973408	H	0.79828126338793	13.34853662277659	14.18719065257870
C	3.38776008259884	13.66064875641100	16.13910738551902	C	10.59361767224570	12.93640628684395	15.99469315029372
C	7.83714563403857	12.06665188043217	11.34950007355710	H	11.03928265837640	12.47296827065160	15.10665086802751
N	2.65266907602956	8.41209750793509	12.88658284243552	H	10.00994333537520	12.17045209252555	16.51966907562702
N	4.66222568041713	13.81091650255465	15.96997282397075	H	11.41601310764379	13.24354983594104	16.65212696194006
C	8.84342640683790	11.61423536684360	10.50597518309637	C	10.56549366878692	15.19609478218600	14.89437542674254
H	9.88302084001322	11.71252264269871	10.80752705987616	H	9.96379407221781	16.07263688380242	14.62423862098223
C	6.46578175026269	11.95709783801517	11.00743841065812	H	11.00534422368348	14.79139747939755	13.97516283990951
C	7.15450840608965	10.97144449207245	8.91748335476795	H	11.39142412245470	15.53686688816560	15.53098212318811
H	6.86976275519796	10.56825117216373	7.95005387048788	C	-2.15097011619954	16.73369475787392	11.53525146661774
C	8.51254309316974	11.03519718048232	9.27437217585067	C	-1.89588109597779	17.74093011453006	12.66862985232350
N	2.83505622897289	16.55896054876600	10.94609774129634	H	-1.98360907856982	17.26064189158912	13.65097614133069
C	6.13958158668260	11.43511377583375	9.74792304714987	H	-2.63128065248704	18.55327885386674	12.62323201617258
C	-0.50895570983445	11.87537071374086	12.12760841168220	H	-0.89949835898813	18.19357725092145	12.60030686380809
C	3.69749700273397	11.89027499643950	9.97486057188111	C	-3.58019151788669	16.20424336261195	11.66412790828956
C	6.49090968991492	12.87831339772521	12.99776965120289	H	-3.82885827296820	15.49383535372084	10.86581559925775
C	-0.47156130059209	13.30729549129600	11.93265088359571	H	-4.28899416632565	17.03665572718108	11.58948061378678
C	3.69324978877570	14.51025924280379	11.39457005066506	H	-3.75297231928473	15.71754596669896	12.63223026158886
C	0.90475218687337	13.63755289950556	11.84962225315848	C	9.20376293640432	14.77501500415512	16.93732906516744
C	7.85666647083273	12.69797198054391	12.64914924353157	H	8.62063000985633	14.06186372023856	17.53340031929414
C	4.70510893918873	15.36996708514280	10.95033559072481	H	8.58517595607651	15.66162708476029	17.9439057773987
C	9.56195291391238	10.49930402127744	8.30374064158574	H	10.05135798736740	15.09504424160288	17.55388275292442
C	-1.54611946739144	10.96543280961088	12.24930773272795	H	2.64274602915508	15.05422724151878	17.48786790412700
H	-2.57707153844486	11.31135831227459	12.19865703182712	H	4.43524398119325	14.54940272186049	16.21778244158529
C	0.85151811871149	11.46849858278950	12.17912847947244	H	-0.36914417137114	13.00377284829238	16.44473400648721
C	3.59295298162263	10.44916491624868	12.57034955064480	C	-1.91649509655684	7.17168897158132	12.77838876821668
C	3.73424923330446	13.08017129849735	14.03578513260372	H	-1.27942631529338	6.81124857161304	11.96106351091465
C	0.07374656788364	9.20818943546392	12.52274237828491	H	-2.77253299859673	6.49088928812695	12.84603247792381
H	0.32608921070561	8.16822719649543	12.69747972011908	H	-1.35903683560941	7.08747836439252	13.71974439285631
C	1.25214500496984	12.15759764816635	8.95454472102375	C	-3.20166635658858	8.62158730628424	11.21199452185313
H	1.16637217593626	13.25210626041734	9.0141454773469	H	-3.63000527913099	9.60967484240902	11.00598005353821
H	0.75213873385956	11.76367470835870	9.84155121188061	H	-4.03104850198387	7.90516881932900	11.25383136171334
C	2.74930457229172	13.21853025188731	15.02074263254638	C	-2.56005002906190	8.34687614197090	13.6656508901477
C	1.12730563222174	10.11725081130036	12.40937046273868	C	-3.33831744663491	8.99805620457695	13.69397037017560
