Supporting Information

d–d Dative Bonding Between Iron and the Alkaline-Earth Metals Calcium, Strontium, and Barium

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Supporting Information:

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1. Supporting Experimental Data

1.1. General Experimental Procedures

All experiments were conducted under an inert nitrogen atmosphere using standard Schlenk and glovebox techniques (MBraun, Labmaster SP). Toluene, n-hexane and benzene were degassed with nitrogen, dried over activated aluminium oxide (Solvent Purification System: Pure Solv 400−4−MD, Innovative Technology) and stored over 3Å molecular sieves under N₂. THF was refluxed over a sodium mirror, distilled under N₂ and stored over 3Å molecular sieves under N₂. Benzene-d₆ (99.6% D, Sigma Aldrich), THF-d₈ (99.6% D, Sigma Aldrich) and pyridine-d₅ (99.5% D, Sigma Aldrich) were dried over 3Å molecular sieves and stored under N₂. 1-H₂ was synthesized starting from ferrocene-1,1-diamine according to the protocol of Siemeling et al. Ferrocene-1,1-diamine was synthesized starting from cyclopentadiene according to the protocol of Tamm et al. The dimeric amides Ca[N(SiMe₃)₂]₂, Sr[N(SiMe₃)₂]₂ and Ba[N(SiMe₃)₂]₂ were synthesized according to literature procedures of Westerhausen. Mg(nBu)₂ (1.0 M in heptane) was purchased by Sigma Aldrich and used without further purification. NMR spectra were recorded with a Bruker Avance III HD 400 MHz or a Bruker Avance III HD 600 MHz spectrometer. The spectra were referenced to the respective residual signals of the deuterated solvents. Elemental analysis was performed with an Hekatech Eurovector EA3000 analyzer.

1.2. Synthesis

Synthesis of 1-Mg:

1-H₂ (110 mg, 0.309 mmol) was dissolved in THF (3 mL) and cooled to -78°C. A solution of Mg(nBu)₂ (0.280 mL, 1.0 M in heptane) was added drop wise via syringe and the reaction was slowly warmed to room temperature while the orange solution turned red. The red solution was stirred for 1 h at room temperature and filtered over celite. The solvent volume was reduced to approximately 0.5 mL under reduced pressure and n-hexane (2 mL) was added. A red-orange precipitate formed and THF (approximately 0.1 mL) was added until the precipitate almost completely redissolved. The slightly turbid
solution was filtered over celite and stored at -30°C for 2 days. Large red-orange plate shaped crystals formed and were isolated by decantation. The crystals were suitable for X-ray diffraction. Subsequent washing with n-hexane (2x 0.5 mL) and drying in vacuum gave 80 mg of red-orange crystals. The mother liquor was evaporated and the leftover solid was suspended in n-hexane (1 mL). THF (approximately 0.3 mL) was added until the precipitate almost completely redissolved. The suspension was filtered over celite. Prolonged storage at -30°C furnished a second batch of crystals. Decantation, washing with n-hexane (2x 0.5 mL) and drying in vacuum gave an additional 50 mg of red-orange crystals. Yield: 120 mg, 0.230 mmol 74%. ¹H NMR (600 MHz, C₆D₆ + THF-d₈, 25°C): δ 3.96 (s, 2H, CH), 3.86 (s, 2H, CH), 3.56 (m, CH₂, β-THF), 3.04 (s, 2H, CH₂), 1.45 (m, CH₂, α-THF), 0.99 (s, 9H, CH₃) ppm. ¹³C{¹H} APT NMR (151 MHz, C₆D₆ + THF-d₈, 25°C): δ 124.1 (CN), 67.9 (CH₂, β-THF), 67.1 (CH₂, β-THF-d₈), 66.2 (CH₂), 61.8 (CH), 60.4 (CH), 36.1 (C(CH₃)₃), 28.8 (CH₃), 25.8 (CH₂, α-THF) 24.8 (CH₂, α-THF-d₈), ppm. Anal. Calcd. for C₂₈H₄₆FeMgN₂O₂ (MW = 522.84 g/mol): C, 64.32; H, 8.87; N, 5.36. Found: C, 63.91; H, 8.62; N, 5.40.

**Synthesis of 1-Ca:**

A 10 mL glass ampoule was charged with a solution of Ca[N(SiMe₃)₂]₂ (55 mg, 0.152 mmol) in THF (4 mL) and a solution of 1-H₂ (50 mg, 0.140 mmol) in THF (4 mL) was added. Subsequently the ampoule was frozen in liquid nitrogen and vacuum sealed. After warming to room temperature the ampoule was placed in a pre-heated oil bath at 125°C for 2 days which led to conversion of the orange solution to a red solution. Subsequently the oil bath was slowly cooled to room temperature and large bright red crystals formed. To complete crystallization the ampoule was stored at room temperature for one week. The crystals were isolated by decantation, washed with THF (3x 0.5 mL) and dried under vacuum. 25 mg of bright red crystals suitable for X-ray diffraction were obtained. The mother liquor was dried under reduced pressure and the resulting powder was transferred in a 10 mL glass ampoule, suspended in THF (8 mL) and placed into a pre heated oil bath at 125°C until all solid had dissolved. Subsequently the oil bath was slowly cooled to room temperature and the ampoule was stored at room temperature for prolonged time (about
1 month) forming a second crop of crystals. Subsequently the crystals were isolated by
decantation, washed with THF (3x 0.5 mL) and dried under vacuum. An additional 8 mg of
bright red crystals were obtained. Yield: 32 mg, 0.069 mmol, 49 %. ¹H NMR (600 MHz,
pyridine-ᵈSBATCH, 100°C): δ 3.98 (s, 2H, CH), 3.83 (s, 2H, CH), 3.66 (CH₂, β-THF), 3.14 (s, 2H,
CH₂), 1.62 (CH₂, α-THF), 1.16 (s, 9H, CH₃) ppm. ¹³C{¹H} APT NMR (151 MHz, Pyridine-
ᵈSBATCH, 100°C): δ 112.0 (CN), 67.5 (CH₂, β-THF), 62.8 (CH), 59.7 (CH₂), 55.9 (CH), 31.0
(C(CH₃)₃), 27.4 (CH₃), 25.5 (CH₂, α-THF) ppm. Anal. Calcd. for C₄₈H₇₆Ca₂Fe₂N₄O₂
(MW = 933.00 g/mol): C, 61.79; H, 8.21; N, 6.01; Found: C, 61.57; H, 8.49; N, 6.09. Note:
NMR spectra were recorded in pyridine at 100°C due to the poor solubility of the
compound.

Synthesis of 1-Sr:

A 10 mL glass ampoule was charged with a solution of Sr[N(SiMe₃)₂]₂ (100 mg,
0.245 mmol) in THF (4 mL) and a solution of 1-Hz (70 mg, 0.196 mmol) in THF (4 mL) was
added. Subsequently the ampoule was frozen in liquid nitrogen and vacuum sealed. After
warming to room temperature the ampoule was placed in a pre-heated oil bath at 125°C
for 1 day which led to formation of a red solution in which small red crystals started to
form. Subsequently the oil bath was slowly cooled to room temperature and large bright
red crystals formed. To complete crystallization the ampoule was stored at room
temperature for one week. The crystals were isolated by decantation, washed with THF
(3x 0.5 mL) and dried under vacuum. 60 mg of bright red crystals suitable for X-ray
crystallography were obtained. The mother liquor was dried under reduced pressure and
the resulting powder was transferred in a 10 mL glass ampoule, suspended in THF (8 mL)
and placed into a pre heated oil bath at 125°C until all solid had dissolved. Subsequently
the oil bath was slowly cooled to room temperature and the ampoule was stored at room
temperature for prolonged time (about 2 weeks) forming a second crop of crystals.
Subsequently the crystals were isolated by decantation, washed with THF (3x 0.5 mL)
and dried under vacuum. An additional 10 mg of bright red crystals were obtained. Yield:
70 mg, 0.136 mmol, 69 %. ¹H NMR (600 MHz, Pyridine-ᵈSBATCH, 100°C): δ 4.11 (s, 2H, CH),
3.73 (s, 13H, CH₂, β-THF, + s, 2H, CH), 3.12 (s, 2H, CH₂), 1.74 (s, 13H, CH₂, α-THF), 1.18
(s, 9H, CH₃) ppm. \(^{13}\)C\(^{1}\)H NMR (151 MHz, Pyridine-\(d_5\), 100°C): \(\delta\) 112.9 (CN), 68.3 (CH₂, \(\beta\)-THF), 63.7 (CH), 60.6 (CH₂), 56.8 (CH), 31.9 (C(CH₃)₃), 28.2 (CH₃), 26.3 (CH₂, \(\alpha\)-THF) ppm. Anal. Calcd. for C₄₈H₇₆Sr₂Fe₂N₄O₂ (MW = 1028.10 g/mol): C, 56.08; H, 7.45; N, 5.45; Found: C, 55.63; H, 7.40; N, 5.79. Note: NMR spectra were recorded in pyridine at 100°C due to the poor solubility of the compound.

