Supporting Information

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1. Spectroscopic data

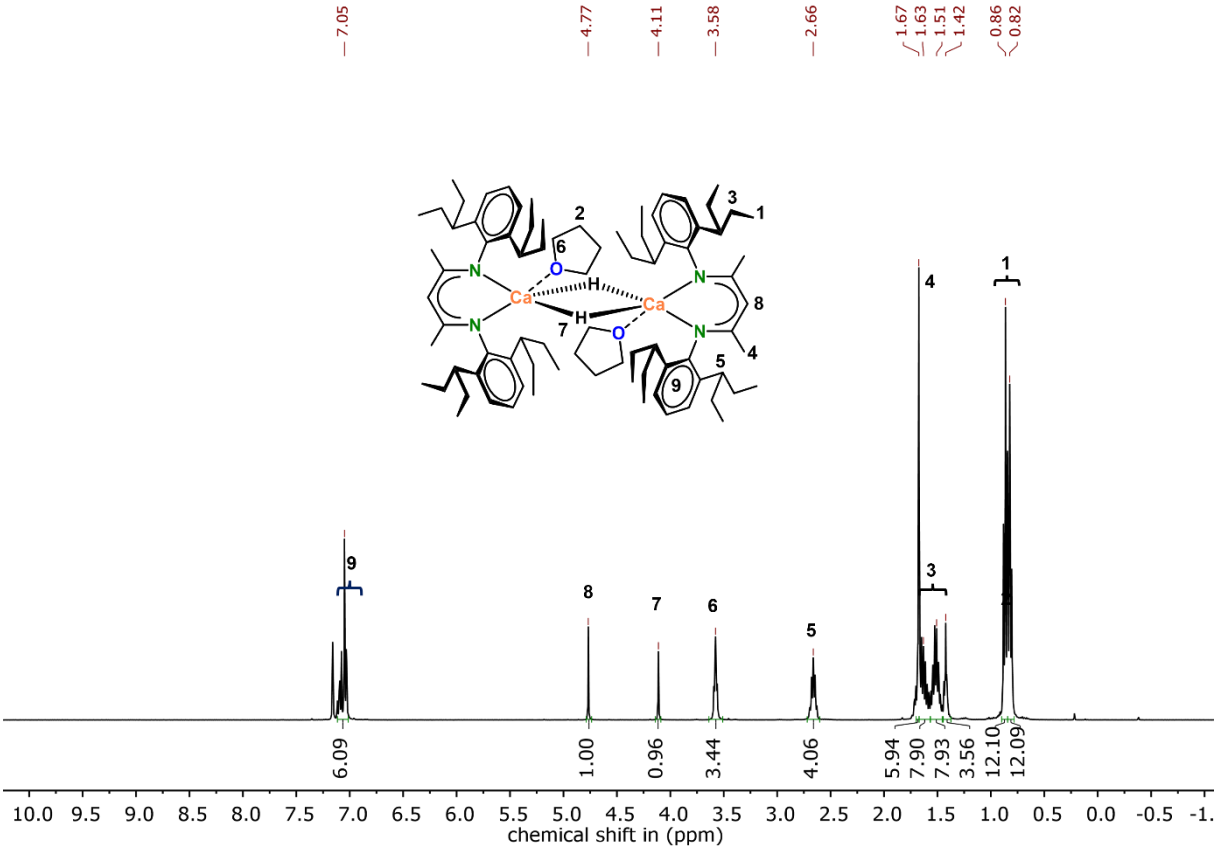


Figure S1. ^{1}H NMR (400.13 MHz, 298 K, C_6D_6) of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**).

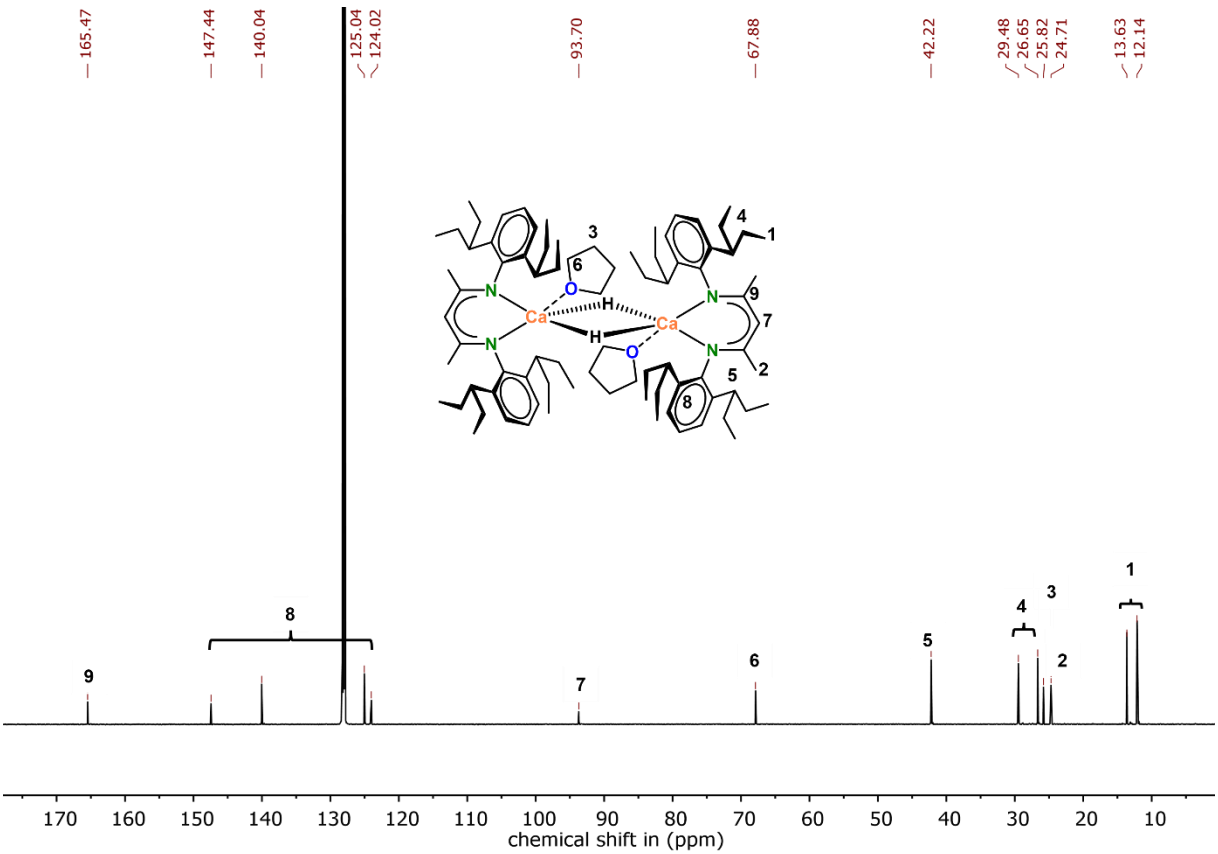


Figure S2. ^{13}C NMR (101 MHz, 298 K, C_6D_6) of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**).

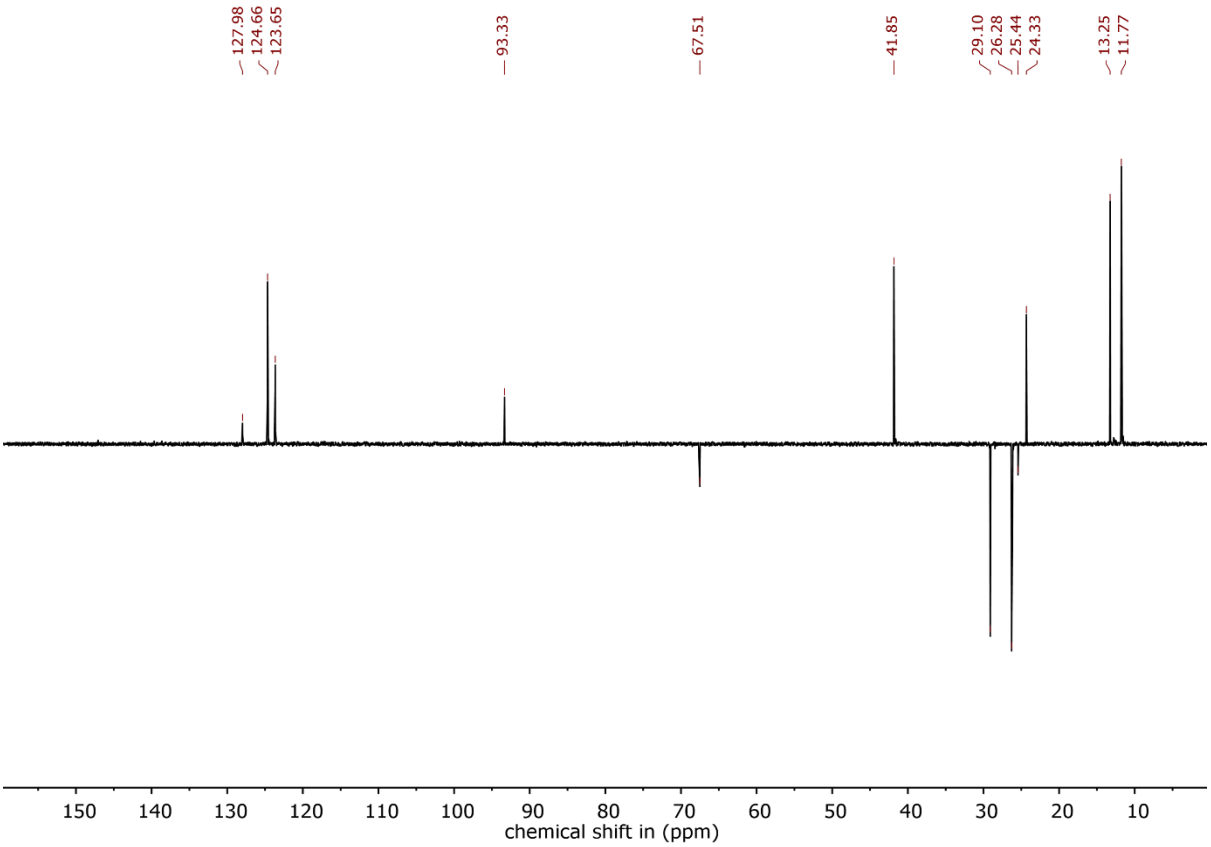


Figure S3. ^{13}C(DEPT 135) NMR spectrum of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**).

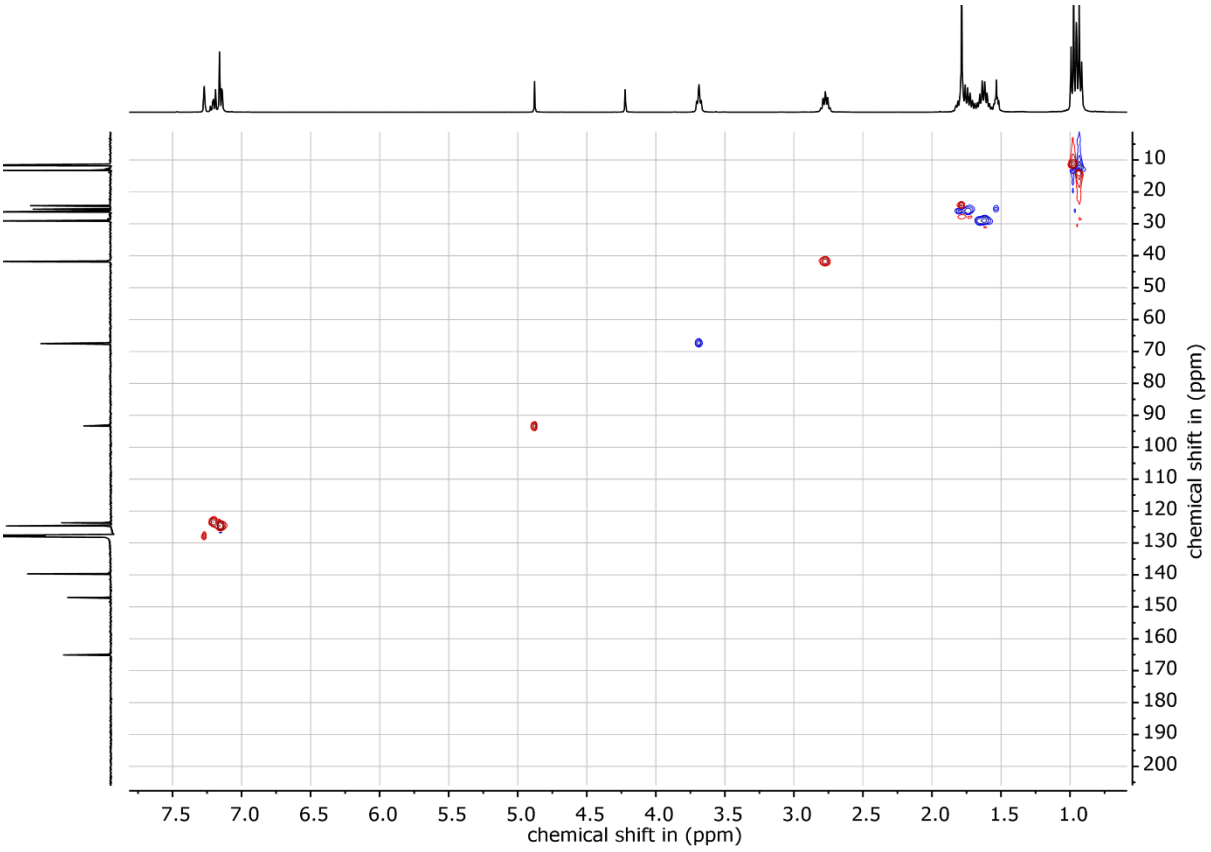


Figure S4. 2D-HSQC NMR spectrum of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**).

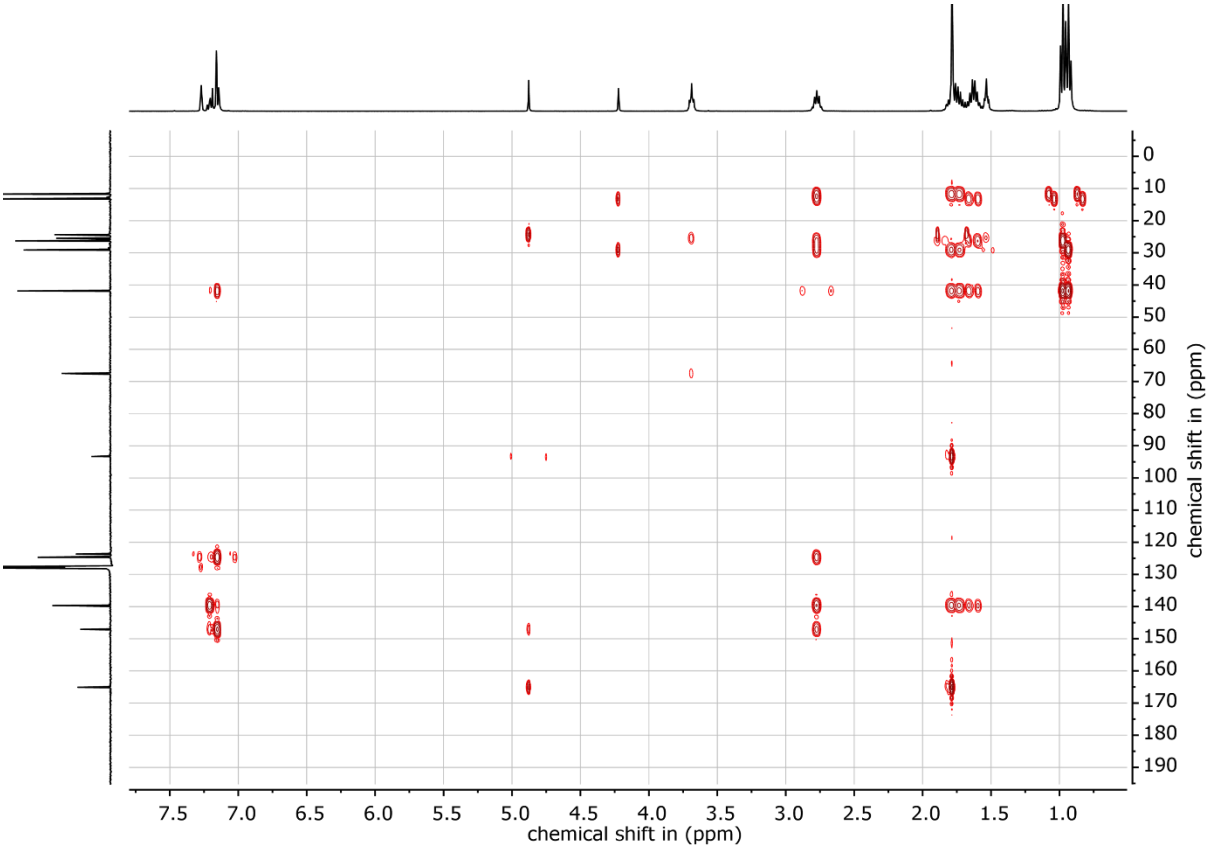


Figure S5. 2D-HMBC NMR spectrum of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**).