C	4.57375382653755	9.51539768834841	12.92168608443647	H	-2.79790140577454	8.99623434772486	14.64851064304781
C	2.69349027949908	11.04533918747048	6.58123041328526	H	-4.16946940005075	8.28727319300309	13.77639863948528
H	2.50010690141935	9.96578355992470	6.53092777730777	H	-3.77411690375999	9.99399897041195	13.55302914352341
H	3.42825279852831	11.29440342225118	5.80982206524711	C	-2.01065795158841	14.473791476548287	10.176013459517734
C	6.19646634362072	13.41452098242356	14.25480880761715	H	-1.01974242981416	17.88780508241193	10.04361844720393
C	1.40639733271971	11.83783755434170	6.45579324717785	H	-2.74996321597187	18.24355149662057	10.09090124108874
H	0.87959223052601	11.5052441525945	5.55443156256407	H	-2.17894071192428	16.73772623122503	9.34863265534815
H	1.63563253055178	12.90376626228105	6.31411602254604	C	1.46942877410852	13.23104217226170	17.96797417882988
C	-1.26714462386839	9.59984119505647	12.43426269787496	H	1.65343521486021	12.15575716583514	17.70500307877314
C	8.88132387802125	13.09826996431201	13.49006087126742	H	0.96360649850437	13.58348806941932	18.47380151271651
H	9.91691767281668	12.94845990415079	13.18960724803754	C	9.29448879826707	9.00649495149484	8.05363143547772
C	0.55105722836996	11.63975206698542	7.69951107508210	H	9.36502515748960	8.43218467345036	8.98558156081481
H	0.32483935112165	10.56985090743913	7.81758643567432	H	10.03488491100069	8.60271931856955	7.35250399876457
H	-0.41313921188950	12.14803525918531	7.59039185674025	H	8.30200389183020	8.83162885027950	7.62170900806082
C	1.24939486539962	14.97196102260446	11.59513135562325	C	9.46364041898892	11.27323544290915	6.97922757716708
C	4.74605014073034	17.79609745465580	10.23884909832330	H	8.48292728283156	11.15707836622137	6.50284829730604
H	4.92304068128112	18.43619606427797	11.11302204160899	H	10.2175978243268	10.9069335853690	6.27196268107370
H	4.02892166643638	18.30357032450532	9.58675019284723	H	9.64000328618075	12.34474228322541	7.13408295552331
C	6.16076955064074	15.19514618566028	10.66323755208845	C	10.98137053916999	10.6550382829780	8.85291171862762
H	6.26437061771634	14.53659964865924	9.78882734871868	H	11.24497897762344	11.70677816666585	9.02052294174771
H	6.63808026556574	14.67427654535315	11.49566221222454	H	11.70086370985111	10.25331867076280	8.13055038039582
H	6.04990051017478	9.59032202542203	13.13413345953347	H	11.12260224907592	10.10497401974737	9.79173404482171
H	6.29203834543892	10.51042417673652	13.67359495637223				
H	6.54678557590778	9.66659066090989	12.15718579453027				
C	-1.46586392682559	14.27210108438060	11.82881243668041				
H	-2.50975039855995	13.97848376114193	11.90286182951129				
C	8.58389031597493	13.69454639734564	14.72817911304262				
C	6.87661416802351	16.52181771981182	10.41292015209349				
H	7.08585497353473	17.01603410675528	11.37306644254586				

155

[Cr(L^{MIC})₂]²⁺_t_PBE0.xyz

Cr	3.68670645430994	12.49198487393432	12.00005673418788
N	3.33620682493816	11.4507461181250	7.85941642238277
N	5.70420205630733</		

N	4.86876088930125	11.81897750121531	9.19283654003968	C	-1.17603944476965	15.40161747046630	10.88191455223168
N	1.66751858680841	12.53006567671805	11.99503290594683	C	0.18966995326390	15.71171509026823	10.74409504657805
N	4.63486438811502	11.54044536986568	7.91124938543091	H	0.49059754802370	16.67906070106449	13.35144134062689
N	2.44108754757903	9.77380599928345	12.90549012326859	C	-2.41034511765792	8.89298375147854	13.68711463329794
N	4.87763587668385	13.12166914956420	14.81897711183700	C	0.66764664408681	14.23847233175709	16.05468144014336
N	2.55216483472940	15.21661145173666	10.98388202527737	C	1.26988341016260	13.54617607091374	14.83578881532645