**Synthesis of 1-Ba:**

A 10 mL glass ampoule was charged with a solution of Ba[N(SiMe₃)₂]₂(THF)₂ (100 mg, 0.166 mmol) in THF (4 mL) and a solution of 1-H₂ (50 mg, 0.140 mmol) in THF (4 mL) was added. Subsequently the ampoule was frozen in liquid nitrogen and vacuum sealed. After warming to room temperature the ampoule was placed in a pre-heated oil bath at 125°C for 2 days which led to formation of a red solution in which small red crystals started to form. Subsequently the oil bath was slowly cooled to room temperature and large bright red crystals formed. To complete crystallization the ampoule was stored at room temperature for one week. The crystals were isolated by decantation, washed with THF (3x 0.5 mL) and dried under vacuum. 47 mg of bright red crystals suitable for X-ray crystallography were obtained. The mother liquor was dried under reduced pressure and the resulting powder was transferred in a 10 mL glass ampule, suspended in THF (8 mL) and placed into a pre heated oil bath at 125°C until all solid had dissolved. Subsequently the oil bath was slowly cooled to room temperature and the ampoule was stored at room temperature for prolonged time (about 2 months) forming a second crop of crystals. Subsequently the crystals were isolated by decantation, washed with THF (3x 0.5 mL) and dried under vacuum. An additional 11 mg of bright red crystals were obtained. Yield: 58 mg, 0.091 mmol, 65 %. \(^1\)H NMR (600 MHz, pyridine-\(d_5\), 100°C): \(\delta\) 4.15 (s, 2H, CH), 3.75 (s, CH₂, \(\beta\)-THF), 3.60 (br s, 2H, CH), 2.99 (s, 2H, CH₂), 1.76 (s, CH₂, \(\alpha\)-THF), 1.19 (s, 9H, CH₃) ppm. \(^{13}\)C\(^{1}\)H NMR (151 MHz, pyridine-\(d_5\), 100°C): \(\delta\) 113.1 (CN), 68.3 (CH₂, \(\beta\)-THF), 67.5 (CH₂, \(\beta\)-THF-\(d_2\)), 65.8 (CH₂), 63.5 (CH₂) 51.2 (CH), 34.7 (C(CH₃)₃), 30.0 (CH₃), 26.3 (CH₂, \(\alpha\)-THF) 25.3 (CH₂, \(\alpha\)-THF-\(d_2\)) ppm. Anal. Calcd. for C₄₈H₇₆Ba₂Fe₂N₄O₂ (MW = 1271.72 g/mol): C, 52.89; H, 7.29; N, 4.41; Found: C, 52.58; H, 7.19, N, 4.46. Note: NMR spectra were recorded in pyridine at 100°C due to the poor solubility of the
compound. THF-\textit{d}_8 was observed in the $^{13}$C-NMR, which was found to be an impurity in the batch of pyridine-\textit{d}_5 used for the $^{13}$C-NMR sample.

**Synthesis of 1-Eu:**

1-H$_2$ (50 mg, 0.140 mmol) and KN(SiMe$_3$)$_2$ (56 mg, 0.281 mmol) were dissolved in THF (2 mL) and stirred over night at room temperature. The solvent was removed under reduced pressure and the resulting residue was dried until a free flowing red powder was obtained. Subsequently the crude 1-K$_2$ was redissolved in THF (10 mL), EuI$_2$ (68.2 mg, 0.168 mmol) was added and the reaction was stirred for 3 days. The precipitated KI was removed by centrifugation and filtration. The Eu complex is clearly better soluble than the corresponding Sr complex. Dark red crystals suitable for X-ray diffraction were grown from the resulting clear solution by slowly evaporating of the solvent. The crystals were isolated by decantation, washed with \textit{n}-hexane (3x 0.5 mL) and dried in vacuum yielding 40 mg of red-orange crystals. Yield: 40 mg; 0.069 mmol 49 %. Anal. Calcd. for C$_{48}$H$_{76}$Eu$_2$Fe$_2$N$_4$O$_2$ (MW = 1156.78 g/mol): C, 49.84; H, 6.62; N, 4.84; Found: C, 49.54; H, 7.08; N, 4.52; Note: NMR spectra could not be recorded due to the paramagnetism of this compound.
1.3. NMR spectra of synthesized compounds

**Figure S1:** $^1$H NMR spectrum of 1-Mg in C$_6$D$_6$ + THF-$d_8$ at 25°C.
Figure S2: $^1$H-$^1$H COSY spectrum of 1-Mg in C$_6$D$_6$ + THF-$d_8$ at 25°C.
Figure S3: $^{13}$C APT NMR spectrum of 1-Mg in C$_6$D$_6$ + THF-$d_8$ at 25°C.
Figure S4: $^1$H NMR spectrum of 1-Ca in pyridine-$d_5$ at 100°C.
Figure S5: $^1$H-$^1$H COSY spectrum of 1-Ca in pyridine-$d_5$ at 100°C.
Figure S6: $^{13}$C APT NMR spectrum of 1-Ca in pyridine-$d_5$ at 100°C.
Figure S7: $^{13}$C NMR spectrum of 1-Ca in pyridine-δ$_5$ at 100°C.
Figure S8: Selective TOCSY NMR spectrum of 1-Ca isolating the cyclopentadiene spin system in pyridine-$d_5$ at 60°C.
Figure S9: $^1$H NMR spectrum of 1-Sr in pyridine-$d_5$ at 100°C.
Figure S10: $^1$H-$^1$H COSY spectrum of 1-Sr in pyridine-$d_5$ at 100°C.
Figure S11: $^{13}$C NMR spectrum of 1-Sr in pyridine-$d_5$ at 100°C.
Figure S12: Selective TOCSY NMR spectrum of 1-Sr isolating the cyclopentadiene spin system in pyridine-$d_5$ at 80°C.
Figure S13: $^1$H NMR spectrum of 1-Ba in pyridine-$d_5$ at 100°C.
Figure S14: $^1$H-$^1$H COSY spectrum of 1-Ba in pyridine-$d_5$ at 100°C.
Figure S15: $^{13}$C NMR spectrum of 1-Ba in pyridine-$d_5$ at 100°C.
Figure S16: Selective TOCSY NMR spectrum of 1-Ba isolating the cyclopentadiene spin system in pyridine-$d_5$ at 100°C.
1.4 Single Crystal X-Ray Diffraction

General experimental information

Crystals were embedded in inert perfluropolyalkyl ether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal under investigation was then flash cooled to 100 K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structures were measured on a SuperNova Dual source diffractometer (Cu at home/near) with Atlas S2 detector using either a CuKα microfocus source (1-Mg, 1-Ca, 1-Sr) or a MoKα microfocus source (1-H₂, 1-Eu, 1-Ba). The measured data was processed with the CrysAlisPro software package. Using Olex2, the structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms (if not otherwise stated below) were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

Crystals of compound 1-H₂ were found to be twinned (racemic twinning) and in addition, the compound is heavily disordered. The fractional contributions of the two twin domains were refined to 0.51(2) and 0.49(2). The disorder was modeled with the help of similarity restraints (SADI) and rigid bond restraints (RIGU). The relative occupancies of the two alternative orientations of the molecule were refined to 0.521(5) and 0.479(5). The positions of the amine hydrogen atoms were observed from difference Fourier maps and refined with restraints (SADI).

In case of 1-Ca, the hydrogen atoms H16A and H16B of the CH₂ group adjacent to N2 were observed from difference Fourier maps and refined. The same applies to 1-Sr.

The THF ligands of compound 1-Ba are disordered. The disorder was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU). The relative occupancies of the two alternative orientations were refined to 0.870(4)/0.130(4) (THF1) and 0.612(14)/0.388(14) (THF2), respectively.
Crystallographic Data has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1996024 for 1-H₂, CCDC 1996025 for 1-Mg, CCDC 1996026 for 1-Ca, CCDC 1996027 for 1-Sr, CCDC 1996028 for 1-Eu and CCDC 1996029 for 1-Ba. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
Table S1: Crystal data and structure refinement for 1-H₂.

| **Identification code**   | hasj190902a          |
|---------------------------|-----------------------|
| **Empirical formula**     | C₂₀H₃₂FeN₂            |
| **Formula weight**        | 356.32                |
| **Temperature/K**         | 100.0(2)              |
| **Crystal system**        | orthorhombic          |
| **Space group**           | C₂₂₂₁                 |
| **a/Å**                   | 6.96288(18)           |
| **b/Å**                   | 9.9016(2)             |
| **c/Å**                   | 27.3847(7)            |
| **α/°**                   | 90                    |
| **β/°**                   | 90                    |
| **γ/°**                   | 90                    |
| **Volume/Å³**             | 1888.00(8)            |
| **Z**                     | 4                     |
| **ρ calc/g/cm³**          | 1.254                 |
| **μ/mm⁻¹**                | 0.801                 |
| **F(000)**                | 768.0                 |
| **Crystal size/mm³**      | 0.487 × 0.182 × 0.07  |
| **Radiation**             | Mo Kα (λ = 0.71073)   |
| **2Θ range for data collection/°** | 7.154 to 59.524 |
| **Index ranges**          | -9 ≤ h ≤ 9, -13 ≤ k ≤ 13, -38 ≤ l ≤ 37 |
| **Reflections collected** | 24928                 |
| **Independent reflections** | 2528 [R_{int} = 0.0353, R_{sigma} = 0.0199] |
| **Data/restraints/parameters** | 2528/83/218          |
| **Goodness-of-fit on F²** | 1.133                 |
| **Final R indexes [I>=2σ (I)]** | R₁ = 0.0228, wR₂ = 0.0525 |
| **Final R indexes [all data]** | R₁ = 0.0245, wR₂ = 0.0533 |
| **Largest diff. peak/hole / e Å⁻³** | 0.28/-0.22            |
Figure S17: Crystal structure of 1-H2 (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms and disorder are omitted for clarity.
Table S2: Crystal data and structure refinement for 1-Mg.