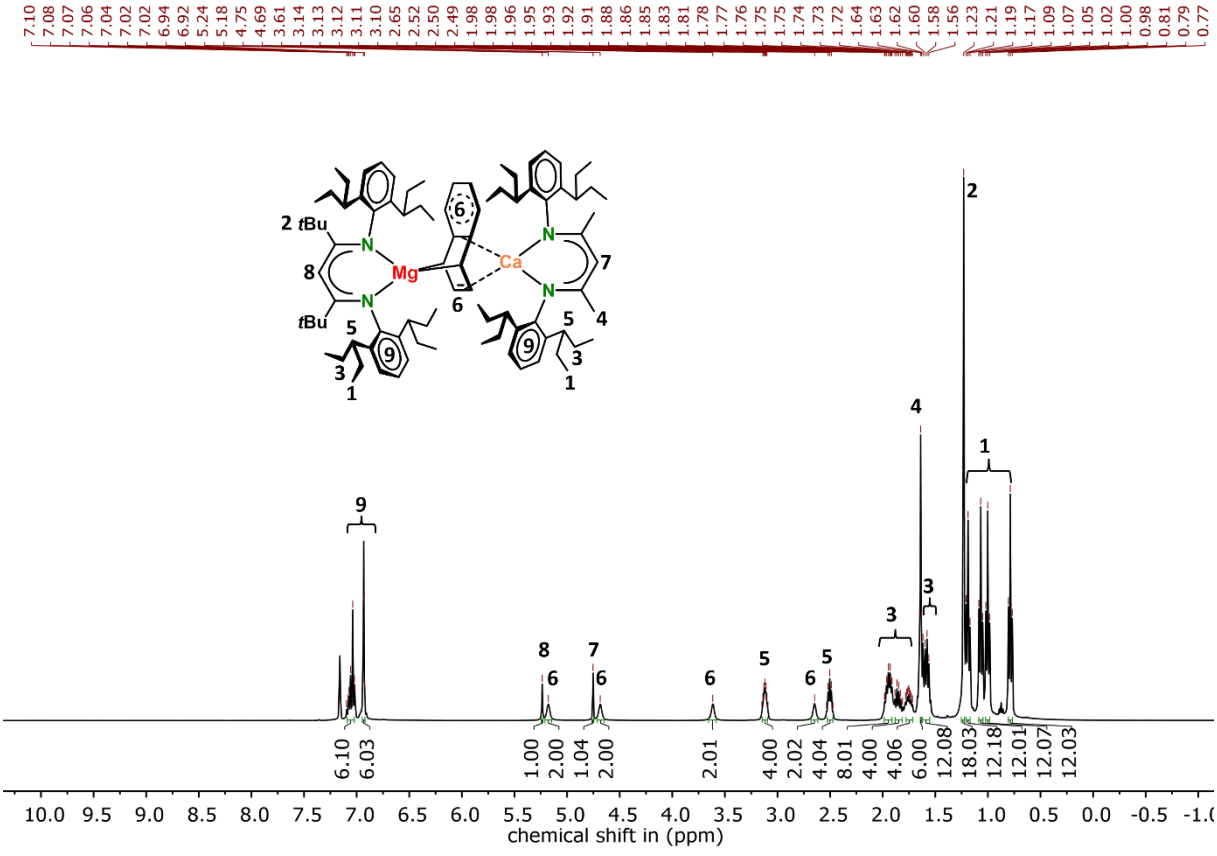


Figure S6. ^{1}H NMR (400.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

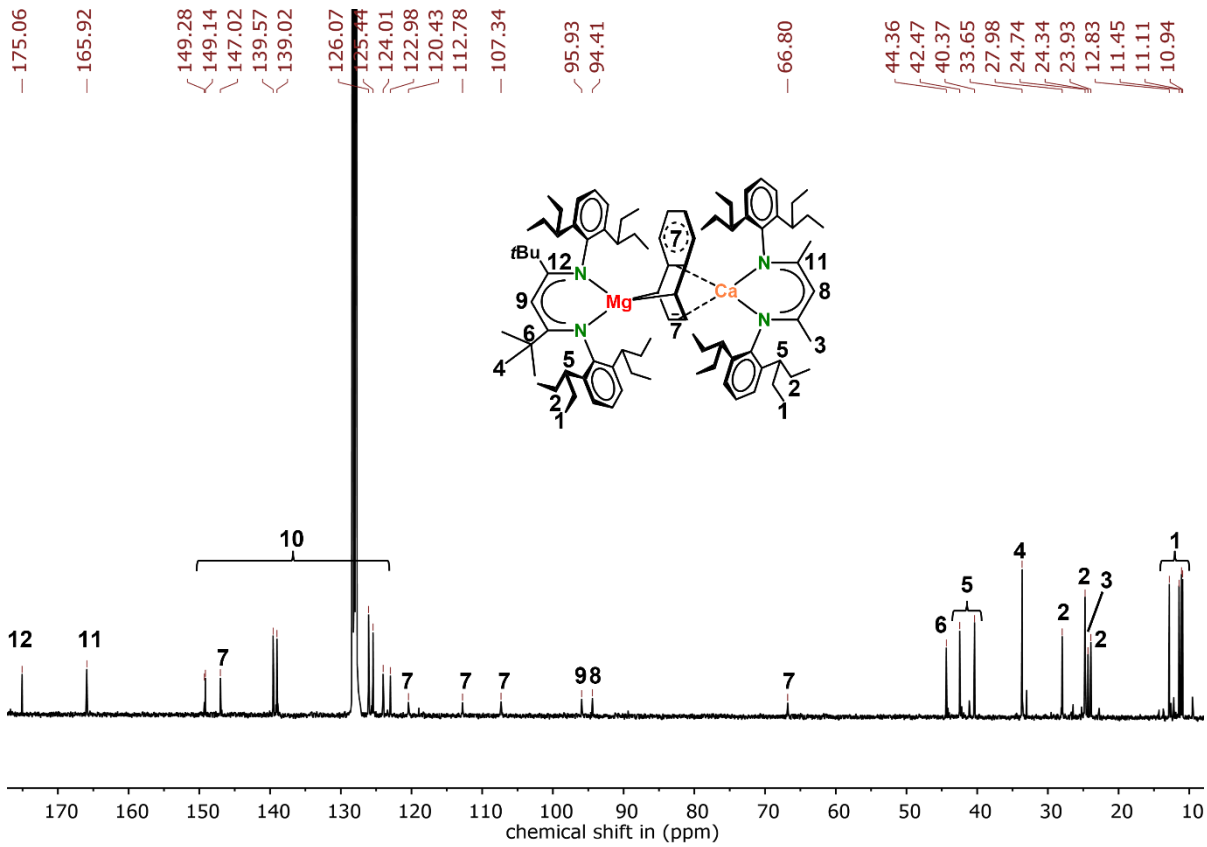


Figure S7. ^{13}C NMR (100 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

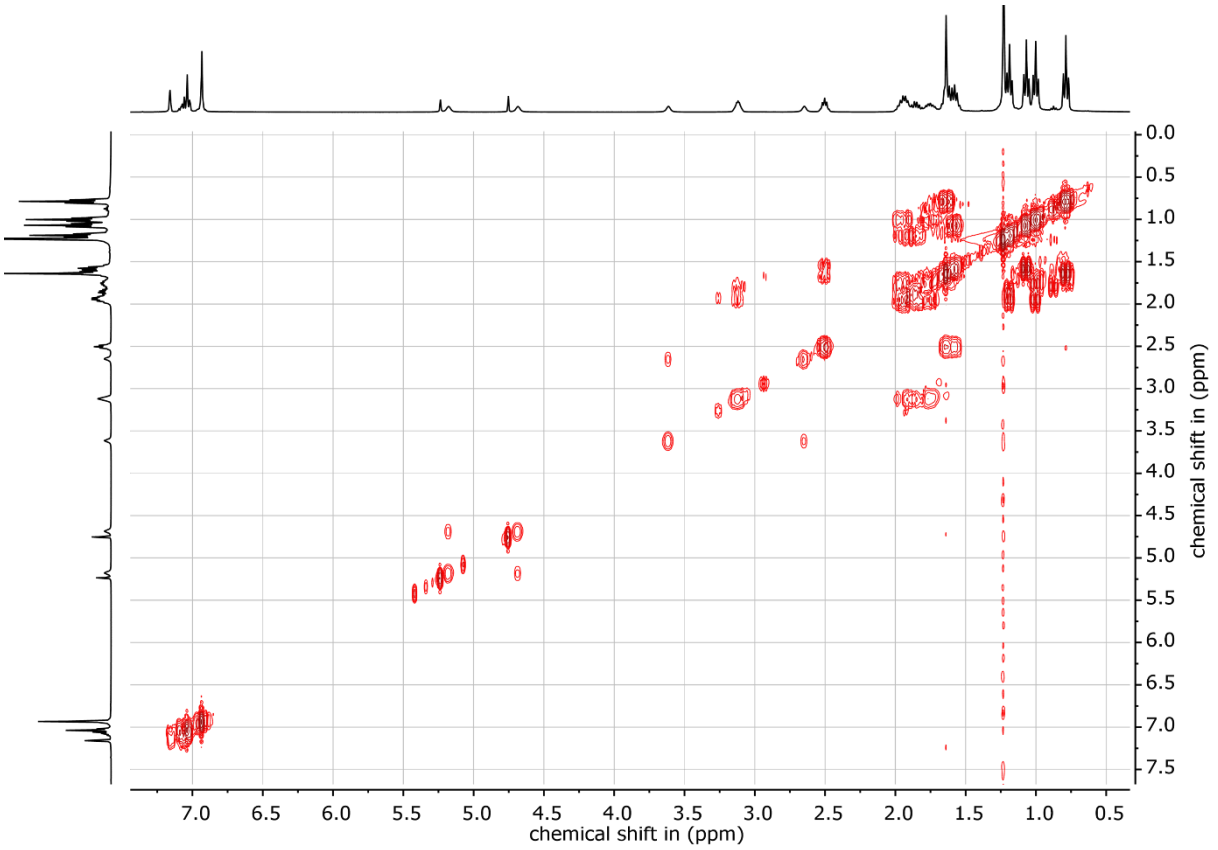


Figure S8. 2D-COSY NMR spectrum (400 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

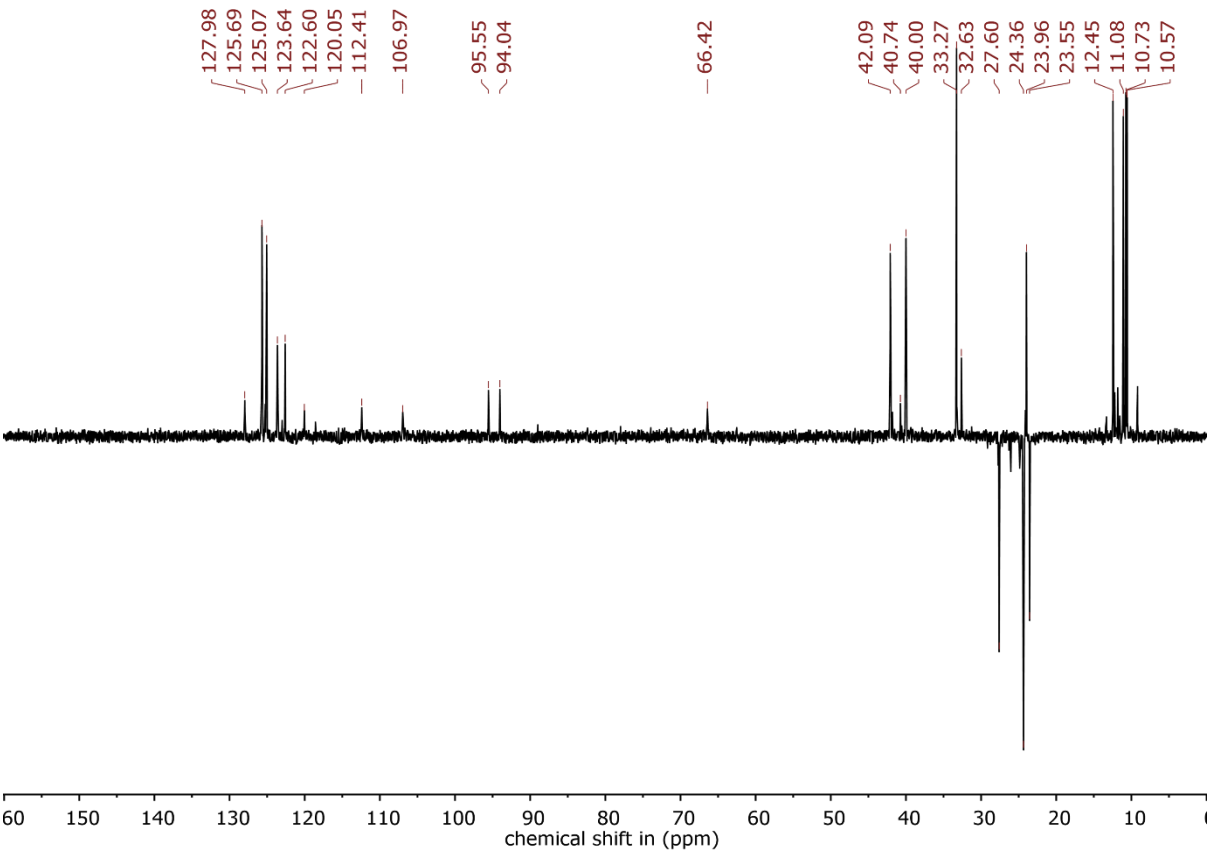


Figure S9. ^{13}C(DEPT 135) NMR spectrum of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

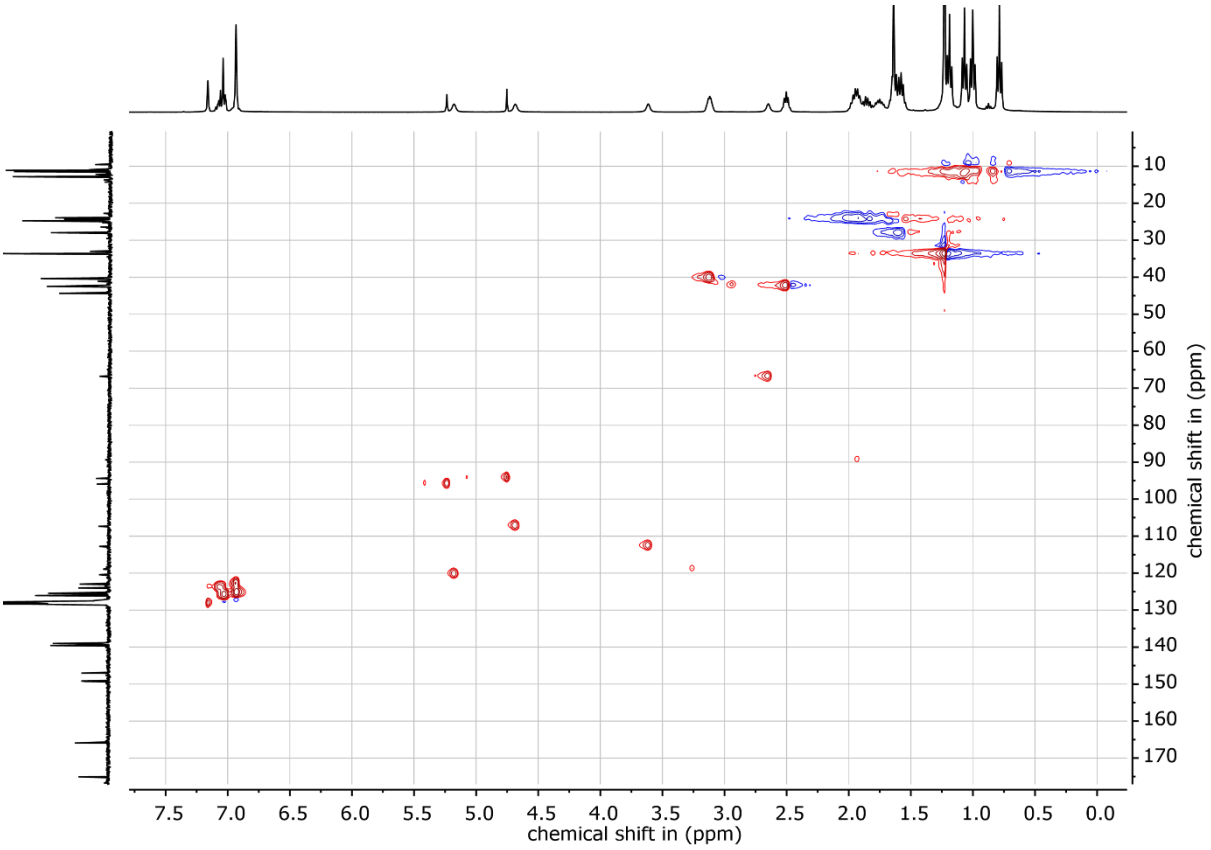


Figure S10. 2D-HSQC NMR spectrum of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