N	4.10591379418381	16.50863717394504	10.56401894673725	H	0.80896854303813	12.55771905215314	14.70237850071726
N	3.92248264683383	8.35307762375751	13.11760437769098	H	1.03466014469536	14.10586748125000	13.92599297822693
N	2.72961343184322	11.65324881325130	9.05505065299343	C	10.47815851428457	11.71431243017718	16.11670271567645
N	3.35923473916366	13.56939577722461	16.14173895813495	H	10.92327596638287	11.44926095343365	15.15041566298636
N	7.89982025206566	12.25301816802328	11.31259385537033	H	9.80392950456606	10.89885820376397	16.40704679734380
N	2.63308127769016	8.49679616355277	13.22572212308623	C	11.28821321200318	11.77016343488526	16.85656804410511
N	4.65125879133682	13.419887468691297	16.09488665328740	C	10.68538611957004	14.16558604897554	15.62885646131239
C	8.92017121972956	12.05392226135710	10.38044201204977	H	10.16482413264962	15.12973108536996	15.57300006127732
H	9.95618738832797	12.10061766746307	10.70832028627349	H	11.13341091675154	13.97256896427038	14.64712794338983
C	6.52507154221138	12.21085069930065	10.94673161289416	H	11.50291569843358	14.25950715528675	16.35655311917577
C	7.24002142586859	11.74336612692984	8.68964751743876	C	-2.21565199043434	16.43652621603532	10.44742047893006
H	6.95561882770623	11.53301208766257	7.6623782322383	C	-2.01468612531130	17.73603503310743	11.24183417992251
C	8.59994939239002	11.80193086657551	9.04713001673904	H	-2.13254091982064	17.55592745587881	12.3176550335043
N	2.80755804197165	16.43071415327253	10.50062372073987	H	-2.75093318589422	18.49261158119751	10.93833305713269
C	6.20630141646723	11.93243112132154	9.60349551287659	H	-1.01592970222169	18.15892976936498	11.08291676301475
C	-0.54182276632995	11.92673586860763	12.31414866218077	C	-3.64500873837771	15.94715333822268	10.8751752394574
C	3.74280574635497	11.92833596510989	9.99095501345793	H	-3.86287924725905	15.03278384324834	10.12149535276803
C	6.52428936917373	12.65003157315110	13.07827191079398	H	-4.36103250763206	16.71423087180660	10.36663921895963
C	-0.51588005670737	13.25537227439044	11.76752156925950	H	-3.82976289649817	15.74423890760706	11.74985145926857
C	3.66353451970495	14.48028543166854	11.35619786502818	C	9.18013675281092	13.37167931104212	17.43758221165421
C	0.86536261878095	13.56175447113038	11.60807783057014	H	8.50332386696049	12.59031345496113	17.80481675781097
C	7.90187595127954	12.52993644361361	12.72268891442168	H	8.64012341829678	14.3265719215746	14.3265719215746
C	4.69217605082300	15.39704389765600	11.07388784832740	H	10.01374454795284	13.4485826801794	18.14705747597115
C	9.65681008576674	11.58153732668588	7.96293691237094	H	2.93713900028102	15.01016487536379	17.57397914588183
C	-1.57122846519552	11.07959735056945	12.71515182156588	H	0.86835612934407	15.32006988885806	16.15155490432225
H	-2.60417106147824	11.41814265051014	12.63525213348833	H	-0.42229396386481	14.12229661580275	16.03505123765616
C	0.82861811953813	11.54034527963709	12.41095758936657	C	-1.89861324741659	7.52801748606985	14.15186091949051
C	3.58449396951385	10.48244062318058	12.58242593252775	H	-1.38023788459301	6.9935414347884	13.34597419363035
C	3.75333410583591	13.05844655493456	14.01579756378471	H	-2.74203410696673	6.90530274397034	14.47598273821366
C	0.06958606129200	9.41691824813733	13.28038499257272	H	-1.20870864128797	7.61921344971478	14.99991465398828
H	0.337762614447804	8.429736214447804	13.63986204075120	C	-3.39931239425539	8.66665481979296	12.53392462304511
C	1.24305310607163	11.56135932033391	9.15609861634506	H	-3.83586561728768	9.60865846223608	12.18229938392871
C	0.82823945770939	12.56967211771314	9.29309864502557	H	-4.22386497940186	8.01541174483518	12.85413927100101