| Identification code       | hasj181122a          |
|---------------------------|----------------------|
| Empirical formula         | C_{28}H_{46}FeMgN_{2}O_{2} |
| Formula weight            | 522.83               |
| Temperature/K             | 100.00(10)           |
| Crystal system            | monoclinic           |
| Space group               | P2_{1}/n             |
| a/Å                       | 11.31510(10)         |
| b/Å                       | 17.8811(2)           |
| c/Å                       | 13.8000(2)           |
| α/°                       | 90                   |
| β/°                       | 98.2170(10)          |
| γ/°                       | 90                   |
| Volume/Å³                 | 2763.44(6)           |
| Z                         | 4                    |
| ρ calcg/cm³               | 1.257                |
| μ/mm⁻¹                    | 4.793                |
| F(000)                    | 1128.0               |
| Crystal size/mm³          | 0.1907 × 0.1246 × 0.0998 |
| Radiation                 | CuKα (λ = 1.54184)   |
| 2Θ range for data collection/° | 8.146 to 145.264     |
| Index ranges              | -13 ≤ h ≤ 13, -21 ≤ k ≤ 21, -17 ≤ l ≤ 16 |
| Reflections collected     | 21206                |
| Independent reflections   | 5375 [R_{int} = 0.0362, R_{sigma} = 0.0325] |
| Data/restraints/parameters| 5375/0/314           |
| Goodness-of-fit on F²     | 1.040                |
| Final R indexes [I>=2σ (I)] | R₁ = 0.0300, wR₂ = 0.0696 |
| Final R indexes [all data]| R₁ = 0.0354, wR₂ = 0.0714 |
| Largest diff. peak/hole / e Å⁻³ | 0.31/-0.2            |
**Figure S18**: Crystal structure of 1-Mg (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms are omitted for clarity.
Table S3: Crystal data and structure refinement for 1-Ca.

| Identification code       | hasj190219a       |
|---------------------------|-------------------|
| Empirical formula         | C₄₈H₇₆Ca₂Fe₂N₄O₂  |
| Formula weight            | 932.98            |
| Temperature/K             | 100.01(10)        |
| Crystal system            | triclinic         |
| Space group               | P-1               |
| a/Å                       | 10.6520(8)        |
| b/Å                       | 11.7910(9)        |
| c/Å                       | 11.9476(7)        |
| α/°                       | 61.304(7)         |
| β/°                       | 65.091(6)         |
| γ/°                       | 69.034(7)         |
| Volume/Å³                 | 1170.80(17)       |
| Z                         | 1                 |
| ρcalcg/cm³                | 1.323             |
| μ/mm⁻¹                    | 7.197             |
| F(000)                    | 500.0             |
| Crystal size/mm³          | 0.1677 × 0.0806 × 0.0376 |
| Radiation                 | CuKα (λ = 1.54184)       |
| 2Θ range for data collection/° | 8.718 to 145.16   |
| Index ranges              | -12 ≤ h ≤ 10, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14 |
| Reflections collected     | 13216             |
| Independent reflections   | 4512 [R_{int} = 0.0366, R_{sigma} = 0.0395] |
| Data/restraints/parameters| 4512/0/276        |
| Goodness-of-fit on F²     | 1.028             |
| Final R indexes [I>=2σ (I)] | R₁ = 0.0351, wR₂ = 0.0854 |
| Final R indexes [all data]| R₁ = 0.0399, wR₂ = 0.0886 |
| Largest diff. peak/hole / e Å⁻³ | 0.39/-0.40     |
**Figure S19**: Crystal structure of 1-Ca (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms are omitted for clarity.
### Table S4: Crystal data and structure refinement for 1-Sr.

| **Identification code** | hasj181105a |
|-------------------------|--------------|
| **Empirical formula**   | C\textsubscript{24}H\textsubscript{38}FeN\textsubscript{2}OSr |
| **Formula weight**      | 514.03       |
| **Temperature/K**       | 100.01(10)   |
| **Crystal system**       | monoclinic   |
| **Space group**          | P\textsubscript{2}\textsubscript{1}/n |
| **a/Å**                  | 10.3443(2)   |
| **b/Å**                  | 24.0480(3)   |
| **c/Å**                  | 10.4400(2)   |
| **α/°**                  | 90           |
| **β/°**                  | 112.803(2)   |
| **γ/°**                  | 90           |
| **Volume/Å\textsuperscript{3}** | 2394.07(8)   |
| **Z**                    | 4            |
| **ρ\textsubscript{calc}g/cm\textsuperscript{3}** | 1.426        |
| **μ/mm\textsuperscript{-1}** | 7.908        |
| **F(000)**               | 1072.0       |
| **Crystal size/mm\textsuperscript{3}** | 0.2605 × 0.2017 × 0.0771 |
| **Radiation**            | CuKα (λ = 1.54184) |
| **2Θ range for data collection/°** | 7.352 to 146.778 |
| **Index ranges**         | -12 ≤ h ≤ 12, -29 ≤ k ≤ 29, -12 ≤ l ≤ 12 |
| **Reflections collected**| 22575        |
| **Independent reflections** | 4715 [R_{int} = 0.0402, R_{sigma} = 0.0271] |
| **Data/restraints/parameters** | 4715/0/277   |
| **Goodness-of-fit on F\textsuperscript{2}** | 1.044        |
| **Final R indexes [I≥2σ (I)]** | R\textsubscript{1} = 0.0288, wR\textsubscript{2} = 0.0680 |
| **Final R indexes [all data]** | R\textsubscript{1} = 0.0320, wR\textsubscript{2} = 0.0697 |
| **Largest diff. peak/hole / e Å\textsuperscript{-3}** | 0.47/-0.58   |
Figure S20: Crystal structure of 1-Sr (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms are omitted for clarity.
Table S5: Crystal data and structure refinement for 1-Eu.

| Identification code   | hasj190104a |
|-----------------------|-------------|
| Empirical formula     | C₄₈H₇₆Eu₂Fe₂N₄O₂ |
| Formula weight        | 1156.74     |
| Temperature/K         | 100.01(10)  |
| Crystal system        | monoclinic  |
| Space group           | P2₁/n       |
| a/Å                   | 10.3288(4)  |
| b/Å                   | 24.0285(6)  |
| c/Å                   | 10.4407(3)  |
| α/°                   | 90          |
| β/°                   | 112.444(4)  |
| γ/°                   | 90          |
| Volume/Å³              | 2394.95(14) |
| Z                      | 2           |
| ρ_calcg/cm³            | 1.604       |
| μ/mm⁻¹                 | 3.217       |
| F(000)                 | 1172.0      |
| Crystal size/mm³       | 0.2952 × 0.2308 × 0.1781 |
| Radiation              | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.812 to 59.052 |
| Index ranges           | -13 ≤ h ≤ 14, -30 ≤ k ≤ 32, -14 ≤ l ≤ 13 |
| Reflections collected  | 21567       |
| Independent reflections| 5969 [R_int = 0.0334, R_sigma = 0.0368] |
| Data/restraints/parameters | 5969/0/268  |
| Goodness-of-fit on F²  | 1.187       |
| Final R indexes [I>=2σ (I)] | R₁ = 0.0326, wR₂ = 0.0568 |
| Final R indexes [all data] | R₁ = 0.0383, wR₂ = 0.0584 |
| Largest diff. peak/hole / e Å⁻³ | 1.14/-0.74 |
Figure S21: Crystal structure of 1-Eu (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms are omitted for clarity.
Table S6: Crystal data and structure refinement for 1-Ba.

| **Identification code** | hasj180926b |
|-------------------------|-------------|
| **Empirical formula**   | C$_{56}$H$_{90}$Ba$_2$Fe$_2$N$_4$O$_4$ |
| **Formula weight**      | 1269.69     |
| **Temperature/K**       | 100.01(10)  |
| **Crystal system**       | monoclinic  |
| **Space group**          | P2$_1$/c    |
| **a/A**                  | 10.2766(2)  |
| **b/A**                  | 15.8347(3)  |
| **c/A**                  | 17.8173(4)  |
| **α/°**                  | 90          |
| **β/°**                  | 101.849(2)  |
| **γ/°**                  | 90          |
| **Volume/A$^3$**         | 2837.57(10) |
| **Z**                    | 2           |
| **ρ$_{calc}$/g/cm$^3$**   | 1.486       |
| **μ/mm$^{-1}$**          | 1.916       |
| **F(000)**               | 1300.0      |
| **Crystal size/mm$^3$**  | 0.1108 × 0.086 × 0.0424 |
| **Radiation**            | MoKα (λ = 0.71073) |
| **2Θ range for data collection/°** | 6.09 to 59.416 |
| **Index ranges**         | -13 ≤ h ≤ 14, -21 ≤ k ≤ 21, -23 ≤ l ≤ 24 |
| **Reflections collected**| 30009       |
| **Independent reflections** | 7098 [R$_{int}$ = 0.0393, R$_{sigma}$ = 0.0401] |
| **Data/restraints/parameters** | 7098/60/354 |
| **Goodness-of-fit on F$^2$** | 1.037   |
| **Final R indexes [I>=2σ (I)]** | R$_1$ = 0.0329, wR$_2$ = 0.0587 |
| **Final R indexes [all data]** | R$_1$ = 0.0474, wR$_2$ = 0.0632 |
| **Largest diff. peak/hole / e A$^{-3}$** | 1.51/-0.45 |
Figure S22: Crystal structure of 1-Ba (top: ball-and-stick representation; bottom: ORTEP plot). Hydrogen atoms and disorder are omitted for clarity.
1.5 UV/Vis Spectra