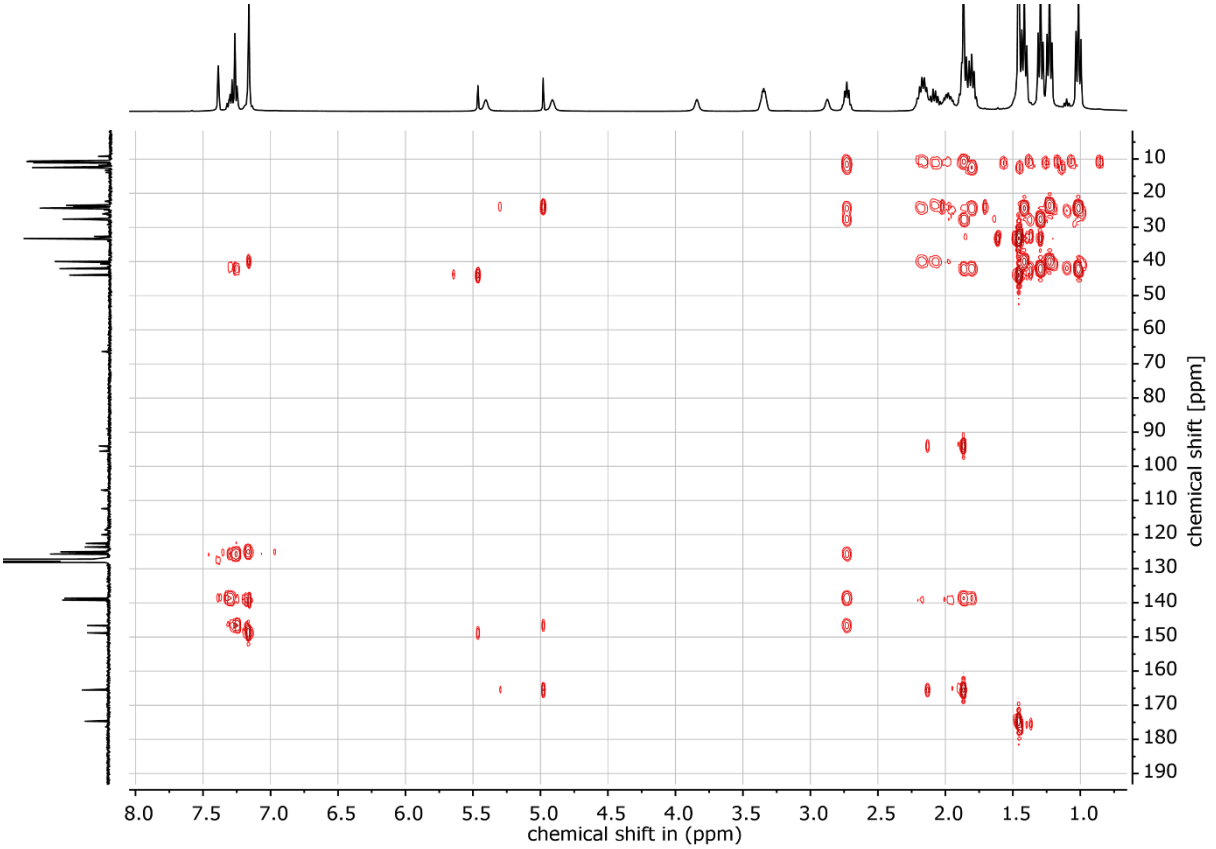


Figure S11. 2D-HMBC NMR spectrum of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).

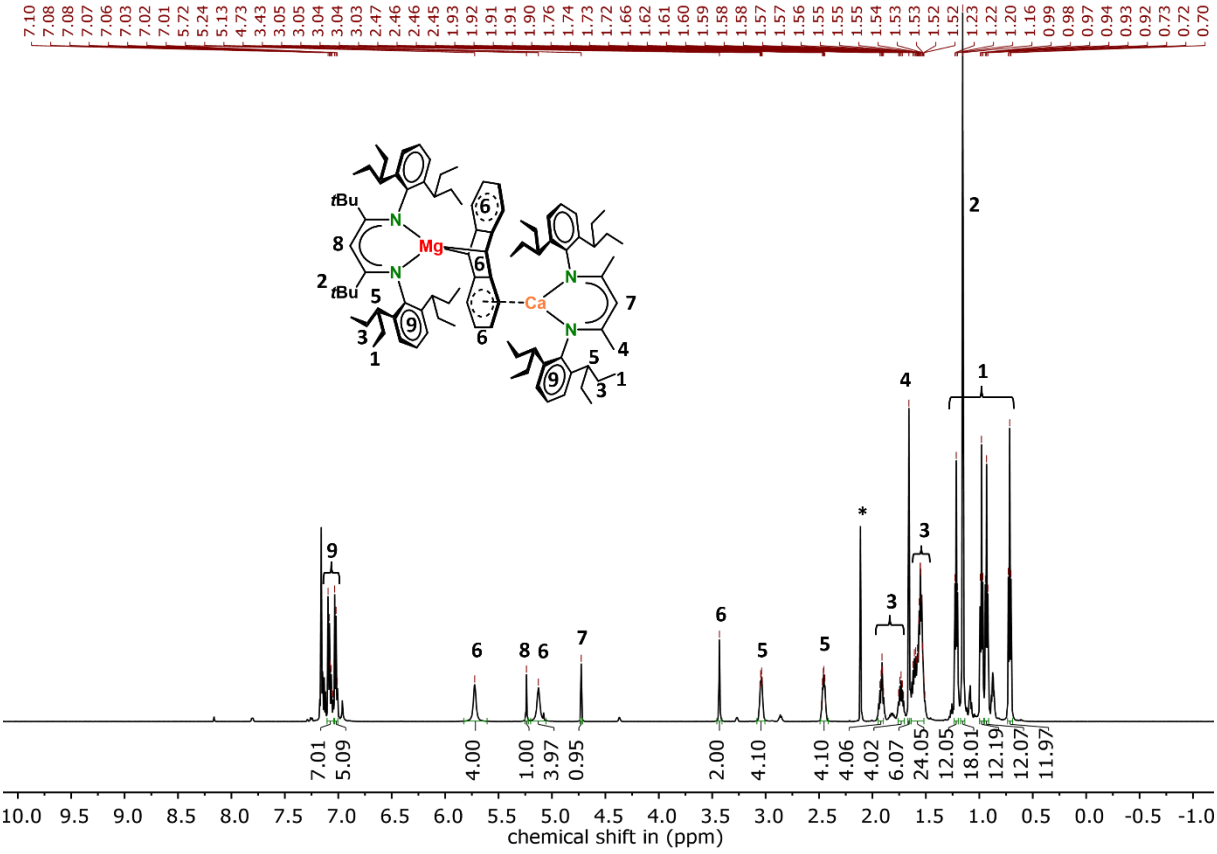


Figure S12. ^{1}H NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**). Signal marked with an asterisk are residue of toluene.

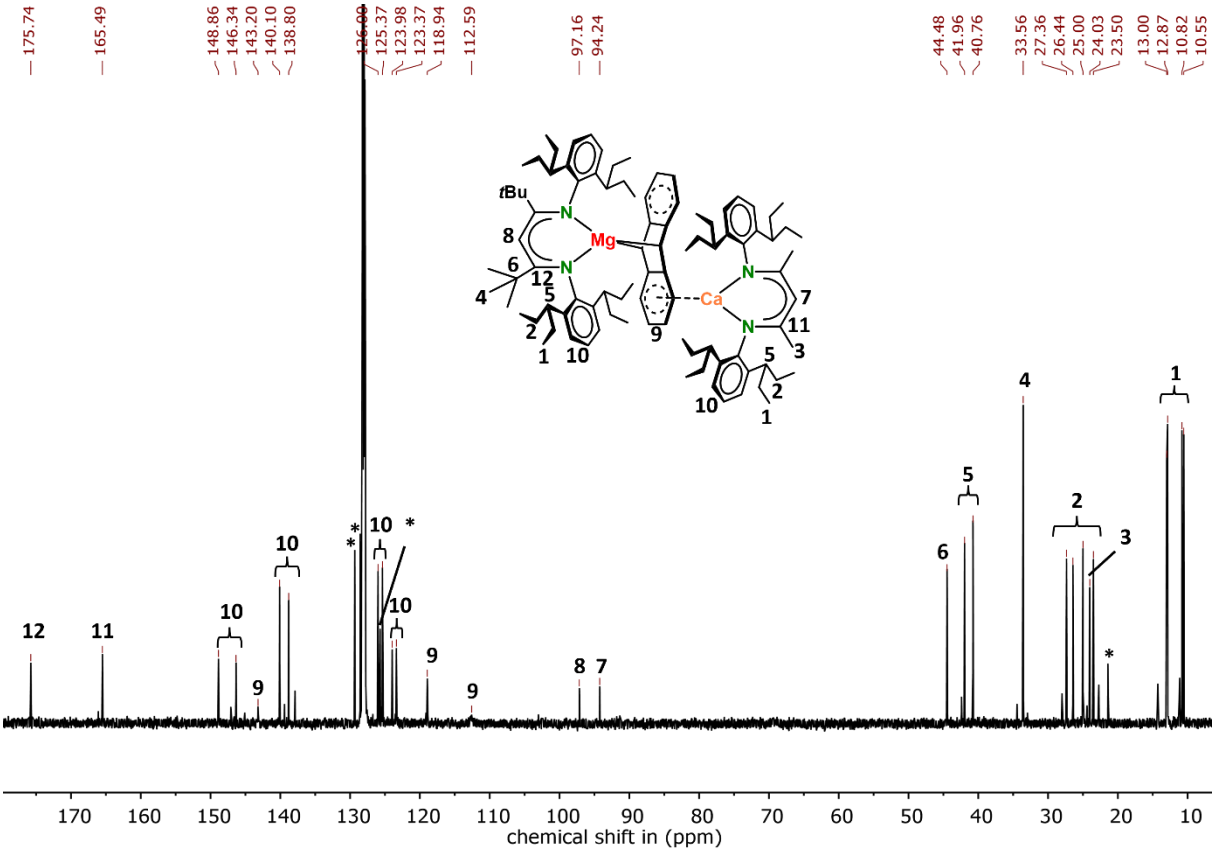


Figure S13. ^{13}C NMR (151.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**). Signals marked with an asterisk are residue of toluene.

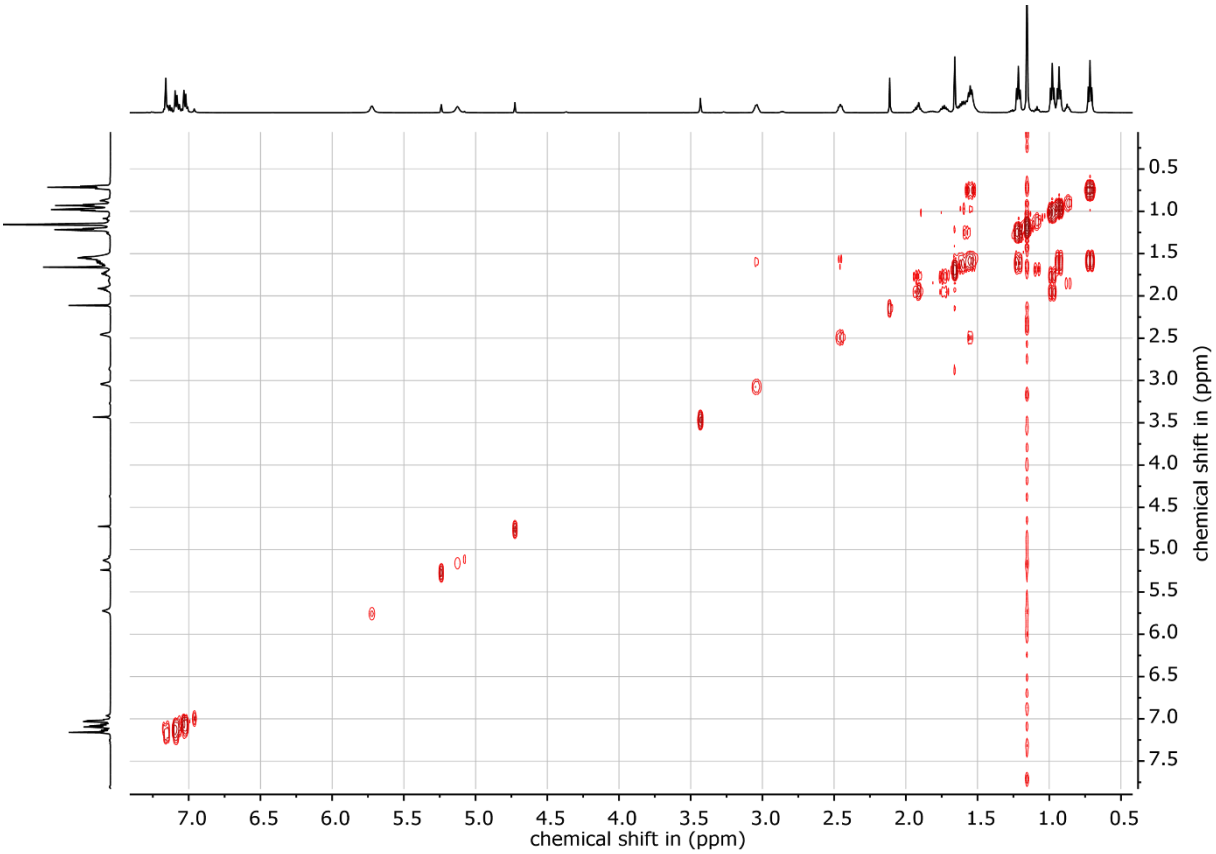


Figure S14. 2D-COSY NMR spectrum (600 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).

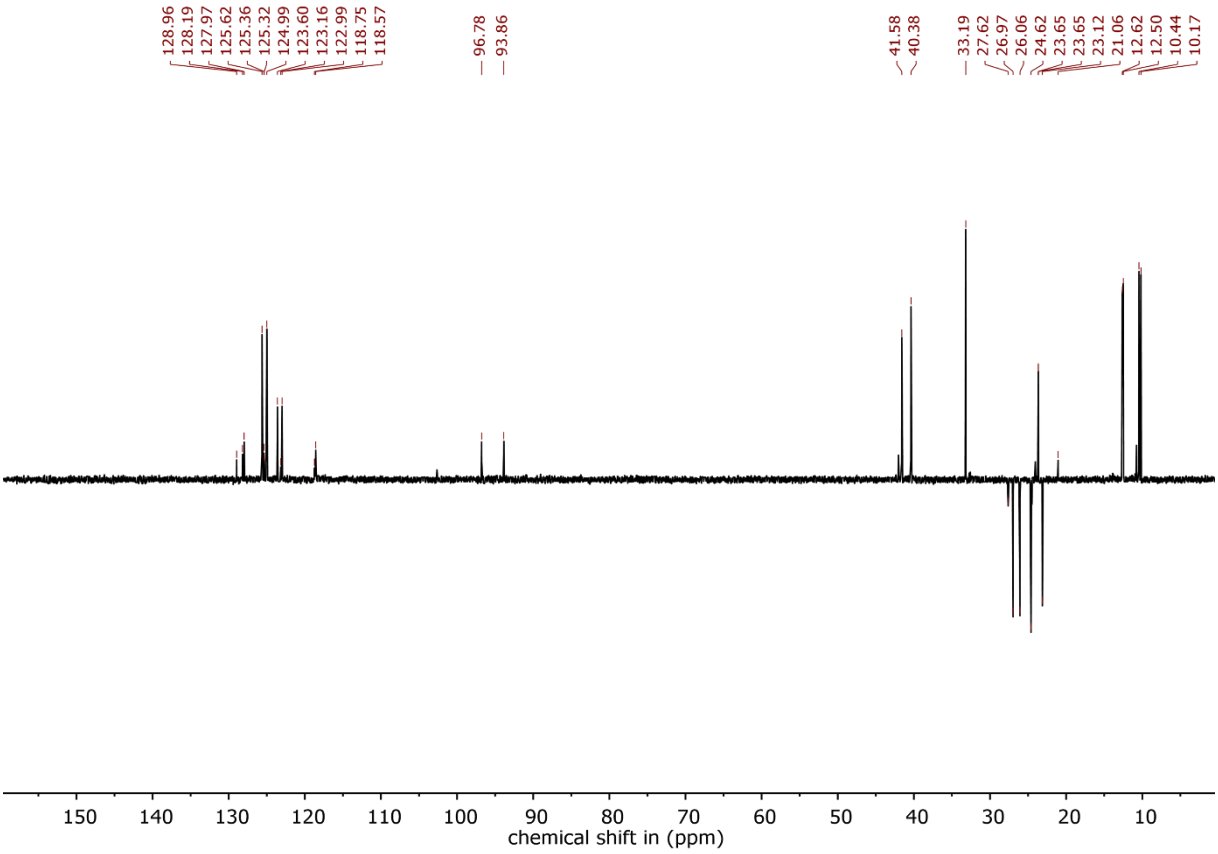


Figure S15. ^{13}C(DEPT 135) NMR spectrum of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).