H	0.97679832993404	11.00852015112567	10.06169185327324	H	-2.89970257274849	8.19186599714786	11.68029472082716
C	2.74926485512502	13.38618659612632	14.94437142873018	C	-3.14168831396297	9.55983013019800	14.86255133310955
C	1.11794288328728	10.24699024827886	12.87788253416423	H	-2.45588833548695	9.72148638839403	15.70360046823309
C	4.56538851899189	9.48709083256318	12.74362038195185	H	-3.97158151836515	8.93082711100497	15.2126917343329
C	2.70663207254647	11.11451612726539	6.59517438735373	H	-3.55508146007809	10.53482882403609	14.57854699073873
H	2.85540879570855	10.04067070346881	6.41479994212032	C	-2.04836018777649	16.72396975220501	8.94751371564041
H	3.23790119715752	11.66133243381957	5.80900423135453	H	-1.04717020199659	17.108550821008118	8.72001084976265
C	6.21221704063232	12.93846014863944	14.41751591775932	H	-2.78047066499490	17.47047397417716	8.61079845534557
C	1.22839297268297	11.45325496769888	6.64692083055675	H	-2.19543899431391	15.81001936869044	8.35840123974233
H	0.74113990433198	11.03721471736004	5.75663695121783	C	1.24769673466572	13.67289700619415	13.67289700619415
H	1.09520284907763	12.54420702191616	6.60676554335948	H	1.06325603415049	12.58974668642793	17.39231656352909
C	-1.27609286157821	9.80886290354102	13.21906281657495	H	0.77649182253168	14.11833826455679	12.2889228846919
C	8.91624599435658	12.6639918355319	13.66722058138367	C	9.47216203908858	10.18858350328259	7.34136017343334
H	9.95498279719767	12.55525304693387	13.35536970989291	H	9.58117668221935	9.40587407724237	8.10251266571940
C	0.61643742843965	10.90549933504034	7.92934282089733	H	10.22097858925634	10.01129278121203	6.55743882271513
H	0.76793929394473	9.81562932020305	7.965688542336342	H	8.48025844662275	10.07631938092191	6.88831414790740
H	-0.46728273476888	11.07041906826687	7.94415386717389	C	9.49680175010934	12.65238411560504	6.87293544110946
C	1.20720164445489	14.83067269658764	11.10208479062237	H	8.50587274828291	12.60750607564724	6.40604484608621
C	4.75532410001556	17.73834702895916	10.14609460622513	H	10.24733711423211	12.51819483264653	6.08208427587190
H	4.59908279821781	18.48988070918559	10.93255945648186	H	9.62018035740027	13.65727834133252	7.29585548324975
H	4.24327113332338	18.08881770567285	9.24373207159578	C	11.07755294673064	11.67215335869803	8.52229666442034
C	6.17657990305854	15.34682592481500	11.22191320722671	H	11.28040961679907	12.65872563194550	8.95755117613634
H	6.59304168505370	14.67674182359078	10.45704520604245	H	11.80630587843920	11.50761561291527	7.71856699554893
H	6.42931666209274	14.89004403549878	12.18309059010999	H	11.25842017770898	10.91366645661209	9.29423610559119
C	6.04159155086793	9.46206185651162	12.52120737817411	155			
H	6.49646985631603	10.34015045703293	12.98527950945193				
H	6.23674409693211	9.56111619667880	11.44378207269111				
C	-1.51924871784502	14.15787825432415	11.41054431485421	[Cr(L ^{MIC}) ₂] ²⁺ _t_r2SCAN3c.xyz			
H	-2.56081202054494	13.87561542773901	11.54611809351125	Cr	3.67626406637430	12.48924171527703	11.98881893774395
C	8.59879136265683	12.92804092959099	15.00297919340061	N	3.36881985115031	11.28360207452356	7.84480067634700
C	6.81760685306974	16.72594229129021	11.10154229726893	N	5.65636542310861	12.43191105366881	11.99394708208315
H	6.65100422091462	17.30132859606631	12.02517030000156	N	4.82942354664021	11.33646515388155	9.31476280203576
H	7.90280169945637	16.61310469117523	10.99467228575988	N	1.69853899799408	12.53232224360154	11.98452521747534
C	7.24589409198006	13.06641654908534	15.34726675255899	N	4.62356733010206	10.96837647563103	8.04962921603004
H	6.95904725712966	13.28663816786322	16.36940552867625	N	2.43742026508961	9.64843804534785	12.42560534388359