General Information

All UV/Vis spectra were recorded under rigorous exclusion of moisture and oxygen in screw sealed, gas tight, glass cuvettes, using an Agilent Technologies Cary 60 UV-vis spectrometer. All samples were prepared in a glovebox. The cuvettes were treated with t-BuLi (1.7M in pentane) and washed with n-pentane prior to usage. All compounds were measured in freshly distilled and thoroughly dried pyridine. (Sigma Aldrich, ACS reagent grade, distillation over freshly ground CaH₂, additional drying over activated MS 3Å). All complexes are intensely colored. Due to the very high air and moisture sensitivity of the compounds and unavoidable traces of water in the pyridine (< 10 ppm) a dilution to the level necessary for applying Lambert-Beer-Law (absorbance below 1.0 a.u. with respect to the first peak in the UV-region) could not be achieved without considerable complex hydrolysis. The UV/vis spectra were recorded at the concentrations of given in Table S7. Since we could not dilute these solutions any further due to hydrolysis, only a rough estimation of the extinction coefficients is given. The characteristic absorption for complexes with a κ³-bis(donor)ferrocenyl-metal bonding mode[^S9] is located around 500 nm. All spectra were recorded at room temperature and in all cases a background spectrum was measured first and subtracted from the spectrum of the compound of interest. The measured extinction coefficients are summarized in table S7.
Figure S23: UV/Vis of 1-H₂.

Figure S24: UV/Vis of 1-Mg.
Figure S25: UV/Vis of 1-Ca.

Figure S26: UV/Vis of 1-Sr.
Figure S27: UV/Vis of 1-Ba.

Figure S28: UV/Vis of 1-Eu.
Figure S29: UV/Vis of 1-H₂, 1-Mg, 1-Ca, 1-Sr, 1-Ba, 1-Eu.

Table S7: Extinction coefficients and absorption maxima measured in pyridine.¹

| Metal | ε [L mole⁻¹ cm⁻¹] | λ [nm] | Concentration [mmol mL⁻¹] |
|-------|-----------------|-------|------------------------|
| H     | 198             | 450   | 8.05 *10⁻⁴             |
| Mg    | 275             | 455   | 8.55 *10⁻⁴             |
| Ca    | 602             | 506   | 1.43 *10⁻³             |
| Sr    | 484             | 479   | 1.53 *10⁻³             |
| Ba    | 651             | 474   | 1.07 *10⁻³             |
| Eu    | 679             | 447   | 1.04*10⁻³              |

¹Due to the very high air and water sensitivity the dilution of these highly colored solutions is limited by trace amounts of water (< 10 ppm) in the pyridine.
1.6 Cyclic Voltammetry

General Information

The cyclic voltammograms were recorded under rigorous exclusion of moisture and oxygen inside an argon filled glovebox with a PalmSens 4 (PalmSens) by working in freshly distilled and degassed THF (Sigma Aldrich, ACS reagent grade, distillation over sodium mirror, additional drying over activated MS 3Å; water content: below 8 ppm H$_2$O) with 0.1 M NBu$_4$PF$_6$ (dried, > 99.0%, electrochemical grade, Fluka) as electrolyte. The electrochemical cell was treated with t-BuLi (1.7M in pentane) and was washed with n-pentane and THF prior to its usage. Concentrations of the compounds were $\sim$ 1·10$^{-4}$ M. A three-electrode setup was used with a glassy carbon working electrode, a coiled platinum wire as counter electrode, and a coiled silver wire as a pseudo-reference electrode. The ferrocene/ferrocenium couple was used as internal reference. The ferrocene was sublimated prior to its use. All determined values are depicted in table S8.

![Cyclic voltammograms](image)

**Figure S30:** Cyclic voltammograms of the ligand 1-H$_2$ and the complexes 1-(Mg, Ca, Sr, Ba) in THF at 100 mV/s, NBu$_4$PF$_6$ as supporting electrolyte.
**Figure S31:** Cyclic voltammogram of the first oxidation of the ligand 1-H₂ in THF at 100 mV/s, NBu₄PF₆ as supporting electrolyte.

**Figure S32:** Cyclic voltammogram (scan 1 and 2) of the first oxidation (including rereduction processes) of complex 1-Mg in THF at 100 mV/s, NBu₄PF₆ as supporting electrolyte.
Figure S33: Cyclic voltammograms of the first oxidation (including rereduction processes) of complex 1-Ca in THF at different scan rates as indicated in the legend, NBu₄PF₆ as supporting electrolyte.

Figure S34: Cyclic voltammogram of complex 1-Sr in THF at 100 mV/s, NBu₄PF₆ as supporting electrolyte.
Figure S35: Cyclic voltammogram of the first oxidation of complex 1-Ba in THF at 100 mV/s, NBu₄PF₆ as supporting electrolyte.

Table S8: Half-wave potentials and cathodic/anodic potentials of the compounds measured in THF (100 mV/s) with NBu₄PF₆ as electrolyte. The FcH/FcH⁺ couple was used as an internal standard.

| Metal | \( E_{1/2}(\text{Ox1}) \) | \( E_{1/2}(\text{Ox2}) \) | \( E_{1/2}(\text{Ox3}) \) | \( E_{1/2}(\text{Ox4}) \) | \( E_P(\text{Ox5}) \) | \( E_P(\text{Rered}) \) |
|-------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1-H₂  | –0.77           | –               | –               | –               | –               | –               |
| 1-Mg  | –1.57<sup>a</sup> | –0.97<sup>c</sup> | –0.65          | –               | –               | –               |
| 1-Ba  | –1.75           | –0.89<sup>b</sup> | –0.77          | –0.45          | 0.33<sup>b</sup> | –3.55<sup>b</sup> |
| 1-Sr  | –1.75           | –0.82<sup>b</sup> | –0.75          | –0.43          | 0.31<sup>b</sup> | –3.39<sup>b</sup> |
| 1-Ca  | –1.67<sup>a</sup> | –0.75<sup>d</sup> | –0.75          | –0.43          | 0.29<sup>b</sup> | –3.35<sup>b</sup> |

<sup>a</sup> Half-wave potentials for irreversible processes
<sup>b</sup> Peak potentials for irreversible processes.
<sup>c</sup> Only visible at slow scan rates (25 mV/s)
<sup>d</sup> Probably contains two oxidation processes
<sup>e</sup> Also contains the irreversible reduction of pyridine
2. Computational Details

The geometry optimization followed by the harmonic vibrational frequencies calculations of 1-Ae (Ae = Mg, Ca, Sr, Ba) complexes were performed at the BP86-D3(BJ)/def2-SVP level. Effective core potential was used for the 28 and 46 core electrons of Sr and Ba atoms, respectively, to take care of the relativistic effects. Superfine integration grid was used for all computations. All these calculations were carried out with Gaussian 16 program package. The natural bond orbital (NBO) analysis was done with the Gaussian 16 program. Quantum theory of atoms in molecules (QTAIM) analysis was performed with wave functions generated at the BP86-D3(BJ)/def2-SVP//BP86-D3(BJ)/def2-SVP level, where an all-electron x2c-SVPall basis set was used for Sr and Ba atoms to avoid the use of ECP in the program, by using AIMALL program.

The bonding situations were analysed by means of an energy decomposition analysis (EDA) together with the natural orbitals for chemical valence (NOCV) method by using the ADF 2018.105 program package. The EDA-NOCV calculations were carried out at the BP86-D3(BJ)/TZ2P+/ZORA level using the BP86-D3(BJ)/def2-SVP optimized geometries. TZ2P+ is a triple-ζ quality basis set augmented by two sets of polarization functions. In this analysis, the intrinsic interaction energy ($\Delta E_{\text{int}}$) between two fragments is divided into four energy components as follows:

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$$ (1)

The electrostatic $\Delta E_{\text{elstat}}$ term is originated from the quasiclassical electrostatic interaction between the unperturbed charge distributions of the prepared fragments, whereas the Pauli repulsion $\Delta E_{\text{Pauli}}$ corresponds to the energy change associated with the transformation from the superposition of the unperturbed electron densities of the isolated fragments to the wavefunction, which properly obeys the Pauli principle through explicit antisymmetrization and renormalization of the production wavefunction. Since D3(BJ) is coupled with the functional, it gives additional dispersion contribution between two interacting fragments. The orbital term $\Delta E_{\text{orb}}$ is originated from the mixing of orbitals, charge transfer and polarization between the isolated fragments, which can be further decomposed into contributions from each irreducible representation of the point group of the interacting system as follows:
\[ \Delta E_{\text{orb}} = \sum_r \Delta E_r \quad (2) \]

The combination of the EDA with NOCV enables the partition of the total orbital interactions into pairwise contributions of the orbital interactions which is very vital to get a complete picture of the bonding. The charge deformation \( \Delta \rho_k(r) \), resulting from the mixing of the orbital pairs \( \psi_k(r) \) and \( \psi_{-k}(r) \) of the interacting fragments presents the amount and the shape of the charge flow due to the orbital interactions (Equation 3), and the associated energy term \( \Delta E_{\text{orb}} \) provides with the size of stabilizing orbital energy originated from such interaction (Equation 4).