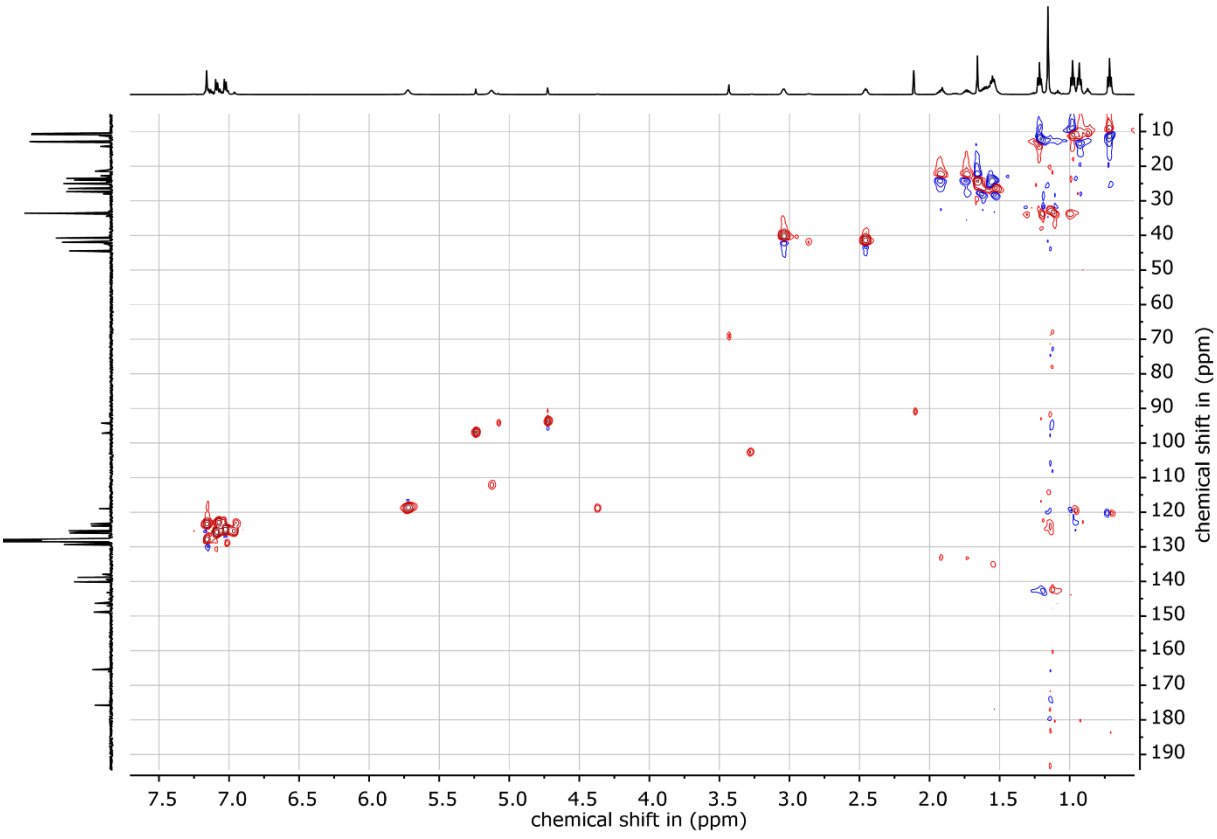


Figure S16. 2D-HSQC NMR spectrum (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).

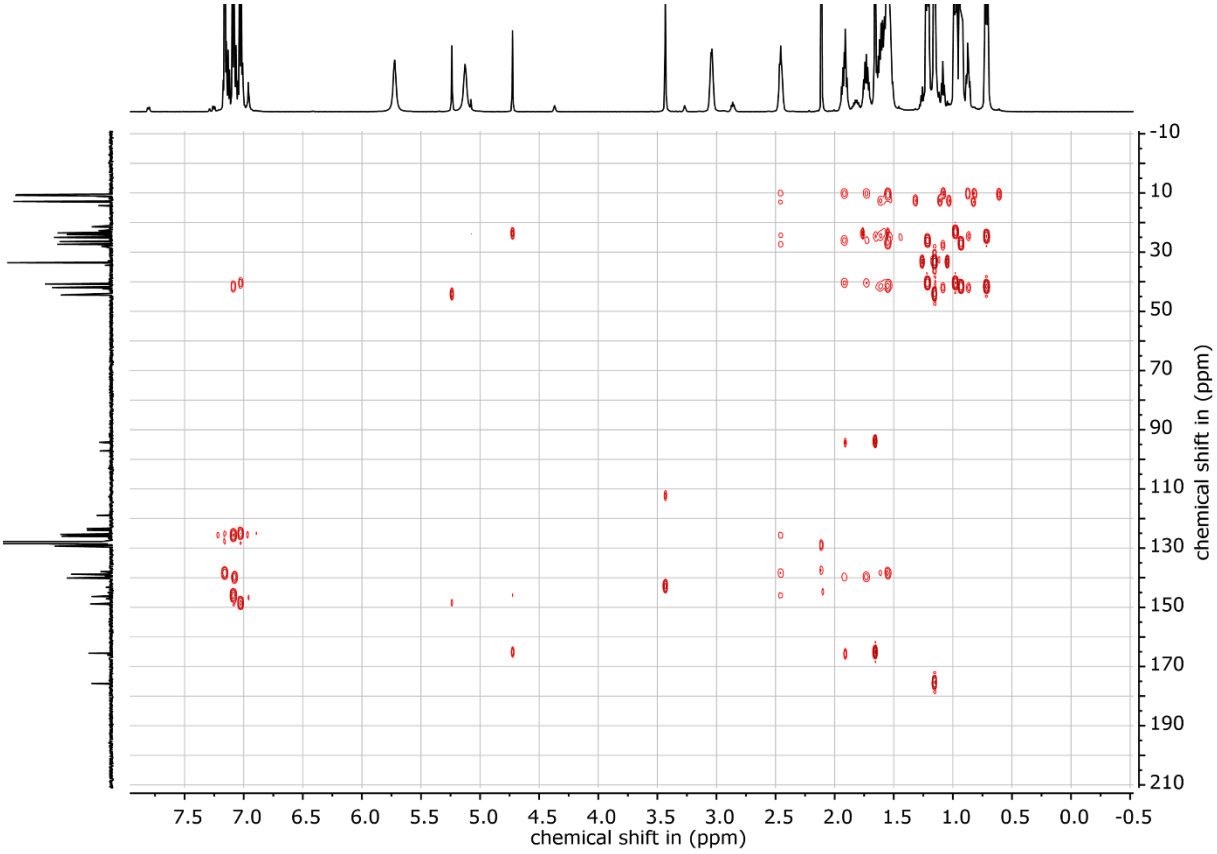


Figure S17. 2D-HMBC NMR spectrum (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).

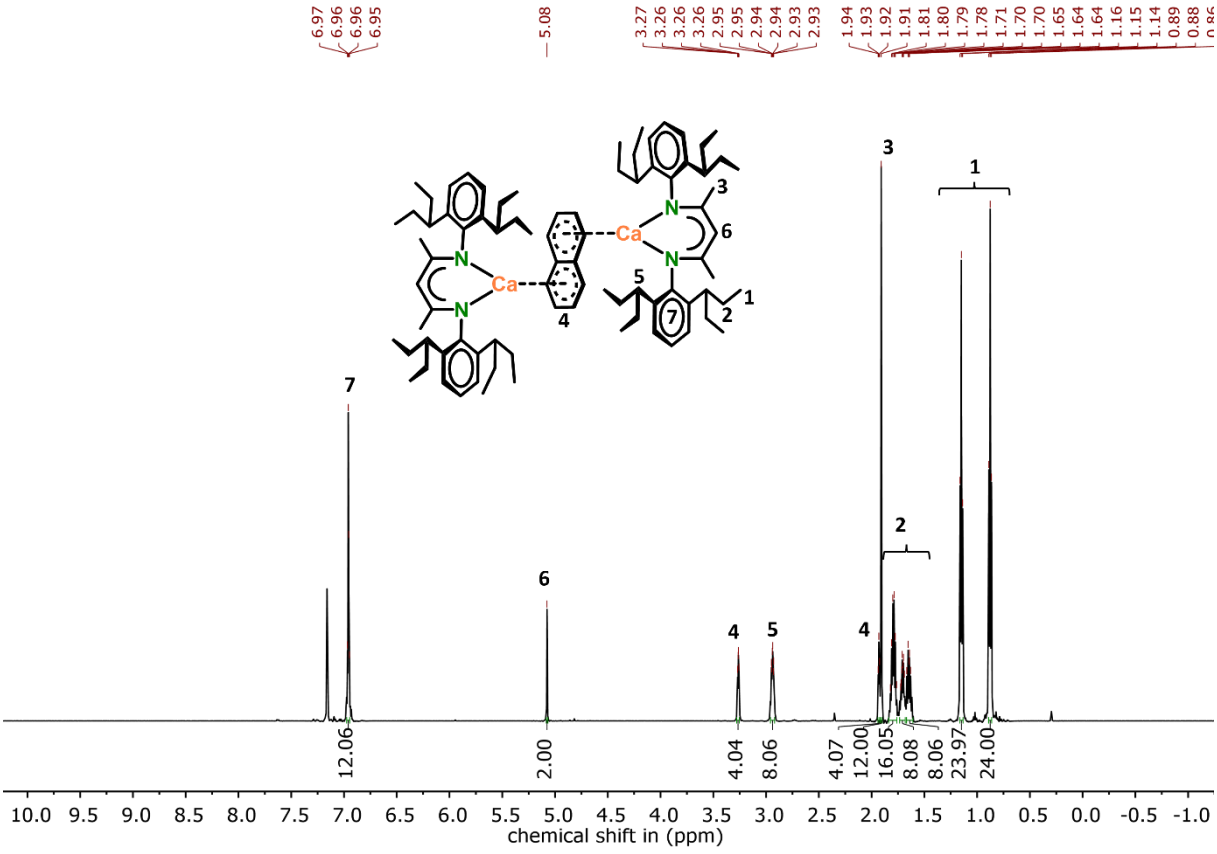


Figure S18. ^{1}H NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^6,μ^6-naphthalene)Ca(^{DIPeP}BDI) (**6**).

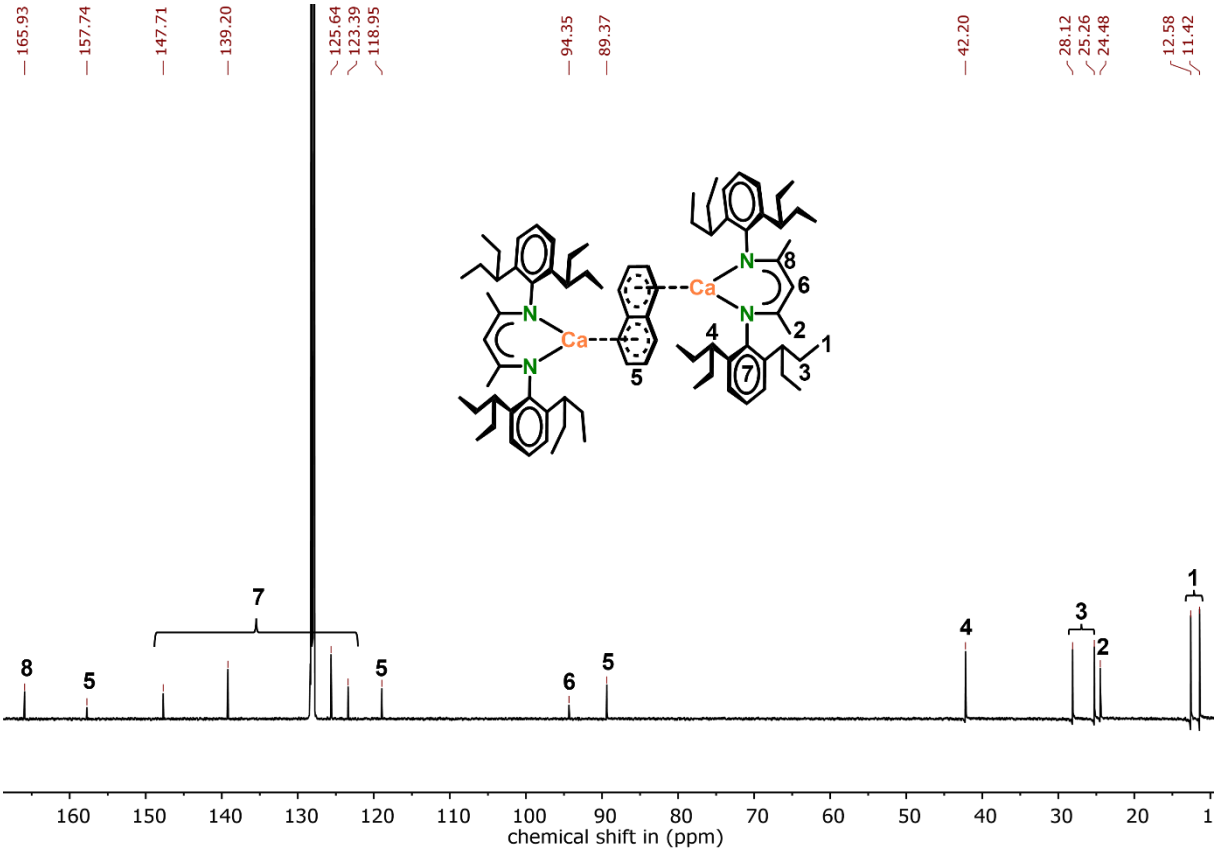


Figure S19. ^{13}C NMR (151.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**).

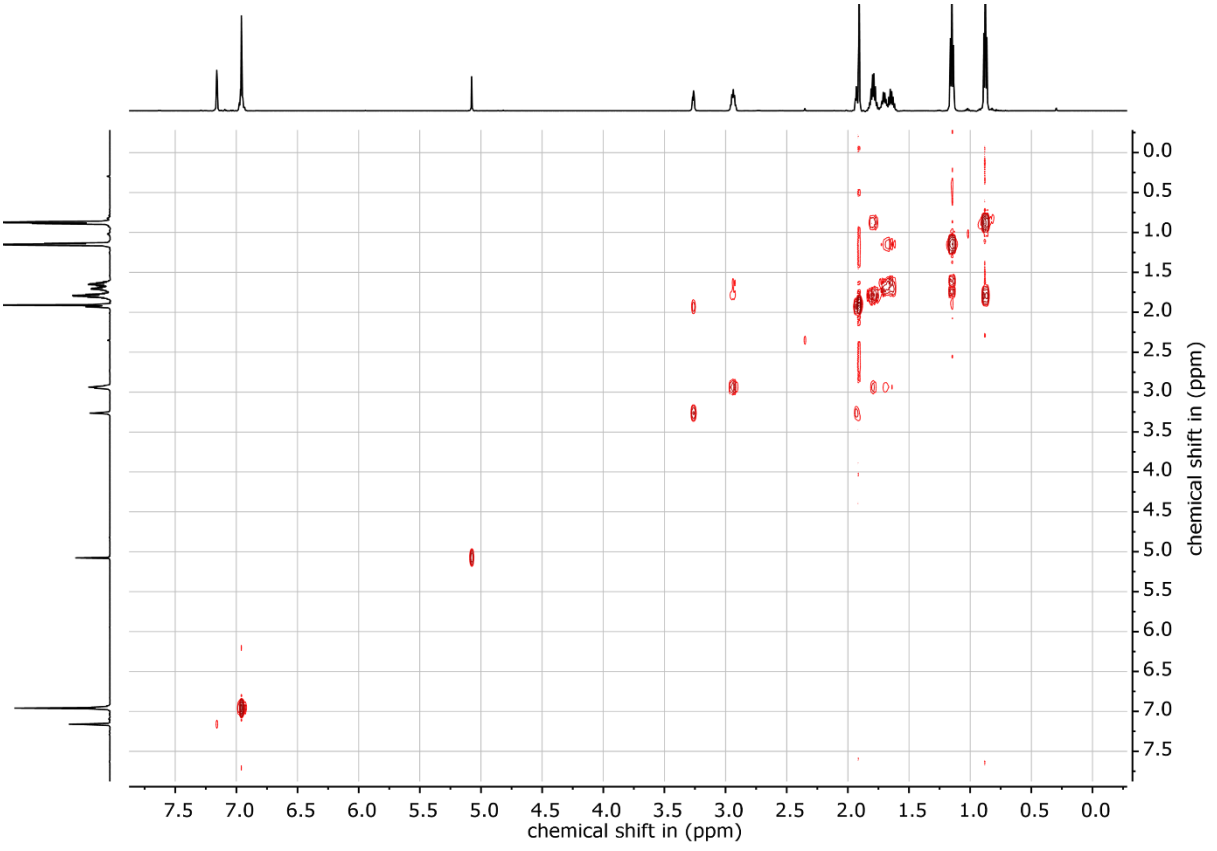


Figure S20. 2D-COSY NMR spectrum (600 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**).