C	6.33588213065577	17.49269940312569	9.92143251056676	N	4.88477111728673	13.57663139307596	14.66637076997828
H	6.28184505240660	16.91644905437808	8.99616144992003	N	2.56600853132621	15.3712146700475	11.67833357031890
H	6.73504457770846	18.45911880466776	9.78050644243656	N	4.05749673714273	16.61926889475955	10.76049558766216
C	4.51455222823776	7.06040570213077	13.40985736284419	N	3.90348975595832	8.30117099382620	13.00469815152509
H	3.81121187771301	6.29556124557035	13.06501334382843	C	2.78850529300647	11.84347081047629	8.93523899512222
H	4.60895708848925	6.96257591946576	14.50050351653353	N	3.42718673495971	13.69969640372651	16.13528905394151
C	9.71694033526546	13.04736439000885	16.04190486321042	C	7.84874371595952	12.00513846095791	11.37492095767133
C	2.37993464842646	13.94306698168633	17.40098126534157	N	2.63029764175633	8.35726886996069	12.69941921662465
H	3.24187182321018	13.37808041965399	18.19344564857032	N	4.69634429904056	13.95135378494593	15.93246914656129
C	5.87260415304402	6.95721856207417	12.74120184728405	C	8.85553040988509	11.47286244942911	10.58212266953341
H	6.36805678493905	6.04185475942492	13.08727304156834	H	9.89098178474345	11.58497109759975	10.88343814092370
H	5.74361466688137	6.86256216940405	11.65298723174291	C	6.47989241923428	11.87531237997140	11.03274808869115
C	6.69905749685591	8.19517281555757	13.06202087805369	H	7.17248591915827	10.72805148235178	9.0

C	4.73934009374368	17.79598184652382	10.09434935920653	H	10.40942725256327	11.41704006722592	6.19081186590089
H	4.73867485249191	18.51037205157490	10.92991271694768	H	9.79786954116113	12.79175397143065	7.14253815989019
H	4.11058724582063	18.20129640954893	9.29348350255731	C	11.14198819481591	11.02061593930308	8.77410404676280
C	6.20939732833839	15.29677530928251	10.89801188519582	H	11.37061821017344	12.06541827216552	9.02861403509451
H	6.47942276187592	14.62521400628013	10.06815310050207	H	11.88246032397619	10.69188458675155	8.03201996347022
H	6.58021388882529	14.82115981846906	11.81175693806336	H	11.28015034888710	10.40464201095746	9.67410622467076
C	6.06041626778930	9.42885176339910	12.70386063482099				
H	6.42649413153623	10.31925922531675	13.22684408993619				
H	6.40473595612914	9.51752679406426	11.66173270480047				
C	-1.52293465249454	14.25668958559890	11.61799708457471				
H	-2.56639008324780	13.96746182709334	11.74558820897274				
C	8.58441160714086	13.43500654415969	14.88640090875742				
C	6.88059310984060	16.66314072355397	10.70662178578817				
H	6.87534757616386	17.21901437519895	11.65862961606576				
H	7.73397837563051	16.51292997046990	10.43638872765617				
C	2.22165360973942	13.53034173391153	15.22994771521710				
H	6.93144081891707	13.86755690171629	16.22146312002772				
C	6.16029537170826	17.48823572456451	9.63780106156378				
H	6.13541684532126	16.93551365895769	8.68532060335853				
H	6.67886358077458	18.43690361003959	9.44611021534448				
C	4.46368091160160	6.94203134427412	13.27225599824622				
H	3.84669510191828	6.19146259690917	12.76522810335076				
H	4.37653950848920	6.78507209212662	14.35675454713274				
C	9.70636310585245	13.83649930696924	15.85963201038080				
C	2.70119152144357	13.78527699488437	17.45623413782600				
H	3.35661364981575	13.36256809041674	18.22597625073735				
C	5.92154602443990	6.91106633287635	12.82879677657401				
H	6.38408697958160	5.99309206048231	13.21468802358675				
H	5.97673261217259	6.86372469384688	11.72953147640302				
C	6.64661570164871	8.15986370674787	13.33608827198455				
H	7.71894910822009	8.10503466125360	8.10741067398371				
H	6.56019375685053	8.21101282312419	14.43399155976503				