\[
\Delta \rho_{\text{orb}} (r) = \sum_k \Delta \rho_k (r) = \sum_{k=1}^{N/2} \nu_k [-\psi_{-k}^2 (r) + \psi_k^2 (r)] \quad (3)
\]

\[
\Delta E_{\text{orb}} = \sum_k \Delta E_{\text{orb}}^k = \sum_{k=1}^{N/2} \nu_k [-F_{-k,-k}^{TS} + F_{k,k}^{TS}] \quad (4)
\]

More details about the EDA-NOCV method and its application are given in recent reviews articles.\[S20\]
Figure S36. HOMO and LUMO orbitals calculated for 1-H$_2$ at the BP86-D3(BJ)/def2-SVP level. The MO isovalue is 0.04 au.
Figure S37. HOMO and LUMO orbitals calculated for 1-Mg at the BP86-D3(BJ)/def2-SVP level. The MO isovalue is 0.04 au.
**Figure S38.** HOMO and LUMO orbitals calculated for 1-Ca at the BP86-D3(BJ)/def2-SVP level. The MO isovalue is 0.04 au.
Figure S39. HOMO and LUMO orbitals calculated for 1-Sr at the BP86-D3(BJ)/def2-SVP level. The MO isovalue is 0.04 au.
Figure S40. HOMO and LUMO orbitals calculated for 1-Ba at the BP86-D3(BJ)/def2-SVP level. The MO isovalue is 0.04 au.
Figure S41. The molecular graphs of 1-Ae (Ae = Mg, Ca, Sr and Ba) complexes at the BP86-D3(BJ)/def2-SVP/x2c-SVPall//BP86-D3(BJ)/def2-SVP level. Small green, red and blue circles represent bond critical point, ring critical point and cage critical points, respectively.
Figure S42. The contour plot of the Laplacian of electron density, $\nabla^2 \rho(r)$ of 1-Sr and 1-Ba in the Fe-Ae-N plane. The blue solid lines indicate regions of charge depletion ($\nabla^2 \rho(r) > 0$) and red dotted lines indicate regions of charge accumulation ($\nabla^2 \rho(r) < 0$). Small green circles represent bond critical points.
Figure S43. Shape of the deformation densities $\Delta \rho(1)-(10)$, which are associated with the orbital interactions $\Delta E_{\text{orb}(1)-(10)}$ in 1-Ca complex and eigenvalues $|\nu_n|$ of the charge flow. The isosurface value is 0.0006. The color code of the charge flow is red → blue.
Figure S44. Shape of the deformation densities $\Delta \rho_{(1)-(10)}$, which are associated with the orbital interactions $\Delta E_{\text{orb}(1)-(10)}$ in 1-Sr complex and eigenvalues $|\nu_n|$ of the charge flow. The isosurface value is 0.0006. The color code of the charge flow is red $\rightarrow$ blue.
Figure S45. Shape of the deformation densities $\Delta \rho_{1-10}$, which are associated with the orbital interactions $\Delta E_{\text{orb}(1)-10}$ in 1-Ba complex and eigenvalues $|\nu_n|$ of the charge flow. The isosurface value is 0.0006. The color code of the charge flow is red $\rightarrow$ blue.
| n  | Deformation Density | ΔE<sub>orb</sub>(n) | | n  | Deformation Density | ΔE<sub>orb</sub>(n) |
|----|---------------------|---------------------|----|---------------------|---------------------|
| 1  | Δρ<sub>1</sub>       | -33.6               | 0.42| 2  | Δρ<sub>2</sub>       | -32.2               | 0.37|
| 3  | Δρ<sub>3</sub>       | -22.8               | 0.33| 4  | Δρ<sub>4</sub>       | -16.4               | 0.27|
| 5  | Δρ<sub>5</sub>       | -13.8               | 0.23| 6  | Δρ<sub>6</sub>       | -17.1               | 0.22|
| 7  | Δρ<sub>7</sub>       | -13.9               | 0.20| 8  | Δρ<sub>8</sub>       | -7.5                | 0.15|
| 9  | Δρ<sub>9</sub>       | -7.0                | 0.14| 10 | Δρ<sub>10</sub>      | -4.9                | 0.11|

**Figure S46.** Shape of the deformation densities Δρ<sub>1</sub>-Δρ<sub>10</sub>, which are associated with the orbital interactions ΔE<sub>orb</sub>(1)-ΔE<sub>orb</sub>(10) in 1-Mg complex and eigenvalues |ν<sub>n</sub>| of the charge flow. The isosurface value is 0.001. The color code of the charge flow is red → blue.
**Figure S47.** Shape of the deformation densities $\Delta \rho(5)$ and the shape of the associated orbitals of the fragments in 1-Mg complex and eigenvalues $|\nu_n|$ of the charge flow. The MO energy eigen values are in eV.

**Table S9.** Some selected experimental and computed geometrical parameters of 1-Ae complex. Bond distances are in Å and bond angles are in degree.
|       | Mg-N1   | Mg-N2   | Mg-O1   | Mg-O2   | <N1MgN2| <FeMgN1| <FeMgN2 |
|-------|---------|---------|---------|---------|--------|--------|--------|
| 1-Mg  | 1.987   | 1.975   | 2.041   | 2.049   | 121.7  | 65.8   | 65.2   |
|       |         |         |         |         |        |       |        |
|       |         |         |         |         |        |       |        |
| 1-Ca  |         |         |         |         |        |       |        |
| Ca-Fe | 3.113   | 3.061   |         |         |        |       |        |
| Ca-N1 | 2.371   | 2.370   |         |         |        |       |        |
| Ca-N2 | 2.502   | 2.475   |         |         |        |       |        |
| Ca-O1 | 2.359   | 2.372   |         |         |        |       |        |
| Ca-N2' | 2.407   | 2.389   |         |         |        |       |        |
| <N1CaN2 | 140.2   | 142.8   |         |         |        |       |        |
| <FeCaN1 | 70.8    | 72.4    |         |         |        |       |        |
| <FeCaN2 | 69.4    | 70.6    |         |         |        |       |        |
| 1-Sr  |         |         |         |         |        |       |        |
| Sr-Fe | 3.320   | 3.198   |         |         |        |       |        |
| Sr-N1 | 2.516   | 2.516   |         |         |        |       |        |
| Sr-N2 | 2.603   | 2.610   |         |         |        |       |        |
| Sr-O1 | 2.496   | 2.524   |         |         |        |       |        |
| Sr-N2' | 2.560   | 2.556   |         |         |        |       |        |
| <N1SrN2 | 132.2   | 137.2   |         |         |        |       |        |
| <FeSrN1 | 67.1    | 70.0    |         |         |        |       |        |
| <FeSrN2 | 68.1    | 67.7    |         |         |        |       |        |
| 1-Ba  |         |         |         |         |        |       |        |
| Ba-Fe | 3.454   | 3.442   |         |         |        |       |        |
| Ba-N1 | 2.676   | 2.693   |         |         |        |       |        |
| Ba-N2 | 2.751   | 2.776   |         |         |        |       |        |
| Ba-O1 | 2.830   | 2.765   |         |         |        |       |        |
| Ba-O2 | 2.814   | 2.809   |         |         |        |       |        |
| Ba-N2' | 2.765   | 2.748   |         |         |        |       |        |
| <N1BaN2 | 127.5   | 126.9   |         |         |        |       |        |
| <FeBaN1 | 65.4    | 65.8    |         |         |        |       |        |
| <FeBaN2 | 62.6    | 62.1    |         |         |        |       |        |
Table S10. The results of EDA for 1-Mg complex taking different partitioning schemes at the BP86-D3(BJ)/TZ2P+//BP86-D3(BJ)/def2-SVP level.

| Energies | \(\text{Mg}^{2+}\) (S, 3s\(^0\)) + \[\text{Cp}^*\text{Fe(THF)}_2\]\(^2\) (S) | \(\text{Mg}^+\) (D, 3s\(^1\)) + \[\text{Cp}^*\text{Fe(THF)}_2\]\(^-\) (D) | \(\text{Mg}\) (S, 3s\(^2\)) + \[\text{Cp}^*\text{Fe(THF)}_2\] (S) | \(\text{Mg}\) (T, 3s\(^1\)3p\(^1\)) + \[\text{Cp}^*\text{Fe(THF)}_2\] (T) |
|----------|---------------------------------|-----------------|-----------------|-----------------|
| \(\Delta E_{\text{int}}\)    | -687.9                          | -285.1          | -154.0          | -214.4          |
| \(\Delta E_{\text{Pauli}}\)  | 91.8                            | 270.2           | 504.3           | 562.3           |
| \(\Delta E_{\text{disp}}\)   | -16.2                           | -16.2           | -16.2           | -16.2           |
| \(\Delta E_{\text{elstat}}\) | -525.1                          | -300.3          | -285.6          | -349.3          |
| \(\Delta E_{\text{orb}}\)    | -238.3                          | -238.9          | -356.5          | -411.3          |

Table S11. The results of EDA for 1-Ca complex taking different partitioning schemes at the BP86-D3(BJ)/TZ2P+//BP86-D3(BJ)/def2-SVP level.