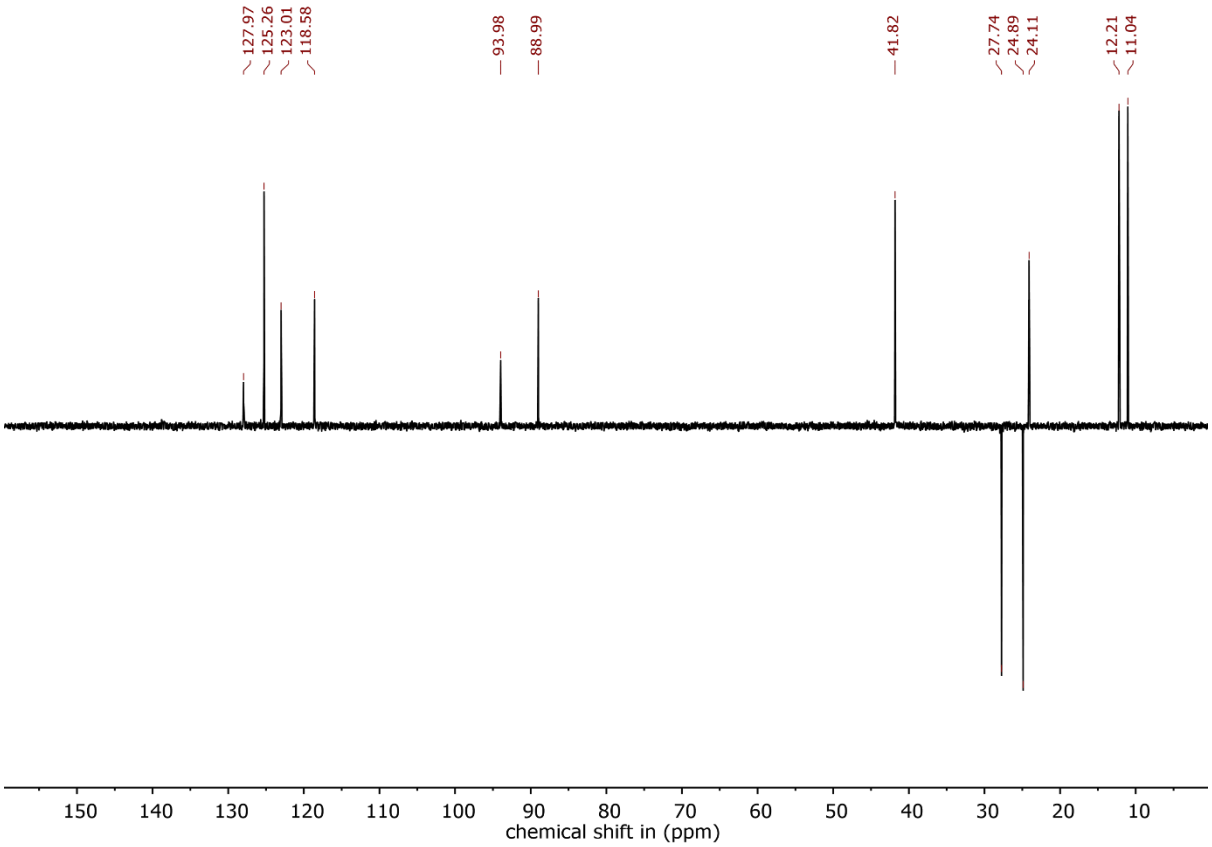


Figure S21. ^{13}C(DEPT 135) NMR spectrum of (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**).

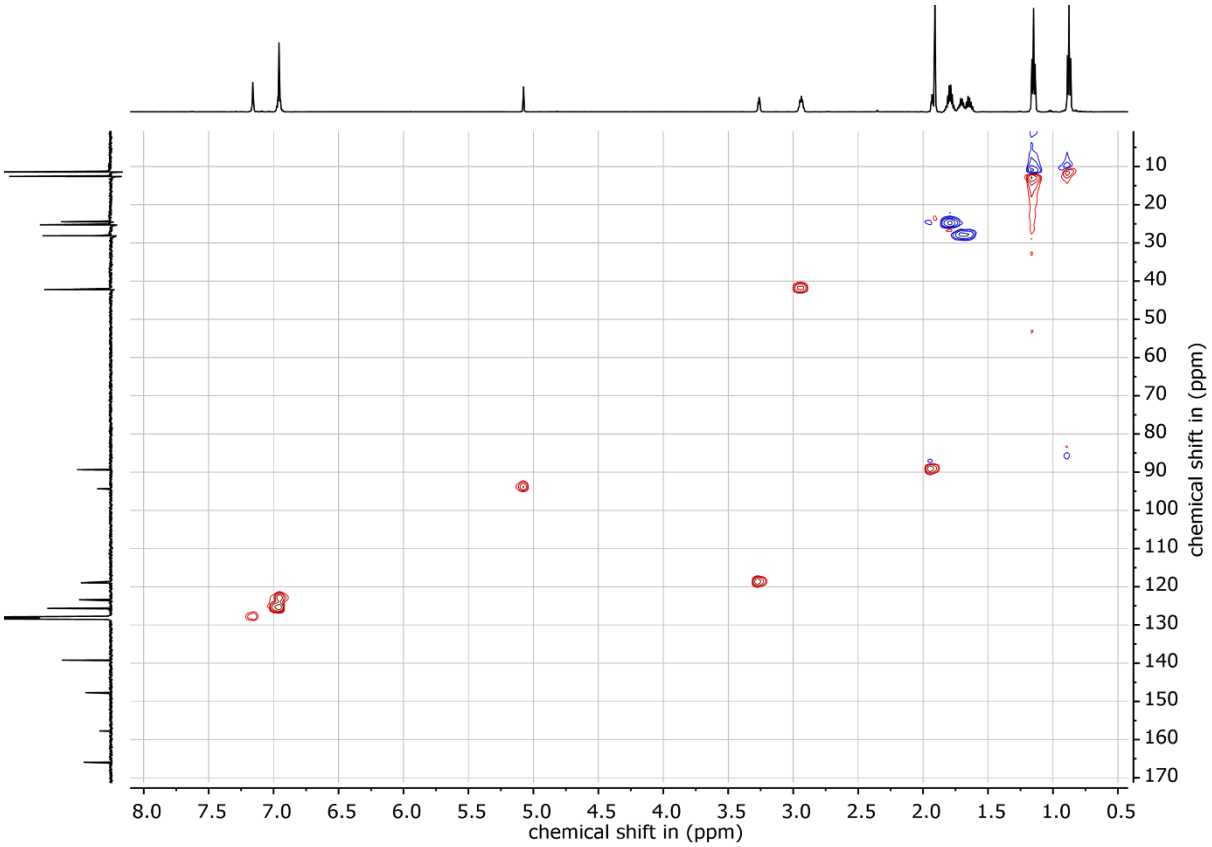


Figure S22. 2D-HSQC NMR spectrum (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**).

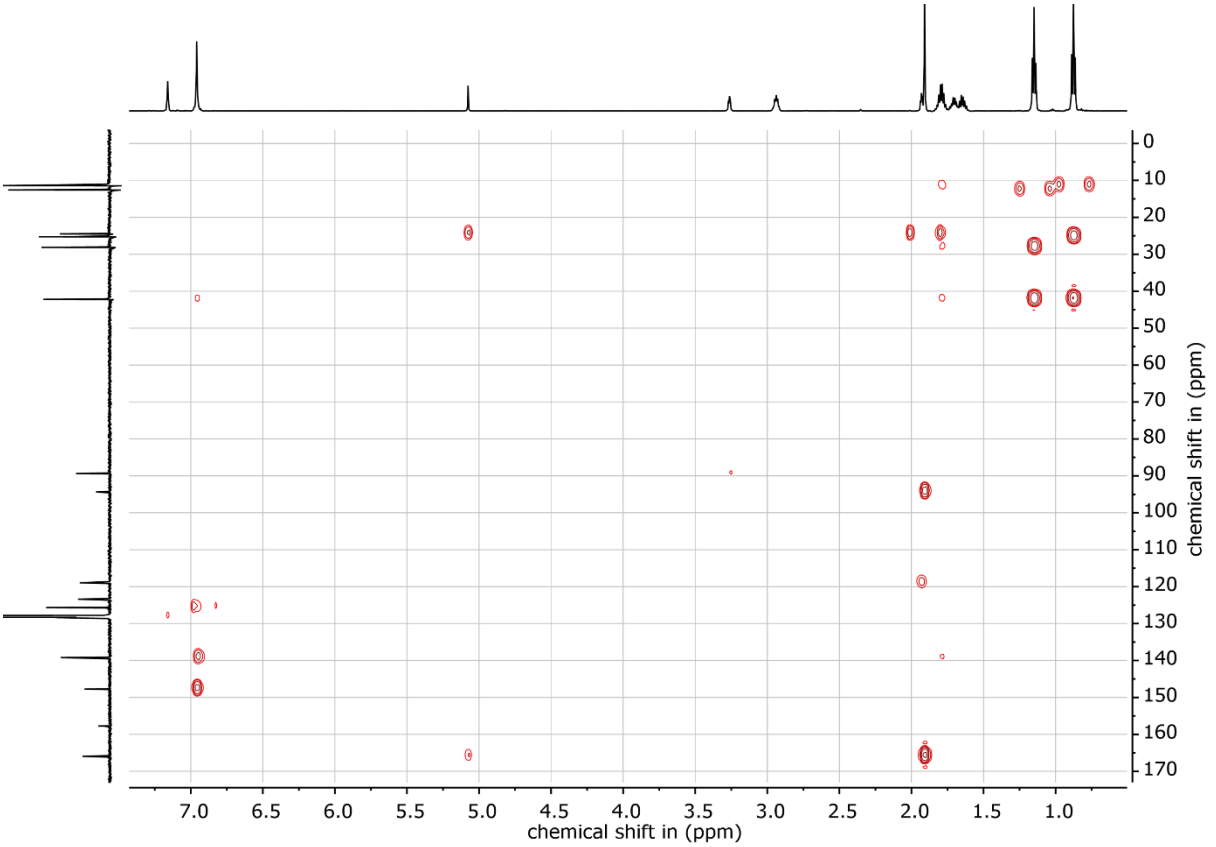


Figure S23. 2D-HMBC NMR spectrum (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**).

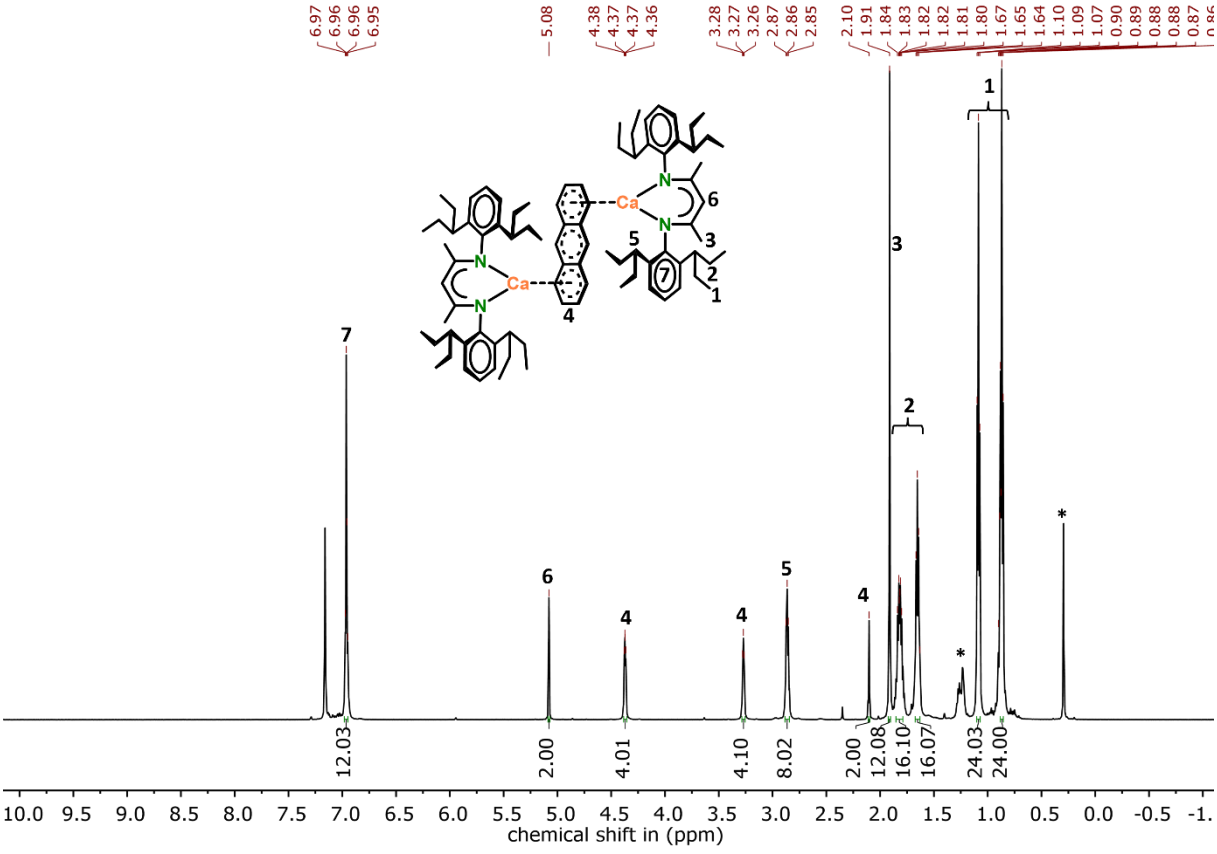


Figure S24. ^{1}H NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**).

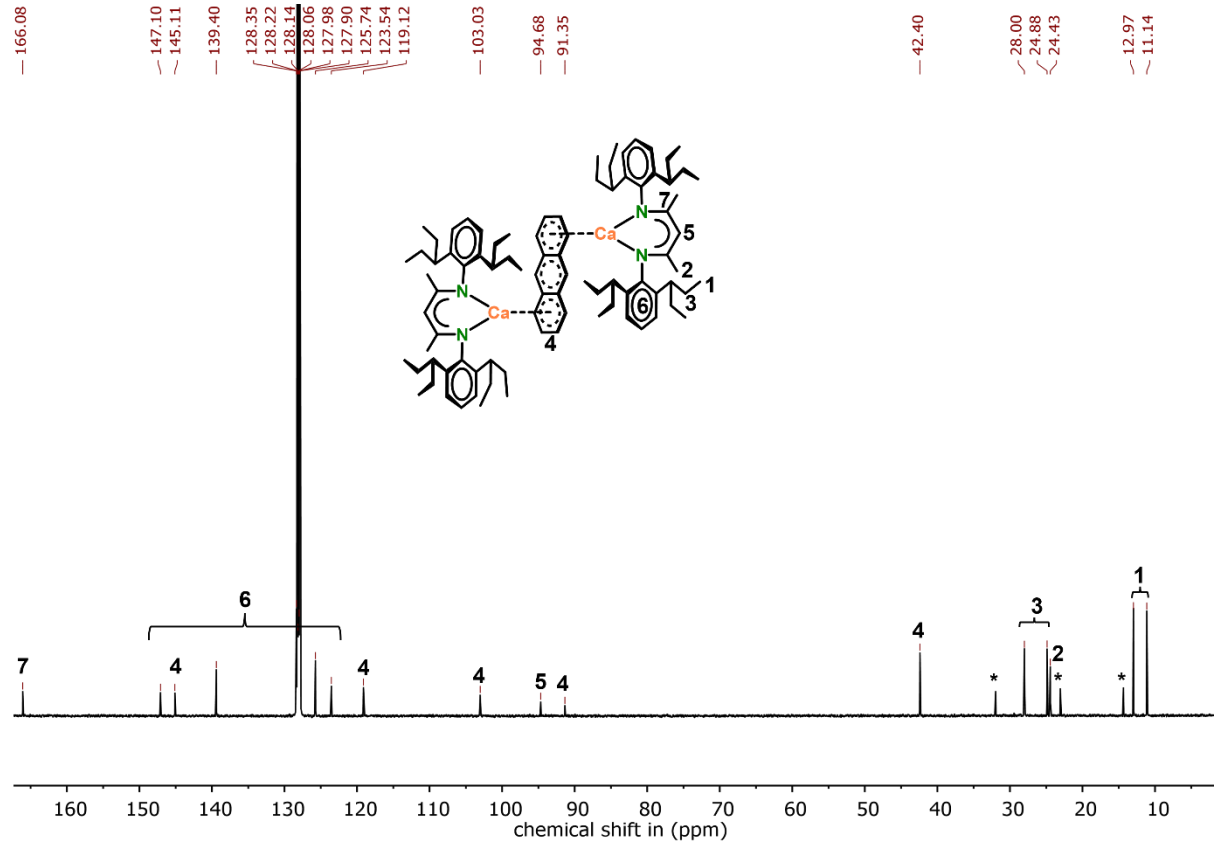


Figure S25. ^{13}C NMR (151.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^{δ},μ^{δ}-anthracene)Ca(^{DIPeP}BDI) (**7**).