C	-1.17783241877860	15.56746400166158	11.29142046053599				
C	0.19409541994287	15.87006466101366	11.13751091150388				
H	0.49695009621546	16.88294446133832	10.87706117111792				
C	-2.48601352032293	8.75896438711417	13.24532133767834				
C	0.53487782534168	13.62098026042829	16.22248904520495				
C	1.19533224674391	13.05511542107625	14.95836998490212				
H	0.094527221866599	11.98779055645349	14.85266271299322				
H	0.79496988477576	13.55526848892812	14.07072228507915				
C	10.64042047498845	12.63253587922683	16.09522472379239				
H	11.10119116502133	12.28404285926710	15.16094928680224				
H	10.08954589976352	11.78891084441327	16.53499387031031				
H	11.45228286343463	12.90712418476584	16.78422556343099				
C	10.51049450261623	14.99933188985074	15.24162634129672				
H	9.86187090629987	15.86762343066237	15.05659204300772				
H	10.96910313825450	14.71216664504063	14.28547349437101				
H	11.31795218386484	15.31261832292396	15.91938409814792				
C	-2.20892617551352	16.69495794008427	11.12093328628748				
C	-1.96153183374170	17.76451831089681	12.20525537513912				
H	-2.04936137598992	17.32664259258827	13.20994494413449				
H	-2.69704744216266	18.57755183291163	12.11985477576818				
H	-0.96020632067548	18.20883699339445	12.11792424073687				
C	-3.64909138411746	16.17883894752253	11.26660872936889				
H	-3.88309231930002	15.41041663995344	10.51598928134810				
H	-4.35543209060571	17.00813332749910	11.12313893122660				
H	-3.83309678121357	15.75761671030813	12.26527015794899				
C	9.15740315637079	14.29466736812657	17.22015419951885				
H	8.58521885313407	13.49845913274411	17.71771525980957				
H	8.51177646018654	15.17931278320856	17.12382916549500				
H	9.99129666213457	14.56528985582482	17.88227895821723				
H	2.67610570295800	14.87670522385865	17.58529815144029				
H	0.50508837670361	14.72170314155588	16.16955723481191				
H	-0.50783767610929	13.28001479085355	16.26630157018899				
C	-1.98518961475083	7.36148520892166	13.64339637002406				
H	-1.44699197557373	6.87072118339072	12.81981314133702				
H	-2.84066185432197	6.72347848903994	13.90454263316964				
H	-1.32158176766848	7.39956605891176	14.51926025375993				
C	-3.44278939388686	8.60862015671707	12.04551231854602				
H	-3.86455058675482	9.57513809152001	11.73760667716192				
H	-4.28143687946228	7.94579164035974	12.30372819096683				
H	-2.92030933341625	8.17754890022290	11.17958464283040				
C	-3.25106419540777	9.35903385917382	14.44314614955299				
H	-2.58418433291731	9.48489514749401	15.30839747745318				
H	-4.07846205018026	8.69887706840051	14.74146788491392				
H	-3.67904441862587	10.34159775035458	14.20180543431355				
C	-2.06286257635133	17.33078644183026	9.72329042438809				
H	-1.06504409772678	17.76448500468325	9.57102183945742				
H	-2.79780162873831	18.13808680780105	9.59205424602934				
H	-2.23157147922101	16.58434945153007	8.93399060657339				
C	1.29511128950834	13.19770864567882	17.48140060957378				
H	1.35069024168164	12.09892816668113	17.53917347596458				
H	0.78759430929669	13.54339669729045	18.39159254452590				
C	9.49664010604243	9.38897576520213	7.84222452839595				
H	9.55835565273209	8.76205881801602	8.74349419019227				
H	10.25774709268113	9.03938777557180	7.12976032820725				
H	8.51094238468532	9.22694295377569	7.38437155931294				
C	9.64018208011690	11.72830309162266	6.91220783247667				
H	8.66333851388714	11.63032982421943	6.41879969266958				

12. References

- [1] M. Moser, B. Wucher, D. Kunz, F. Rominger, *Organometallics* **2007**, *26*, 1024.
- [2] P. Pinter, C. M. Schüßlbauer, F. A. Watt, N. Dickmann, R. Herbst-Irmer, B. Morgenstern, A. Grünwald, T. Ullrich, M. Zimmer, S. Hohloch et al., *Chem. Sci.* **2021**, *12*, 7401.