| Energies | \([\text{Ca}]^+\) (D, 4s\(^0\)4p\(^0\)3d\(^1\)) + \[\text{Ca(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) | \([\text{Ca}]^+\) (D, 4s\(^1\)) + \[\text{Ca(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) | \([\text{Ca}]^+\) (S, 4s\(^0\)) + \[\text{Ca(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) | \([\text{Ca}]^+\) (T, 4s\(^1\)4p\(^1\)3d\(^1\)) + \[\text{Ca(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) |
|----------|---------------------------------|-----------------|-----------------|-----------------|
| \(\Delta E_{\text{int}}\)    | -302.5                          | -275.0          | -576.0          | -189.2          |
| \(\Delta E_{\text{Pauli}}\)  | 145.3                           | 294.9           | 106.4           | 555.5           |
| \(\Delta E_{\text{disp}}\)   | -26.4                           | -26.4           | -26.4           | -26.4           |
| \(\Delta E_{\text{elstat}}\) | -195.6                          | -285.6          | -432.9          | -338.0          |
| \(\Delta E_{\text{orb}}\)    | -225.9                          | -257.9          | -223.3          | -380.3          |

Table S12. The results of EDA for 1-Sr complex taking different partitioning schemes at the BP86-D3(BJ)/TZ2P+//BP86-D3(BJ)/def2-SVP level.

| Energies | \([\text{Sr}]^+\) (D, 5s\(^0\)5p\(^0\)4d\(^1\)) + \[\text{Sr(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) | \([\text{Sr}]^+\) (D, 5s\(^1\)) + \[\text{Sr(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) | \([\text{Sr}]^+\) (S, 5s\(^0\)) + \[\text{Sr(Cp}^*\text{Fe(THF)}_2\] \(\Delta E_{\text{int}}\) |
|----------|---------------------------------|-----------------|-----------------|
| \(\Delta E_{\text{int}}\)    | -295.0                          | -256.6          | -537.3          |
| \(\Delta E_{\text{Pauli}}\)  | 131.1                           | 291.1           | 113.5           |
| \(\Delta E_{\text{disp}}\)   | -28.7                           | -28.7           | -28.7           |
Table S13. The results of EDA for 1-Ba complex taking different partitioning schemes at the BP86-D3(BJ)/TZ2P+/BP86-D3(BJ)/def2-SVP level.

| Energies  | \([\text{Ba}]^+ (D, 6s^6p^65d^1) + [\text{Ba}(\text{Cp}^*_2\text{Fe(THF)}_2)_2]^-(D)\) | \([\text{Ba}]^+(D, 6s^1) + [\text{Ba}(\text{Cp}^*_2\text{Fe(THF)}_2)_2]^-(D)\) | \([\text{Ba}]^{2+} (S, 6s^0) + [\text{Ba}(\text{Cp}^*_2\text{Fe(THF)}_2)_2]^2-(S)\) |
|-----------|-------------------------------------------------|-------------------------------------------------|----------------------------------|
| \(\Delta E_{\text{int}}\) | -283.8                                           | -272.4                                           | -524.0                           |
| \(\Delta E_{\text{Pauli}}\) | 172.0                                            | 298.9                                            | 119.7                            |
| \(\Delta E_{\text{disp}}\) | -31.7                                            | -31.7                                            | -31.7                            |
| \(\Delta E_{\text{elstat}}\) | -220.7                                           | -292.1                                           | -418.2                           |
| \(\Delta E_{\text{orb}}\) | -203.5                                           | -247.6                                           | -193.9                           |
Table S14. The results of EDA-NOCV for 1-Ae (Ae = Mg, Ca, Sr, and Ba) complexes taking Ae$^{2+}$ as one fragment and the rest as another at the BP86-D3(BJ)/TZ2P+/BP86-D3(BJ)/def2-SVP level.

| Energies | [Mg$^{2+}$ (S, 3s$^0$) + [Cp*$_2$Fe(THF)$_2$]$^2$ (S)] | [Ca$^{2+}$ (S, 4s$^0$) + [Ca(Cp*$_2$Fe(THF))$_2$]$^2$ (S)] | [Sr$^{2+}$ (S, 5s$^0$) + [Sr(Cp*$_2$Fe(THF))$_2$]$^2$ (S)] | [Ba$^{2+}$ (S, 6s$^0$) + [Ba(Cp*$_2$Fe(THF))$_2$]$^2$ (S)] |
|-----------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| $\Delta E_{\text{int}}$ | -687.9 | -576.0 | -537.3 | -524.0 |
| $\Delta E_{\text{Pauli}}$ | 91.8 | 106.4 | 113.5 | 119.7 |
| $\Delta E_{\text{disp}}$ [a] | -16.2 (2.1%) | -26.4 (3.9%) | -28.7 (4.4%) | -31.7 (4.9%) |
| $\Delta E_{\text{elstat}}$ [a] | -525.1 (67.4%) | -432.9 (63.4%) | -420.4 (64.6%) | -418.2 (65.0%) |
| $\Delta E_{\text{orb}}$ [a] | -238.3 (30.6%) | -223.3 (32.7%) | -201.7 (31.0%) | -193.9 (30.1%) |
| $\Delta E_{\text{orb}(1)}$ [b] | -33.6 (14.1%) | -35.8 (16.0%) | -29.6 (14.7%) | -25.8 (13.3%) |
| $\Delta E_{\text{orb}(2)}$ [b] | -32.2 (13.5%) | -26.7 (12.0%) | -22.6 (11.2%) | -19.9 (10.3%) |
| $\Delta E_{\text{orb}(3)}$ [b] | -22.8 (9.6%) | -15.9 (7.1%) | -16.4 (8.1%) | -19.0 (9.8%) |
| $\Delta E_{\text{orb}(4)}$ [b] | -16.4 (6.9%) | -13.4 (6.0%) | -12.8 (6.3%) | -12.2 (6.3%) |
| $\Delta E_{\text{orb}(5)}$ [b] | -13.8 (5.8%) | -11.8 (5.3%) | -10.3 (5.1%) | -9.1 (4.7%) |
| $\Delta E_{\text{orb}(6)}$ [b] | -17.1 (7.2%) | -11.0 (4.9%) | -9.1 (4.5%) | -7.5 (3.9%) |
| $\Delta E_{\text{orb}(7)}$ [b] | -13.9 (5.8%) | -7.7 (3.4%) | -6.4 (3.2%) | -5.6 (2.9%) |
| $\Delta E_{\text{orb}(8)}$ [b] | -7.5 (3.1%) | -6.2 (2.8%) | -5.2 (2.6%) | -4.5 (2.3%) |
| $\Delta E_{\text{orb}(9)}$ [b] | -7.0 (2.9%) | -5.7 (2.6%) | -4.5 (2.2%) | -4.2 (2.2%) |
| $\Delta E_{\text{orb}(10)}$ [b] | -4.9 (2.1%) | -5.3 (2.4%) | -4.8 (2.4%) | -4.1 (2.1%) |
| $\Delta E_{\text{orb}(\text{rest})}$ [b] | -69.1 (29.0%) | -83.8 (37.5%) | -80.0 (39.7%) | -82.0 (42.3%) |

[a] The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$

[b] The values in parentheses give the percentage contribution to the total orbital interactions $\Delta E_{\text{orb}}$. 

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S63
**Table S15.** The Cartesian coordinates of 1-Ae at the BP86-D3(BJ)/def2-SVP level.

1-Mg

\[ E = -2817.701781 \text{ au} \]

0 1

Fe -1.10164500 -2.60237500 -0.17602000
Mg 0.07422300 0.42996200 0.02868100
O 0.73496400 2.31300600 -0.56882300
O 0.43046200 0.69975600 2.04107100
N 1.44847900 -0.81597000 -0.65602100
N -1.90069000 0.48328000 -0.26592400
C 0.87430400 -2.09943800 -0.64682000
C -3.07851700 -3.03759600 -0.17283300
H -3.52833300 -3.95551900 -0.57416800
C -2.59421700 -2.84850400 1.17023400
H -2.61571600 -3.59090700 1.97915100
C 0.20054600 -2.75356900 -1.75449000
H 0.05852200 -2.30709600 -2.74769300
C -2.29205700 -0.81993400 -0.00383200
C -2.85272400 -1.81448300 -0.90440800
H -3.08439500 -1.65158600 -1.96435900
C -2.08523600 -1.50368500 1.26308200
H -1.67909400 -1.02920500 2.16583900
C -2.62609100 1.22458800 -1.27294900
H -3.35287000 0.57534700 -1.81698500
H -1.94669300 1.63621000 -2.06397300
C 3.97324900 -0.54102200 -0.83251800
C -3.43323100 2.43308000 -0.69738400
C 0.78492000 -3.02031000 0.48001600
H 1.19324700 -2.83083900 1.48065900
C 0.11037500 -4.21771000 0.05577000
H -0.10481600 -5.09758700 0.67735100
C 2.57955500 -0.62824000 -1.53863000
H 2.48361200 0.31532900 -2.13784300
H 2.63802800 -1.45376100 -2.29058600
C -0.25048500 -4.05317900 -1.33053600
H -0.79362900 -4.78414700 -1.94443500
C 0.83586600 2.62123400 -1.98455400
H -0.12193800 3.07613600 -2.32282600
H 0.99333500 1.66392900 -2.52080600
C 4.20782200 -1.81204800 0.00054600
H 3.40515000 -1.92971700 0.75602500
H 5.18763900 -1.78046800 0.52389600
H 4.18587500 -2.71888000 -0.63956000
C 2.00270300 3.59950200 -2.07098700
H 1.97237000 4.21994900 -2.98801000
H 2.96430500 3.04453700 -2.05718700
C 5.06208200 -0.40401300 -1.91107800
H 5.08102600 -1.29499300 -2.57428700
H 6.07232500 -0.29561100 -1.46143700
H 4.88122000 0.48726500 -2.55162900
C 3.99866200 0.69435800 0.08543100
H 3.91468200 1.63077100 -0.50787500
H 4.93775300 0.75143000 0.67604500
H 3.14138500 0.66203600 0.78982900
C 1.82136400 4.41667900 -0.77808500
H 2.74951000 4.92155600 -0.44542100