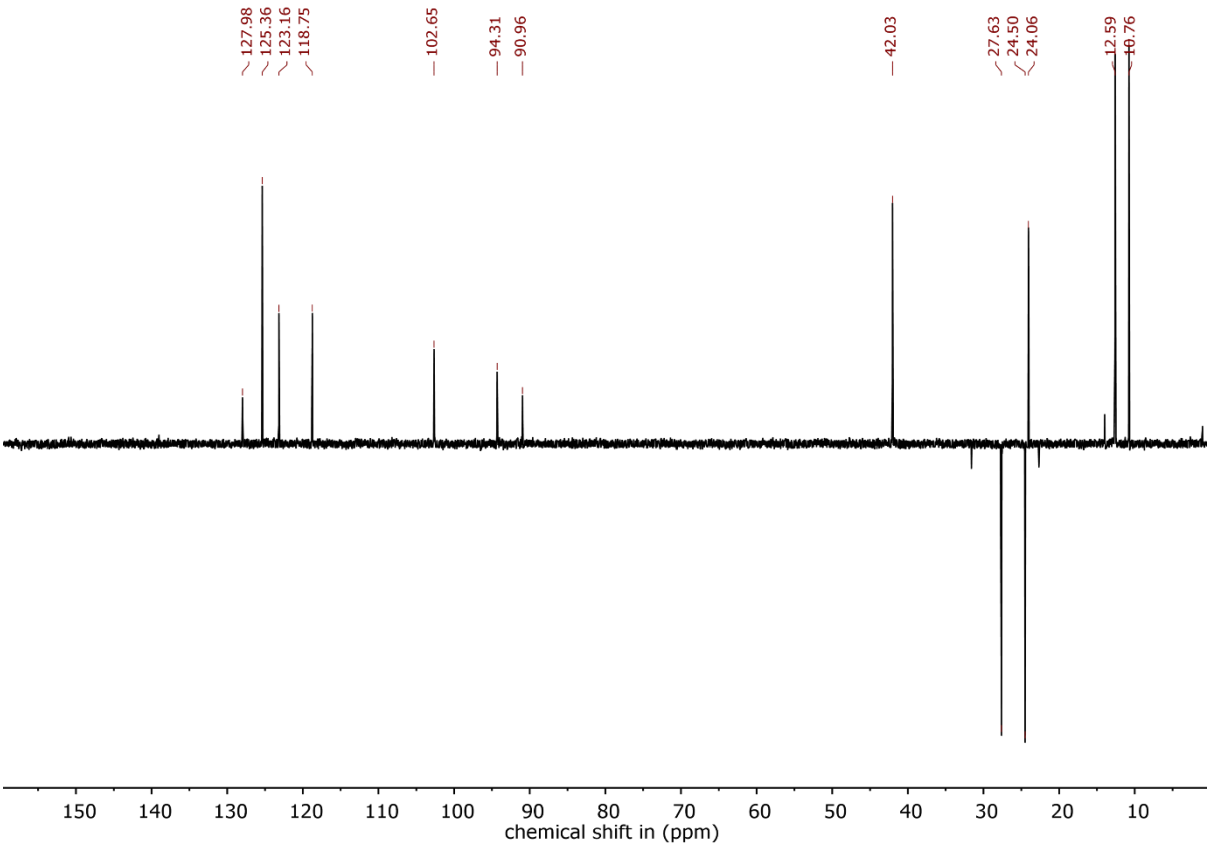


Figure S26. ^{13}C(DEPT 135) NMR spectrum of (^{DIPeP}BDI)Ca(μ^{δ},μ^{δ}-anthracene)Ca(^{DIPeP}BDI) (**7**).

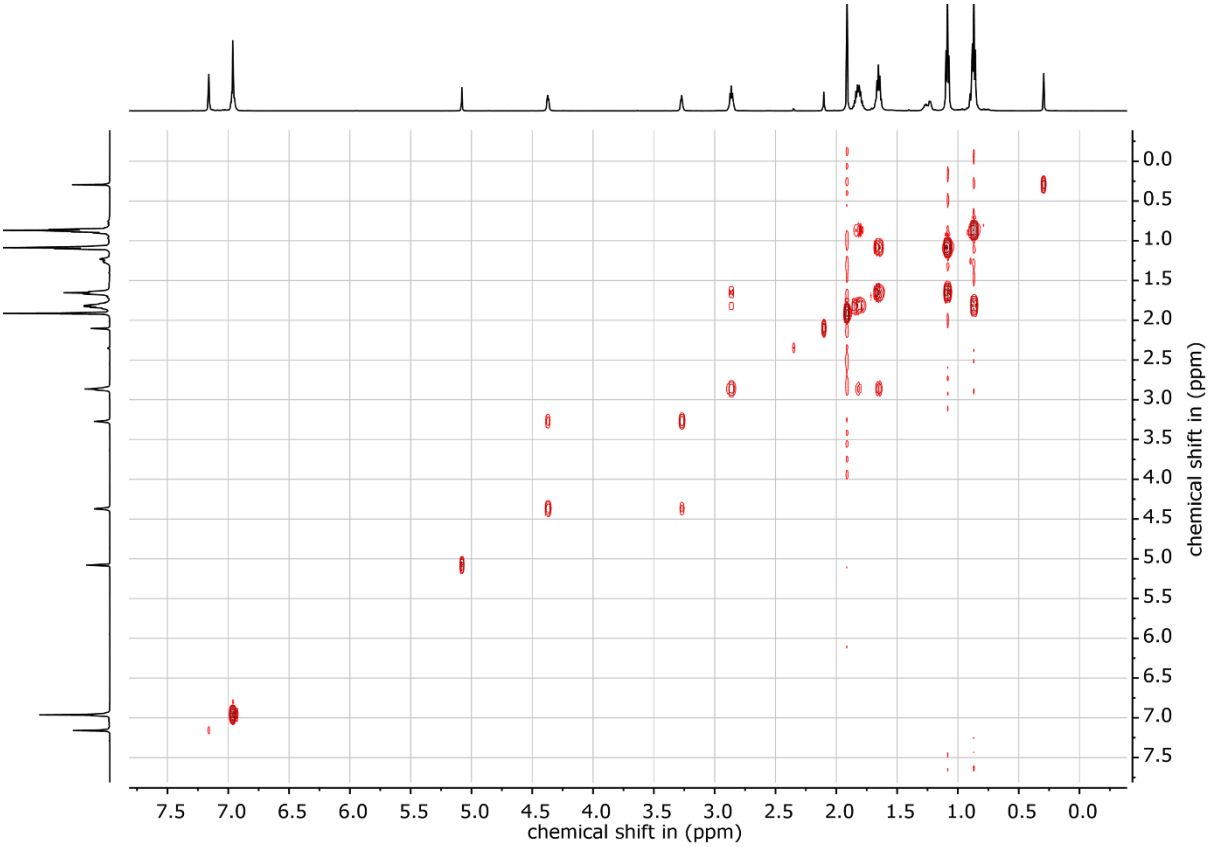


Figure S27. 2D-COSY NMR spectrum (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**).

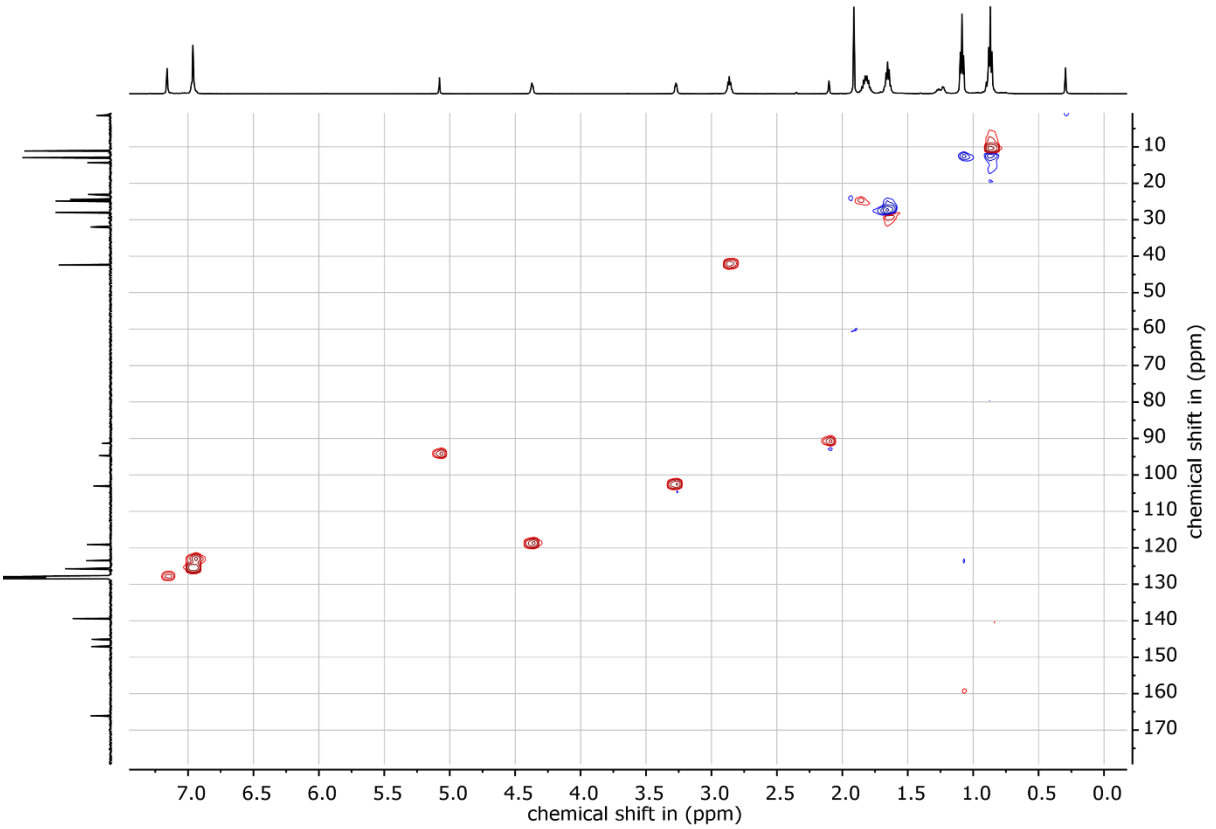


Figure S28. 2D-HSQC NMR spectrum (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**).

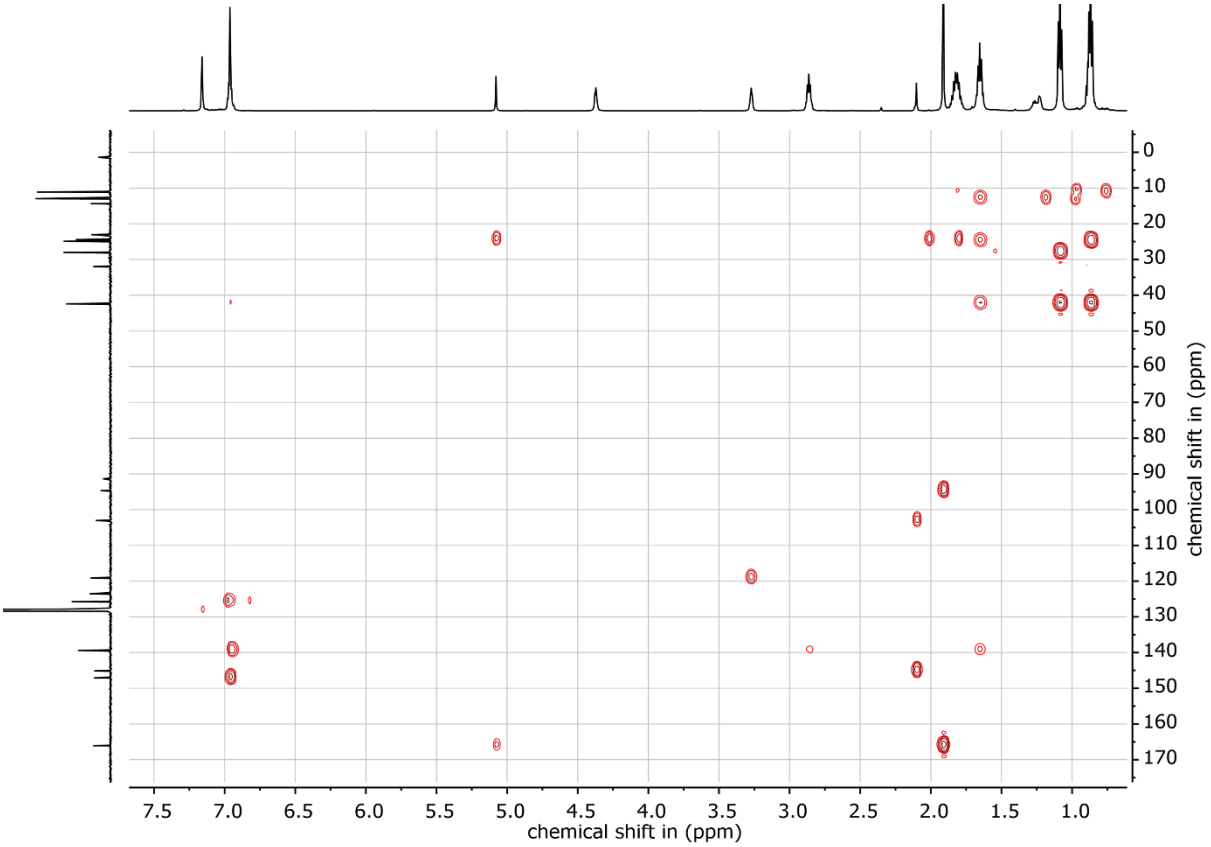


Figure S29. 2D-HMBC NMR spectrum (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**).

2. Selected reactions

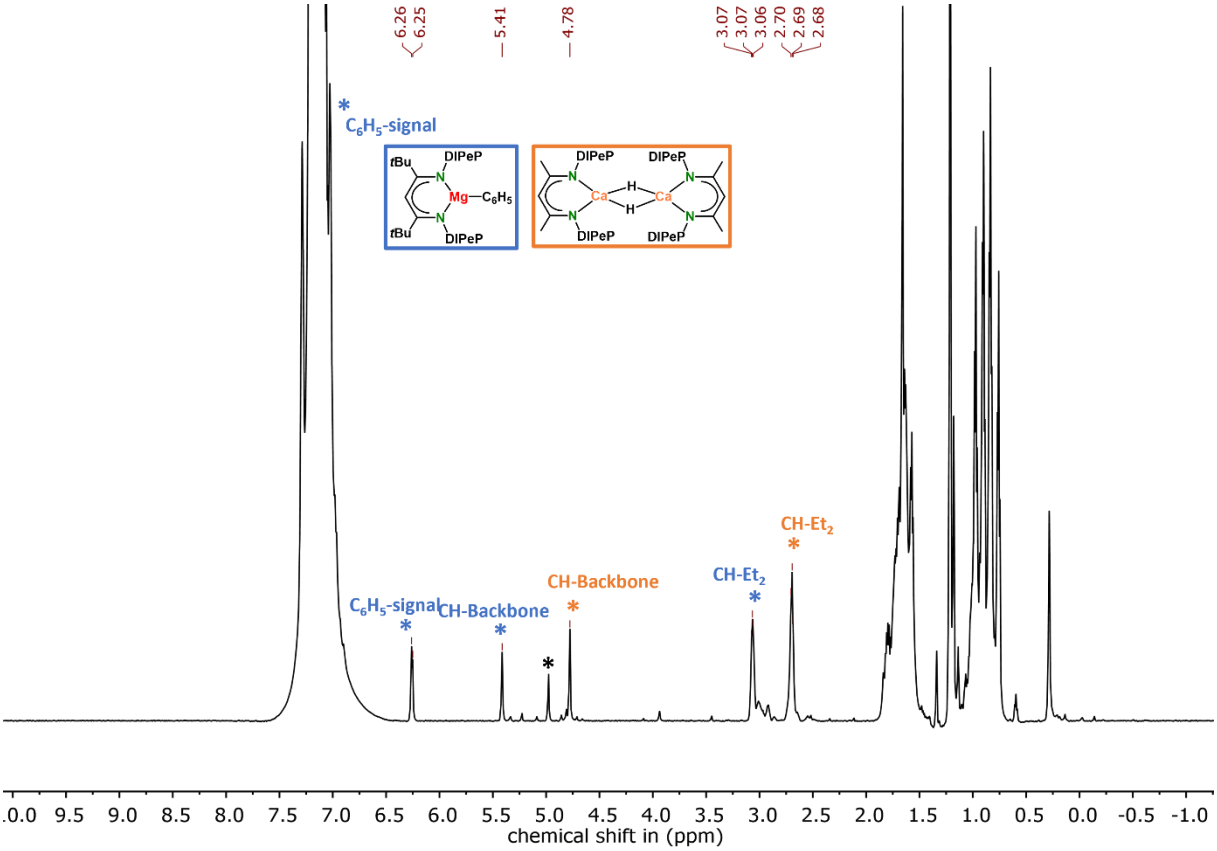


Figure S30. ^{1}H NMR of the reaction of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in C_6H_6 after two days at room temperature. Mainly the two products (^{DIPeP}BDI*)MgPh (**X**) and [(^{DIPeP}BDI)CaH]$_2$ are formed. The signal for the Ca-H is not visible. Unidentified impurities are marked with a black *.