- [3] B. Wittwer, N. Dickmann, S. Berg, D. Leitner, L. Tesi, D. Hunger, R. Gratzl, J. van Slageren, N. I. Neuman, D. Munz et al., *Chem. Commun.* **2022**, *58*, 6096.
- [4] N. Sinha, J.-R. Jiménez, B. Pfund, A. Prescimone, C. Piguet, O. S. Wenger, *Angew. Chem. Int. Ed.* **2021**, *60*, 23722.
- [5] H. E. Gottlieb, V. Kotlyar, A. Nudelman, *J. Org. Chem.* **1997**, *62*, 7512.
- [6] S. Stoll, A. Schweiger, *J. Mag. Res.* **2006**, *178*, 42.
- [7] G. M. Sheldrick, *Acta Cryst A* **2015**, *71*, 3.
- [8] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J Appl Crystallogr* **2009**, *42*, 339.
- [9] G. M. Sheldrick, *Acta Cryst. C* **2015**, *71*, 3.
- [10] A. L. Spek, *Acta Cryst. C* **2015**, *71*, 9.
- [11] D. Rehm, A. Weller, *Isr. J. Chem.* **1970**, *8*, 259.
- [12] D. P. Hari, P. Schroll, B. König, *J. Am. Chem. Soc.* **2012**, *134*, 2958.
- [13] A. Ripak, S. de Kreijger, R. N. Sampaio, C. A. Vincent, É. Cauët, I. Jabin, U. K. Tambar, B. Elias, L. Troian-Gautier, *Chem. Catal.* **2023**, *3*.
- [14] J. Yu, L. Zhang, G. Yan, *Adv. Synth. Catal.* **2012**, *354*, 2625.
- [15] F. Neese, *WIREs Comput Mol Sci* **2012**, *2*, 73.
- [16] F. Neese, *WIREs Comput Mol Sci* **2018**, *8*.
- [17] S. Grimme, A. Hansen, S. Ehlert, J.-M. Mewes, *J. Chem. Phys.* **2021**, *154*, 64103.
- [18] C. van Wüllen, *J. Chem. Phys.* **1998**, *109*, 392.
- [19] C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158.
- [20] E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth, S. Grimme, *J. Chem. Phys.* **2019**, *150*, 154122.
- [21] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
- [22] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.
- [23] T. Yanai, D. P. Tew, N. C. Handy, *Chem. Phys. Lett.* **2004**, *393*, 51.
- [24] F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, *356*, 98.
- [25] R. Izsák, F. Neese, *J. Chem. Phys.* **2011**, *135*, 144105.
- [26] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057.
- [27] D. A. Pantazis, X.-Y. Chen, C. R. Landis, F. Neese, *J. Chem. Theory. Comput.* **2008**, *4*, 908.
- [28] G. L. Stoychev, A. A. Auer, F. Neese, *J. Chem. Theory. Comput.* **2017**, *13*, 554.
- [29] G. Knizia, *J. Chem. Theory. Comput.* **2013**, *9*, 4834.
- [30] V. N. Staroverov, G. E. Scuseria, J. Tao, J. P. Perdew, *J. Chem. Phys.* **2003**, *119*, 12129.
- [31] V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995.
- [32] C. Angeli, R. Cimraglia, S. Evangelisti, T. Leininger, J.-P. Malrieu, *J. Chem. Phys.* **2001**, *114*, 10252.
- [33] S. K. Singh, J. Eng, M. Atanasov, F. Neese, *Coord. Chem. Rev.* **2017**, *344*, 2.
- [34] Chemcraft - graphical software for visualization of quantum chemistry computations. Version 1.8, build 654. <https://www.chemcraftprog.com>.
- [35] M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeersch, E. Zurek, G. R. Hutchison, *J. Cheminform.* **2012**, *4*, 17.

13. Author Contributions

Synthesis was carried out by PY, BW and AS. PY conducted spectroscopic investigations and analysis, photocatalysis experiments. Electrochemical investigations were carried out by PY and FRN. EPR spectroscopic investigations and simulations were carried out by DL. Theoretical investigations were performed by DM. Crystal structure solution and analysis was performed by FT and SH. The idea was conceived by SH and OSW. The manuscript was written by PY, BW, DM, OSW and SH and proof read by all authors.