S65
1-Ca

E = -6126.037138 au

0 1
Fe -1.02048300 3.52248200 -0.21518100
Ca -0.29128100 0.86423600 -1.54546000
O 0.87092900 0.27710300 -3.52803500
N 1.05278900 1.15086100 0.51348900
N -1.85088000 1.96450500 -2.95055500
C -1.32419100 1.83237800 0.89897400
H -1.79775700 0.87627300 0.63672000
C 0.11725900 2.09350900 0.92346000
C -2.01324100 2.98597800 1.43389300
H -3.09754800 3.07451700 1.58129700
C -0.29637200 3.72346300 -2.14730500
H 0.61513300 3.35491100 -2.63988300
C 0.27723800 3.44863500 1.41573400
H 1.22872800 3.97955000 1.52023800
C -1.01836500 3.97665700 1.75992900
H -1.21219300 4.96990900 2.18557200
C 2.45425000 1.40973200 0.82974900
C -1.79063600 5.16182500 -1.09566000
H -2.21420700 6.02164000 -0.55965900
C -3.23477400 1.58491600 -3.14531700
H -3.89699300 2.48196800 -3.22874100
H -3.64683300 0.99746300 -2.27704000
C -3.44698500 0.73558800 -4.42970500
C -2.52058800 4.00981900 -1.56103700
H  -3.59097800  3.82975200  -1.40550800
C   -1.62667300  3.14758000  -2.32878100
C    1.02526000   -0.87884100  -5.57453000
H   1.60487800   -1.62745800  -6.15000500
H   -0.04665500  -0.99381900  -5.83532300
C    -0.40516900   4.98282800  -1.44771200
H    0.41525900  5.68696200  -1.25642600
C     3.39984000   2.00353800  -0.25812300
C    -4.93331700  0.34372800  -4.51637800
H    -5.24155400  -0.24959800  -3.62866300
H    -5.13508500  -0.27022000  -5.41963400
H    -5.58447900  1.24250700  -4.56624400
C     0.99986700  1.30136500  -4.56113600
H    1.71920700   2.06948000  -4.20428100
H    -0.00380300  1.76727700  -4.66622700
C    1.21681700  -1.02703300  -4.06720400
H    0.56278700  -1.77963200  -3.58612500
H    2.27027100  -1.26193500  -3.79693600
C    2.93578300  3.41053800  -0.66847100
H    1.86140600  3.40930500  -0.93332000
H    3.51876400  3.79240100  -1.53354700
H    3.06541000  4.13222900  0.16502000
C    1.48931100  0.56860900  -5.81741000
H    2.59643600  0.61105800  -5.88874900
H    1.07218400  1.01126100  -6.74331900
C    4.80964700  2.07649400  -0.36200100
H    4.81439100  2.71425200   1.27143600
H    5.54070400  2.50540500  -0.35518500
H  -1.22872800  -3.97955000  -1.52023800
C  1.01836500  -3.97665700  -1.75992900
H  1.21219300  -4.96990900  -2.18557200
C  -2.45425000  -1.40973200  -0.82974900
C  1.79063600  -5.16182500  1.09566000
H  2.21420700  -6.02164000  0.55965900
C  3.23477400  -1.58491600  3.14531700
H  3.89699300  -2.48196800  3.22874100
H  3.64683300  -0.99746300  2.27770400
C  3.44698500  -0.73558800  4.42970500
C  2.52058800  -4.00981900  1.56103700
H  3.59097800  -3.82975200  1.40550800
C  1.62667300  -3.14758000  2.32878100
C  -1.02526000  0.87884100  5.57453000
H  -1.60487800  1.62745800  6.15000500
H  0.04665500  0.99381900  5.83532300
C  0.40516900  -4.98282800  1.44771200
H  -0.41525900  -5.68696200  1.25642600
C  -3.39984000  -2.00353800  0.25812300
C  4.93331700  -0.34372800  4.51637800
H  5.24155400  0.24959800  3.62866300
H  5.13508500  0.27022000  5.41963400
H  5.58447900  -1.24250700  4.56624400
C  -0.99986700  -1.30136500  4.56113600
H  -1.71920700  -2.06948000  4.20428100
H  0.00380300  -1.76727700  4.66622700
C  -1.21681700  1.02703300  4.06720400
H  -0.56278700  1.77963200  3.58612500
H -2.27027100 1.26193500 3.79693600
C -2.93578300 -3.41053800 0.66847100
H -1.86140600 -3.40930500 0.93332000
H -3.51876400 -3.79240100 1.53354700
H -3.06541000 -4.13229900 -0.16502000
C -1.48931100 -0.56860900 5.81741000
H -2.59643600 -0.61105800 5.88874900
H -1.07218400 -1.01126100 6.74331900
C -4.80964700 -2.07649400 -0.36200100
H -4.81439100 -2.71425200 -1.27143600
H -5.54070400 -2.50540500 0.35518500
H -5.17364700 -1.06850400 -0.65568800
C -3.44816300 -1.08588400 1.49118600
H -3.78358700 -0.06259700 1.21983400
H -4.15497200 -1.48073600 2.25132400
H -2.46154900 -0.98798500 1.98679600
C 2.58108400 0.53573000 4.37170500
H 1.52035400 0.26930400 4.19462200
H 2.64493900 1.11030000 5.32024900
H 2.90513600 1.20659000 3.55120200
C 3.05090000 -1.57416000 5.65917900
H 3.67908000 -2.48669900 5.73935600
H 3.16791700 -0.99313600 6.59878800
H 1.99553600 -1.90384100 5.57422800
H -2.92702000 -0.44229700 -1.13286500
H -2.53471400 -2.06727500 -1.72798100
S71
I-Sr

$E = -4832.376309 \text{ au}$

\begin{align*}
0 & & 1 \\
\text{Sr} & 0.06287700 & -1.83088900 & -0.50384300 \\
\text{Fe} & 0.74653000 & -2.58319100 & 2.52776500 \\
\text{O} & -1.30626200 & -3.03973200 & -2.24644000 \\
\text{N} & -1.22512900 & -0.33555700 & 1.20422700 \\
\text{N} & 1.50264100 & -3.89334200 & -0.43433100 \\
\text{C} & -0.32462200 & -0.71931200 & 2.18496400 \\
\text{C} & 1.28885800 & -4.06898000 & 0.88820100 \\
\text{C} & 1.77614200 & -1.02402200 & 3.24079600 \\
\text{H} & 2.85798000 & -1.01727800 & 3.42893600 \\
\text{C} & 1.13058000 & -0.62621800 & 2.00715100 \\
\text{H} & 1.65263800 & -0.24004100 & 1.11845600 \\
\text{C} & 1.47528200 & -4.31499300 & 3.23490000 \\
\text{H} & 1.91064000 & -4.43631300 & 4.23567700 \\
\text{C} & -0.53208600 & -1.26235900 & 3.51421200 \\
\text{H} & -1.50520000 & -1.50285700 & 3.95560600 \\
\text{C} & -0.04103700 & -4.21041600 & 1.47473100 \\
\text{H} & -0.96137500 & -4.35036400 & 0.88787700 \\
\text{C} & -2.62477200 & -0.19658300 & 1.58567200 \\
\text{C} & 0.74247600 & -1.40263400 & 4.17054300 \\
\text{H} & 0.89758600 & -1.75583700 & 5.19868500 \\
\text{C} & 0.07946300 & -4.43806600 & 2.89590500 \\
\text{H} & -0.74080300 & -4.69474300 & 3.57925600 \\
\text{C} & 2.19799500 & -3.99418000 & 2.02873500 \\
\text{H} & 3.27680300 & -3.80749700 & 1.96461500 \\
\text{C} & -3.64156400 & -1.31300800 & 1.20244400
\end{align*}
C 2.87460000 -3.70268200 -0.85112900
H 3.57418900 -4.39249300 -0.31384900
H 3.25430900 -2.66758100 -0.60609200
C 2.11304400 -3.02801000 -3.18017800
H 1.05875700 -3.25054500 -3.18017800
H 2.23536400 -3.18613200 -4.27269000
H 2.30210300 -1.95351000 -2.98365100
C -1.30910400 -4.49711100 -2.25372000
H -2.22804800 -4.85442900 -1.73466400
H -0.40682800 -4.81798300 -1.68859600
C 3.06979400 -3.92961100 -2.37520500
C -3.27867700 -2.63481500 1.89804500
H -2.21998100 -2.90323600 1.71450200
H -3.92287600 -3.46860400 1.54640000
H -3.40548500 -2.55570500 2.99805100
C -5.03073600 -0.83630700 1.67221500
H -5.03983700 -0.64676700 2.76660100
H -5.81027100 -1.59623400 1.45423000
H -5.32549800 0.10689700 1.16414600
C -3.67886800 -1.51068600 -0.32347100
H -3.85845400 -0.54983200 -0.85089100
H -4.49167600 -2.21121400 -0.61078400
H -2.74121200 -1.94690500 -0.72225700
C -1.30951400 -4.87247200 -3.73441600
H -0.27427500 -4.84479100 -4.13393400
H -1.72017700 -5.88536800 -3.91603500
C -2.16350500 -3.74794700 -4.34997300
H -1.99021600 -3.60759800 -5.43516500
H  -3.24346100 -3.96108500 -4.20330600
C  -1.74502900 -2.51896800 -3.53296400
H   -0.89526400 -1.96674000 -3.99064900
H   -2.56579600 -1.79462400 -3.35844400
C  2.77686300 -5.40528700  -2.70560600
H   3.48248900 -6.07967400  -2.17573500
H   2.86903000 -5.60134800  -3.79532200
H   1.75141100 -5.67405300  -2.38029200
C  4.52498800 -3.58256500  -2.73914900
H   4.74741900 -2.51567300  -2.52246000
H   4.72200500 -3.75657000  -3.81814300
H   5.24205600 -4.20259600  -2.15999700
H   -2.72078100  -0.03466400  2.68690700
H  -3.02478000  0.73596900  1.11352900
Sr  -0.06287700  1.83088900  0.50384300
Fe  -0.74653000  2.58319100  -2.52776500
O  1.30626200  3.03973200  2.24644000
N  1.22512900  0.33555700  -1.20422700
N  -1.50264100  3.89334200  0.43433100
C   0.32462200  0.71931200  -2.18496400
C  -1.28885800  4.06898000  -0.88820100
C  -1.77614200  1.02402200  -3.24079600
H  -2.85798000  1.01727800  -3.42893600
C  -1.13058000  0.62621800  -2.00715100
H  -1.65263800  0.24004100  -1.11845600
C  -1.47528200  4.31499300  -3.23449000
H  -1.91064000  4.43631300  -4.23567700
C  0.53208600  1.26235900  -3.51421200
H 5.81027100 1.59623400 -1.45423000
H 5.32549800 -0.10689700 -1.16414600
C 3.67886800 1.51068600 0.32347100
H 3.85845400 0.54983200 0.85089100
H 4.49167600 2.21121400 0.61078400
H 2.74121200 1.94690500 0.72225700
C 1.30951400 4.87247200 3.73441600
H 0.27427500 4.84479100 4.13393400
H 1.72017700 5.88536800 3.91603500
C 2.16350500 3.74794700 4.34997300
H 1.99021600 3.60759800 5.43516500
H 3.24346100 3.96108500 4.20330600
C 1.74502900 2.51896800 3.53296400
H 0.89526400 1.96674000 3.99064900
H 2.56579600 1.79462400 3.35844400
C -2.77686300 5.40528700 2.70560600
H -3.48248900 6.07967400 2.17573500
H -2.86903000 5.60134800 3.79532200
H -1.75141100 5.67405300 2.38029200
C -4.52498800 3.58256500 2.73914900
H -4.74741900 2.51567300 2.52246000
H -4.72200500 3.75656700 3.81814300
H -5.24205600 4.20259600 2.15999700
H 2.72078100 0.03466400 -2.68690700
H 3.02478000 -0.73596900 -1.11352900