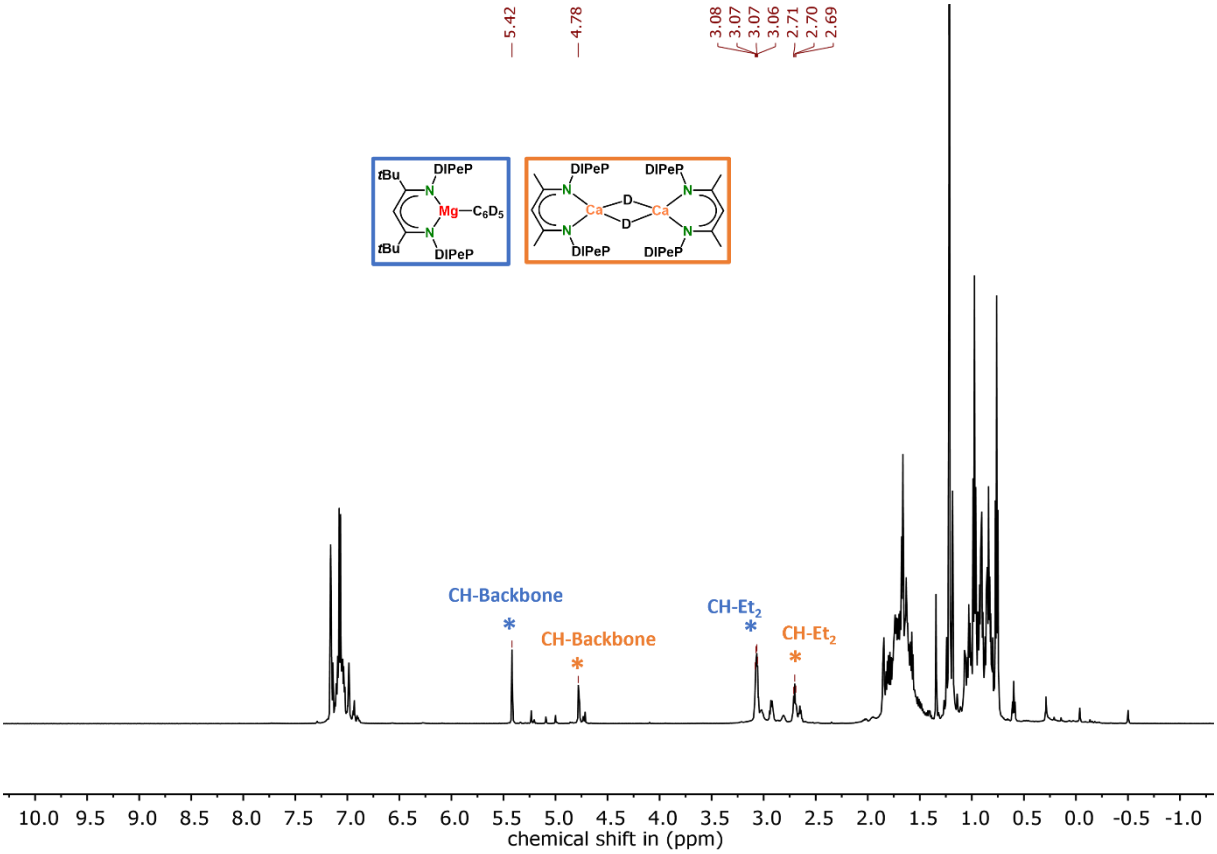


Figure S31. ^{1}H NMR of the reaction of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in C_6D_6 after two days at room temperature. Mainly the two products (^{DIPeP}BDI*)MgPh (**X**) and [(^{DIPeP}BDI)CaD]$_2$ are formed. The Ca-D and the Mg-C_6D_5 signals are not visible in the ^{1}H NMR but can be seen in the ^{2}D NMR spectrum (Figure S32).

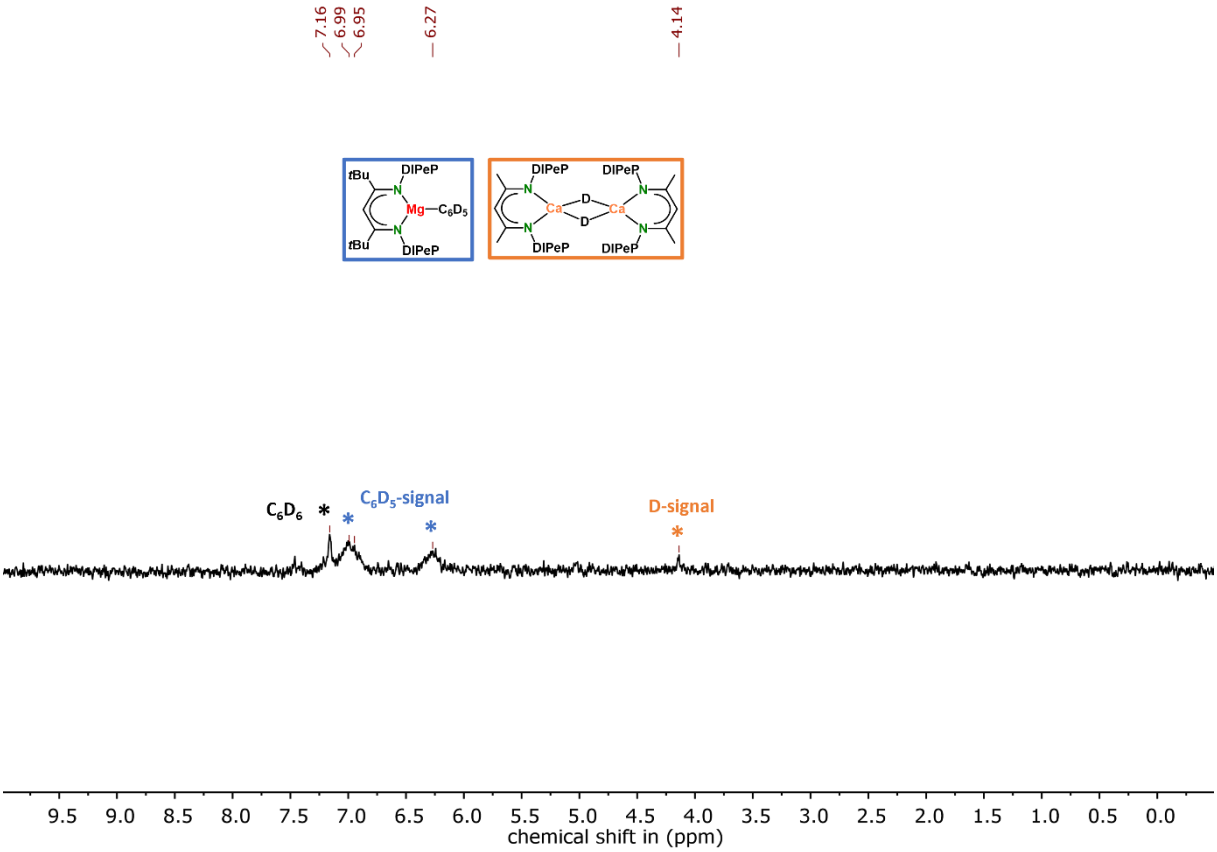


Figure S32. ^{2}D NMR of the reaction of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in C_6D_6 after two days at room temperature. The Ca-D and the Mg-C_6D_5 signals can be observed in the ^{2}D NMR. After the reaction is finished, the solvent was removed and dried under vacuum. The resulting powder was then dissolved in hexanes and measured. Residual C_6D_6 is marked with a black *.

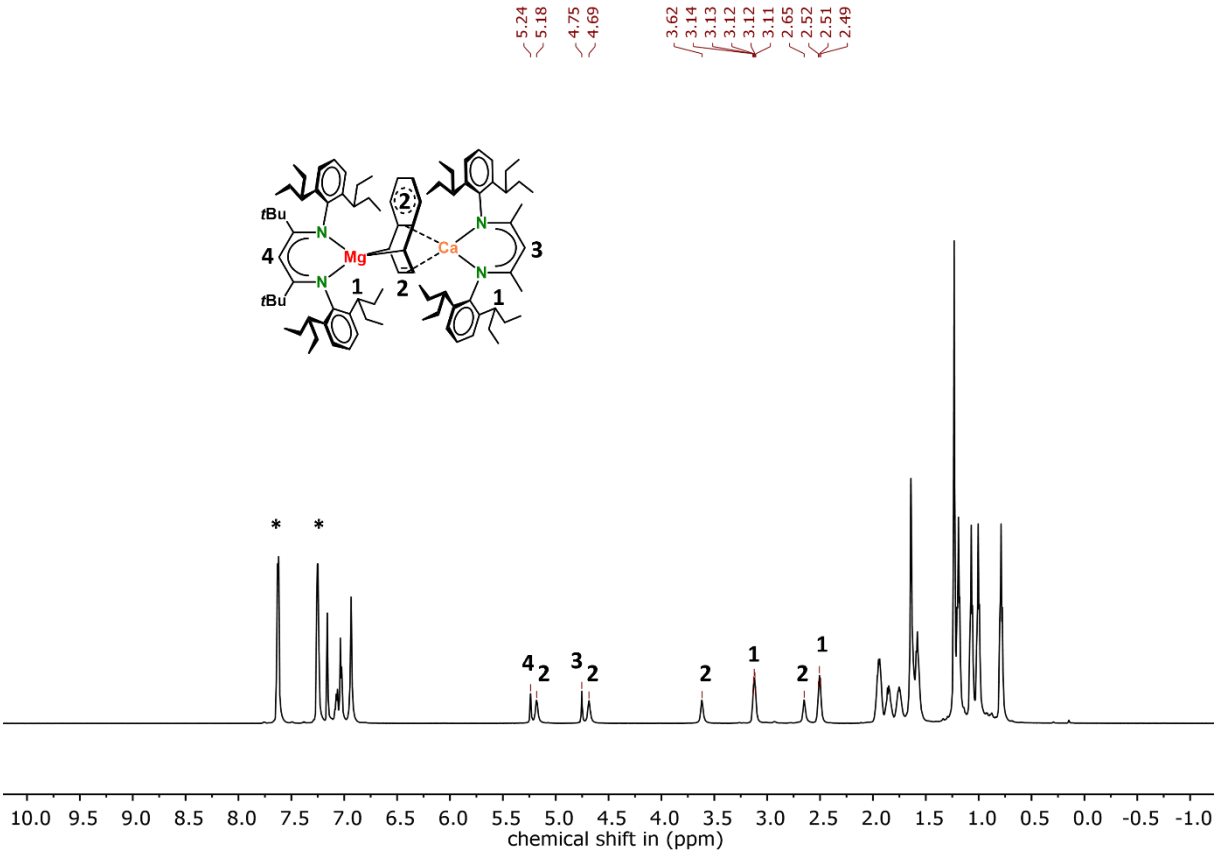


Figure S33. ^{1}H NMR spectrum of the crude reaction of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in the presence of naphthalene in C_6D_6. The spectrum essentially shows the pure product (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**). Residual naphthalene is marked with a *.

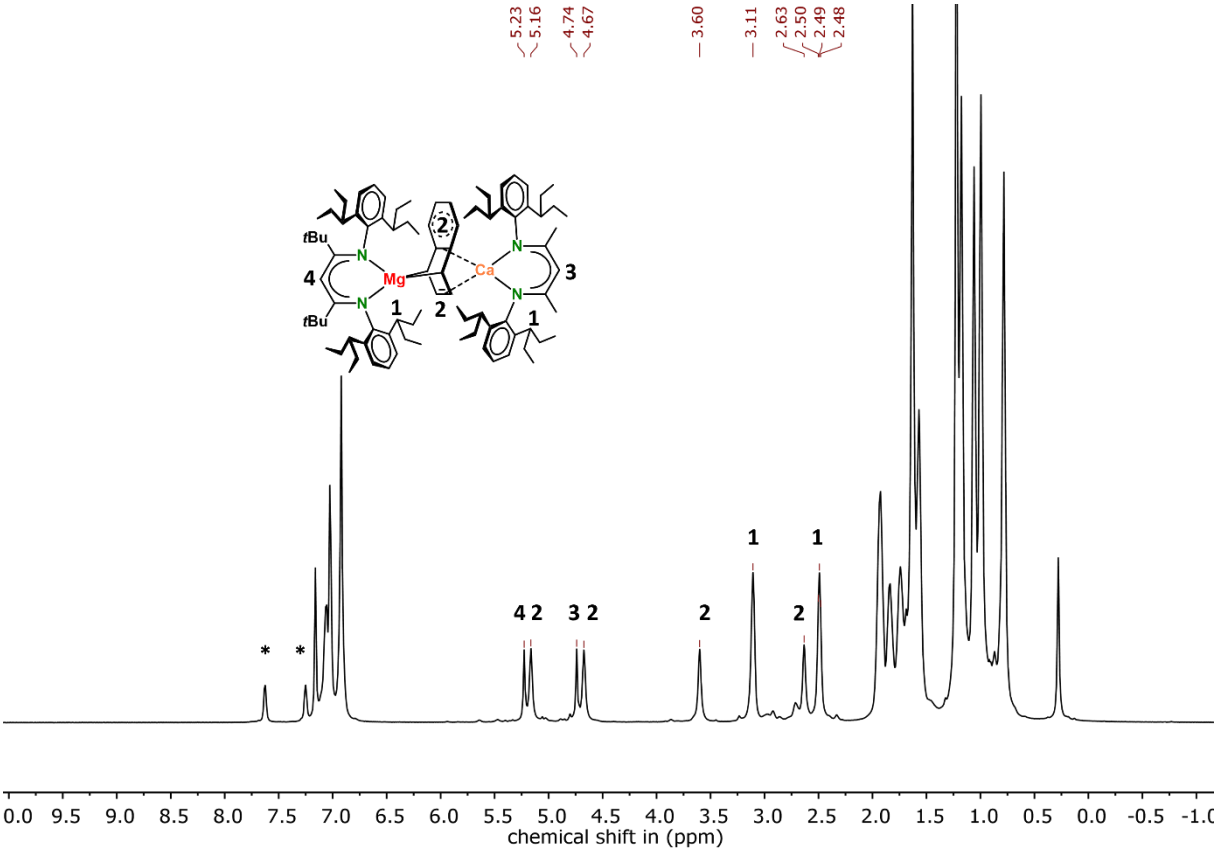


Figure S34. ^{1}H NMR spectrum of the crude reaction product of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in the presence of naphthalene performed in MCH (methylcyclohexane). The NMR spectrum was recorded in C_6D_6 for better comparison. For this purpose, the solvent was removed from the reaction mixture and the crude product was redissolved in C_6D_6. The spectrum essentially shows the pure product (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**). Residual naphthalene is marked with a *.

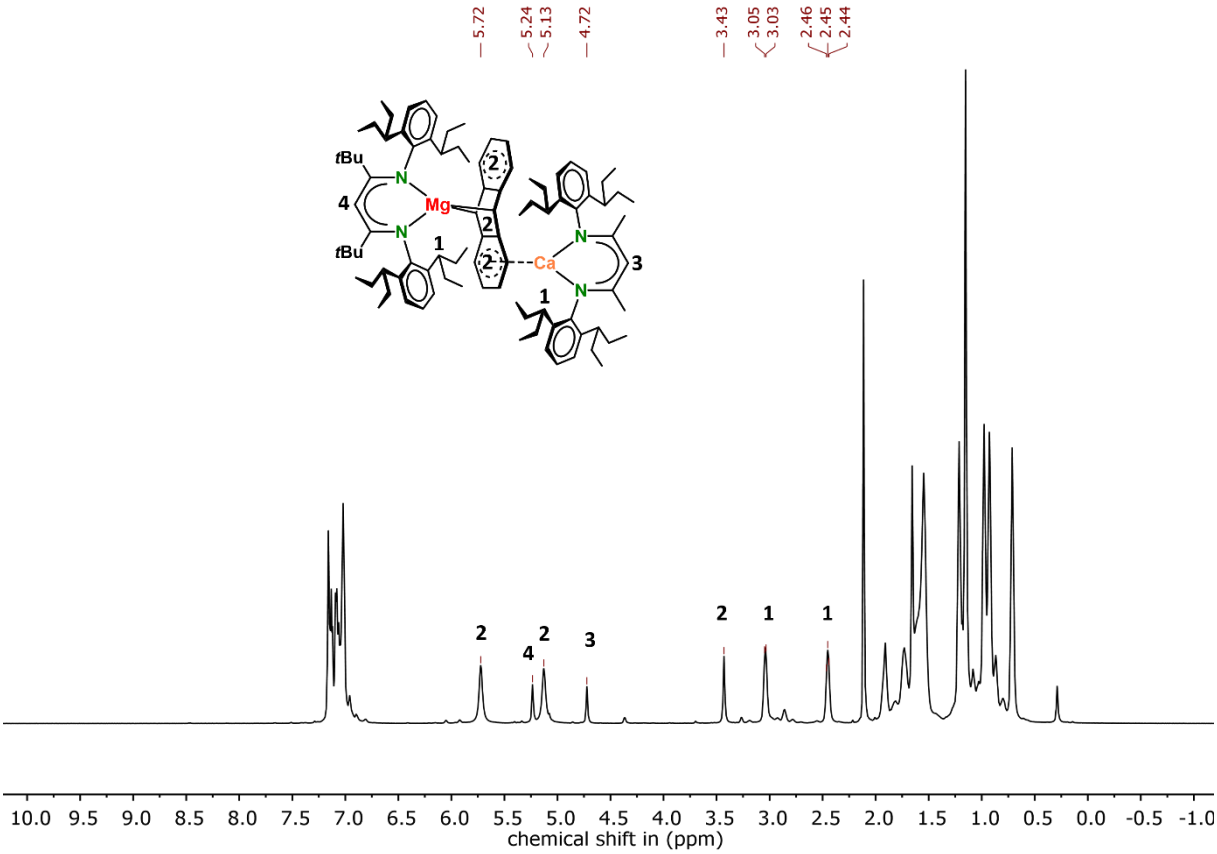


Figure S35. ^{1}H NMR spectrum of the crude reaction product of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in the presence of anthracene in C_6D_6. The spectrum essentially shows the pure product ((^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).