I-Ba
E = -5286.561130 au

| Atom | X    | Y    | Z    |
|------|------|------|------|
| Ba   | 0.33187500 | -2.03368700 | -0.38955300 |
| Fe   | 3.12916800  | -0.84145200  | -2.00242100  |
| N    | 0.11900200  | 0.37433900   | -1.75424600  |
| O    | -1.17440500 | -4.09583400  | 0.78095500   |
| N    | 2.35636800  | -3.80386500  | -0.54049000  |
| C    | 1.48176700  | 0.57240300   | -1.79223700  |
| C    | -0.53943400 | 0.13056300   | -3.02771300  |
| H    | -1.11062500 | -0.83203700  | -2.98345400  |
| H    | 0.19963600  | -0.02311900  | -3.84894800  |
| C    | 2.33655900  | 0.47346200   | -0.60230700  |
| H    | 1.99434300  | 0.26052000   | 0.42123700   |
| C    | -1.55972300 | 1.20986600   | -3.49653200  |
| C    | 3.10706600  | -4.26313600  | 0.60992300   |
| H    | 2.42957400  | -4.30978200  | 1.49896400   |
| H    | 3.92648500  | -3.56332400  | 0.91118000   |
| C    | -2.75907800 | 1.27726200   | -2.53252200  |
| H    | -3.24296600 | 0.28355000   | -2.42474400  |
| H    | -3.52661000 | 1.99084000   | -2.89734200  |
| H    | -2.48414800 | 1.61286400   | -1.51307200  |
| C    | 3.03185700  | -3.08807500  | -1.47115300  |
| C    | 2.47406000  | -2.67816800  | -2.75865500  |
| C    | 3.70496900  | 0.77505500   | -0.97575400  |
| H    | 4.56215000  | 0.83054800   | -0.29154000  |
| C    | 2.37475000  | 0.86948100   | -2.89915400  |
| H    | 2.07437800  | 0.97344800   | -3.94836900  |
| C    | 3.50644000  | -2.04316200  | -3.54714600  |
H 3.42020700 -1.74796300 -4.60159500
C 4.33852700 -2.43351000 -1.41117700
H 5.02030500 -2.46466600 -0.55322800
C 4.67138800 -1.90757100 -2.70952300
H 5.63645000 -1.47459300 -3.00583000
C -2.68769000 -3.16189100 -2.30928000
H -3.02465300 -2.34625400 -2.90490200
H -2.97452800 -2.88902400 -1.19072200
C -2.07169300 0.79882400 -4.89029700
H -1.24032600 0.74939300 -5.62498800
H -2.82398600 1.51986000 -5.27395700
H -2.55113000 0.20351000 -4.85784400
C 4.75319900 -5.70018400 -0.70139600
H 4.25802900 -5.44032300 -1.65866700
H 5.21058900 -6.70703500 -0.81059700
H 5.57197900 -4.96909800 -0.53949000
C -0.87159400 2.58172200 -3.57716000
H -0.38810400 2.83967200 -2.61300200
H -1.59546400 3.38555100 -3.82689000
H -0.07303700 2.58341000 -4.34842800
C 3.74630800 -5.68414700 0.46351000
C 3.71780900 1.03027200 -2.39880500
H 4.59758700 1.30211600 -2.99800400
C -0.83595300 -4.62583600 -2.54532300
H 0.05716100 -4.83766000 -1.91721100
H -0.54252300 -4.73259200 -3.61476400
C 4.46898000 -6.01525900 1.78204100
H 5.28026200 -5.28459200 1.98911400
N  -0.11900200  -0.37433900  1.75424600
O  1.17440500  4.09583400  -0.78095500
N  -2.35636800  3.80386500  0.54049000
C  -1.48176700  -0.57240300  1.79223700
C   0.53943400  -0.13056300  3.02771300
H  1.11062500  0.83203700  2.98345400
H  -0.19963600  0.02311900  3.84894800
C  -2.33655900  -0.47346200  0.60230700
H  -1.99434300  -0.26052000  -0.42123700
C  1.55972300  -1.20986600  3.49653200
C  -3.10706600  4.26313600  -0.60992300
H  -2.42957400  4.30978200  -1.49896400
H  -3.92648500  3.56332400  -0.91118000
C  2.75907800  -1.27726200  2.53252200
H  3.24296600  -0.28355000  2.42474400
H  3.52661000  -1.99084000  2.89734200
H  2.48414800  -1.61286400  1.51307200
C  -3.03185700  3.08807500  1.47115300
C  -2.47406000  2.67816800  2.75865500
C  -3.70496900  -0.77505500  0.97575400
H  -4.56215000  -0.83054800  0.29154000
C  -2.37475000  -0.86948100  2.89915400
H  -2.07437800  -0.97344800  3.94836900
C  -3.50644000  2.04316200  3.54714600
H  -3.42020700  1.74796300  4.60159500
C  -4.33852700  2.43351000  1.41117700
H  -5.02030500  2.46466600  0.55322800
C  -4.67138800  1.90757100  2.70952300
| Atom| X Coordination| Y Coordination| Z Coordination |
|-----|----------------|----------------|----------------|
| H   | 4.1794700      | 4.78623800     | 2.13953500     |
| C   | -2.64818000    | 6.72967900     | -0.19432800    |
| H   | -1.97671200    | 6.84333900     | -1.07214100    |
| H   | -3.08795200    | 7.72749600     | 0.01737000     |
| H   | -2.03409800    | 6.42097100     | 0.67648300     |
| C   | 2.48156100     | 4.09341800     | -1.38342200    |
| H   | 3.14168000     | 4.80643000     | -0.83031300    |
| H   | 2.89293900     | 3.07049100     | -1.30279600    |
| C   | 0.52186200     | 5.29194500     | -1.24604800    |
| H   | -0.56657400    | 5.13777500     | -1.13425300    |
| H   | 0.81395500     | 6.14680700     | -0.59087200    |
| C   | 1.01121900     | 5.50626800     | -2.69779800    |
| H   | 0.22371400     | 5.24333800     | -3.43023000    |
| H   | 1.28255200     | 6.56706300     | -2.86906600    |
| C   | 2.23583400     | 4.55715600     | -2.82370400    |
| H   | 3.12551500     | 5.05043800     | -3.26258300    |
| H   | 1.99332600     | 3.67490000     | -3.44806300    |
| O   | 1.24347700     | 3.25263900     | 2.30682800     |
| C   | 2.06310400     | 5.47162100     | 2.20520400     |
| H   | 2.06689300     | 6.44980800     | 2.72554600     |
| H   | 2.10104000     | 5.65729800     | 1.11268500     |
| H   | -1.49743100    | 2.99764300     | 3.15052100     |
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