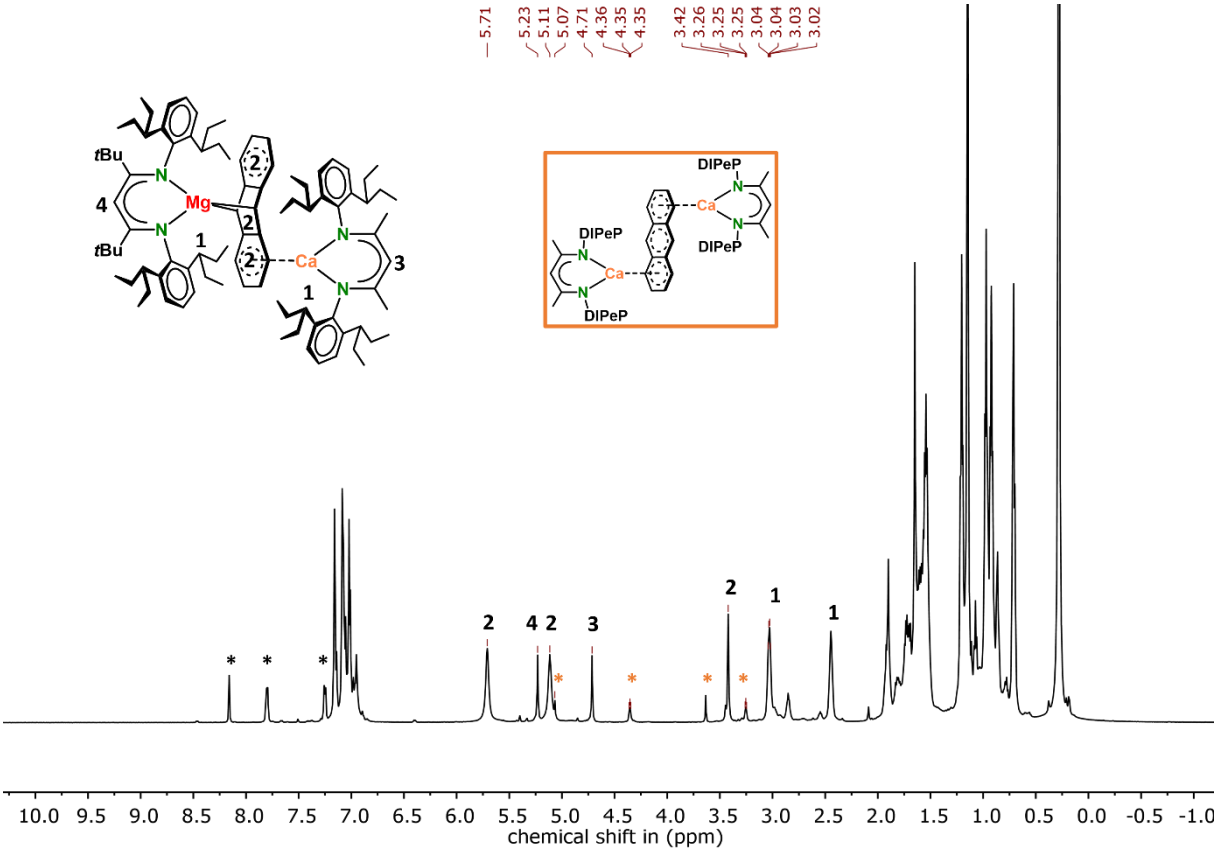


Figure S36. Crude ^{1}H NMR spectrum of the reaction of [(^{DIPeP}BDI*)Mg^{-}Na^{+}]$_2$ complex (**VII**) with [(^{DIPeP}BDI)CaI]$_2$ (**IX**) in the presence of anthracene performed in MCH (methylcyclohexane). The NMR spectrum was recorded in C_6D_6 for better comparison. For this purpose, the solvent was removed from the reaction mixture and the crude product was redissolved in C_6D_6. Besides the product ((^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) a small amount of the homometallic (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**) is visible. Residual anthracene is marked with a *.

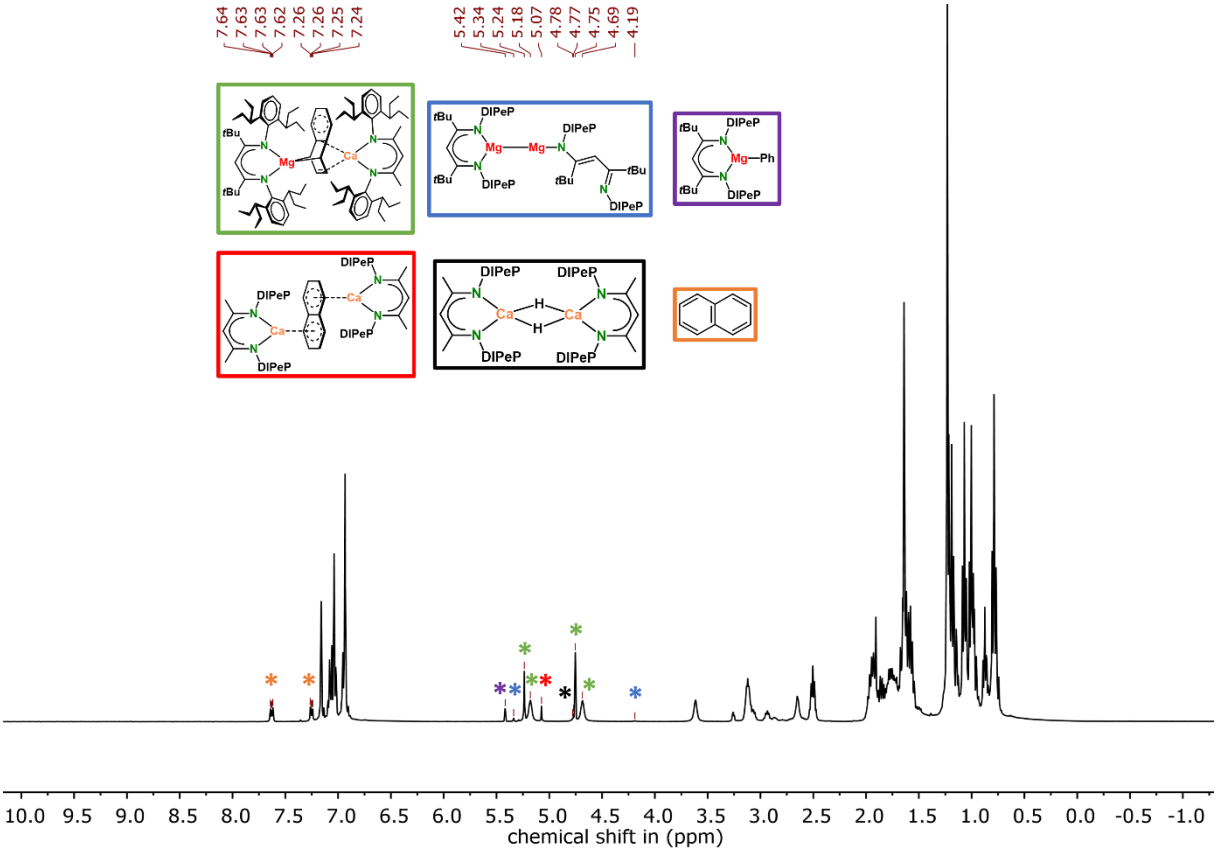


Figure S37. ^{1}H NMR (600.15 MHz, C_6D_6): Decomposition of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) after 1 day at rt.

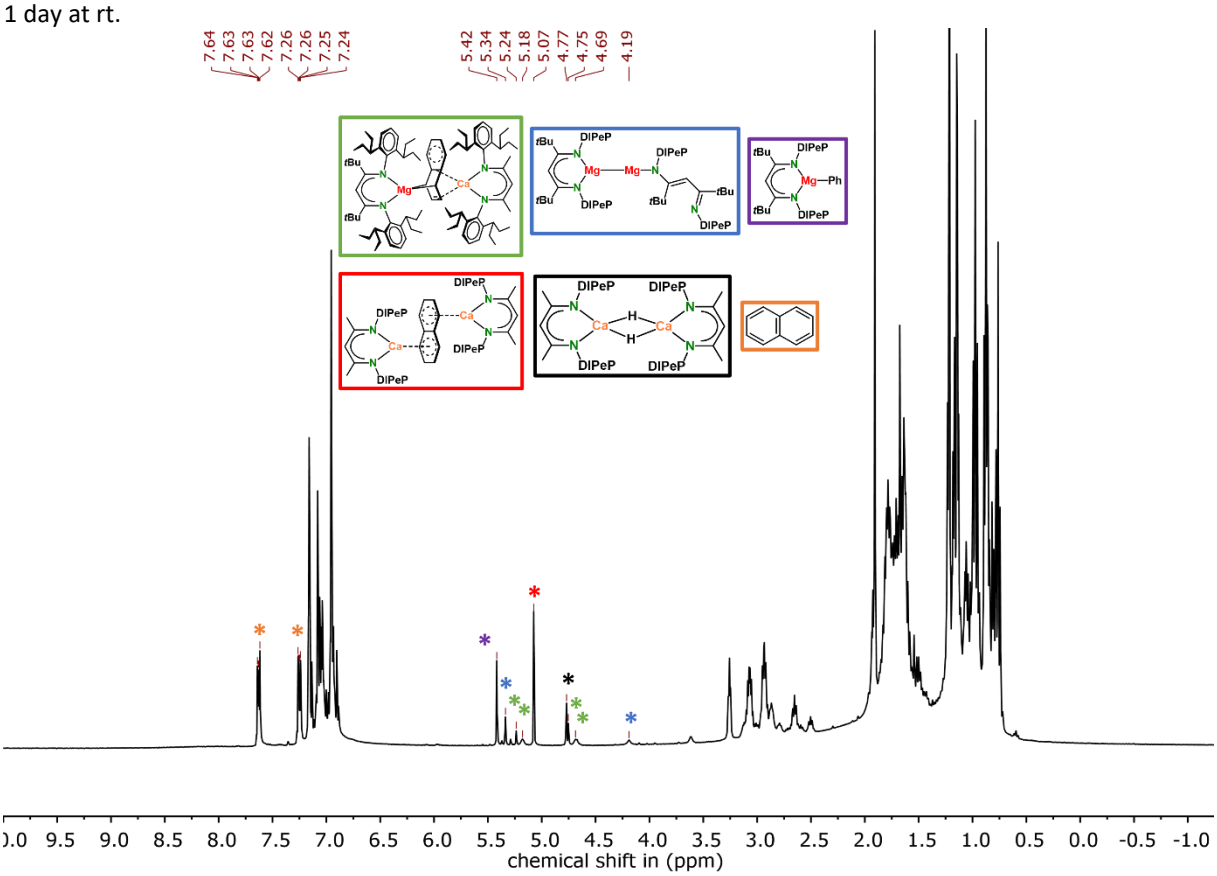


Figure S38. ^{1}H NMR (600.15 MHz, C_6D_6): Decomposition of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) after 13 days at rt.

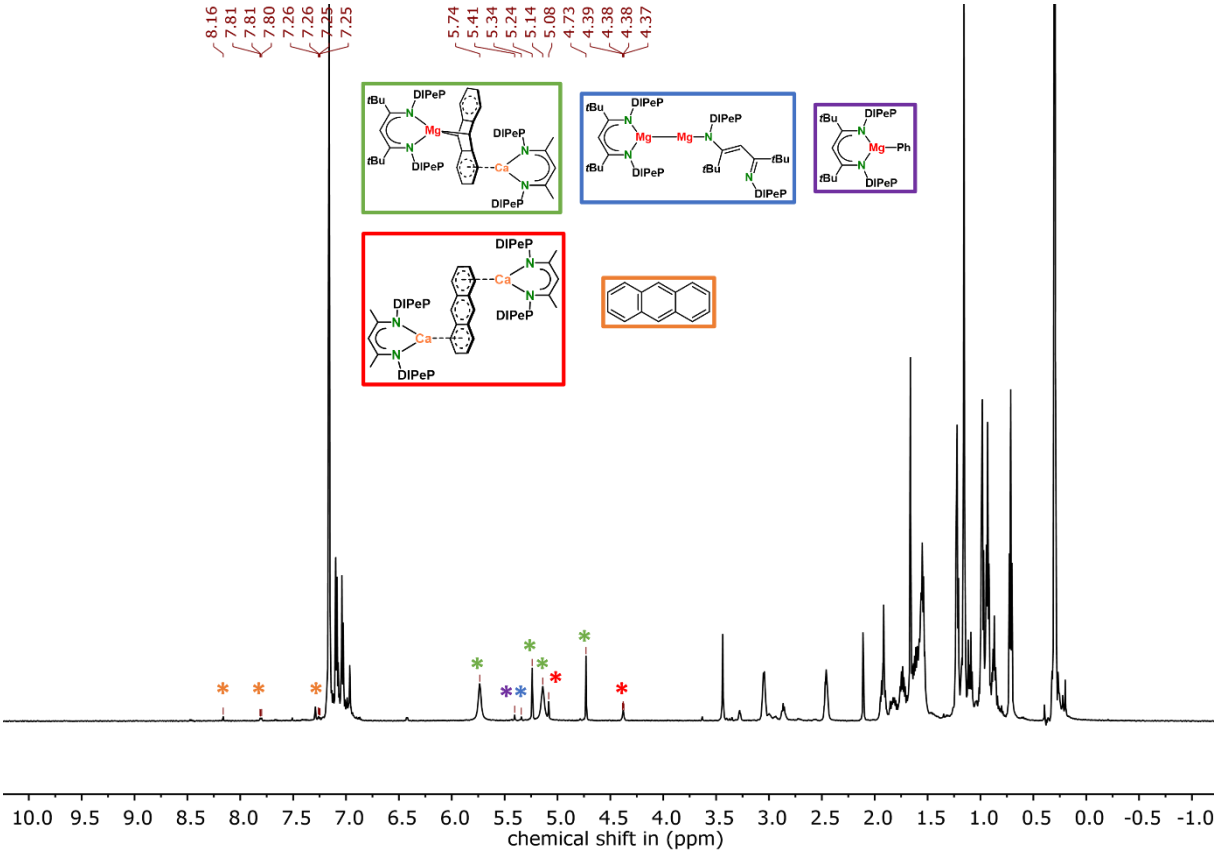


Figure S39. ^{1}H NMR (600.15 MHz, C_6D_6): Decomposition of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) after 1 day at rt.

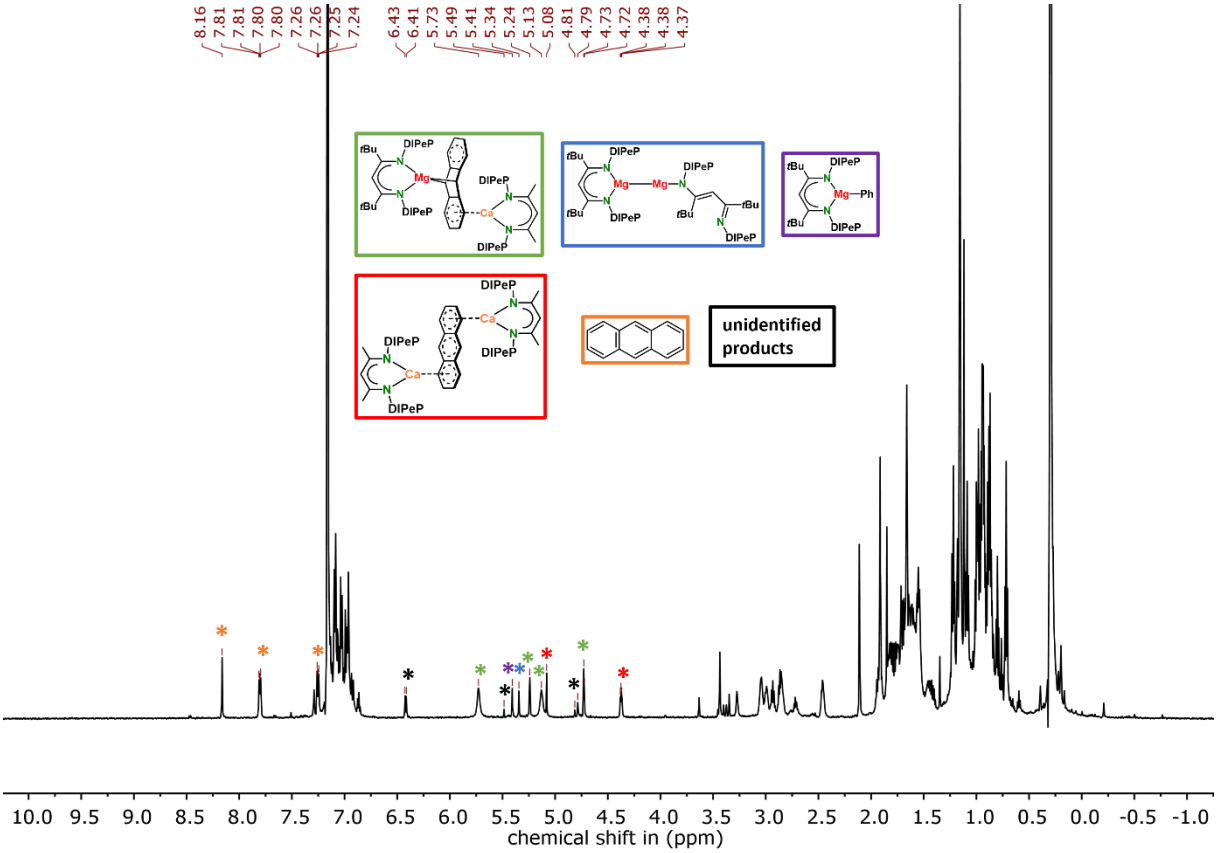


Figure S40. ^{1}H NMR (600.15 MHz, C_6D_6): Decomposition of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) after 16 days at rt.

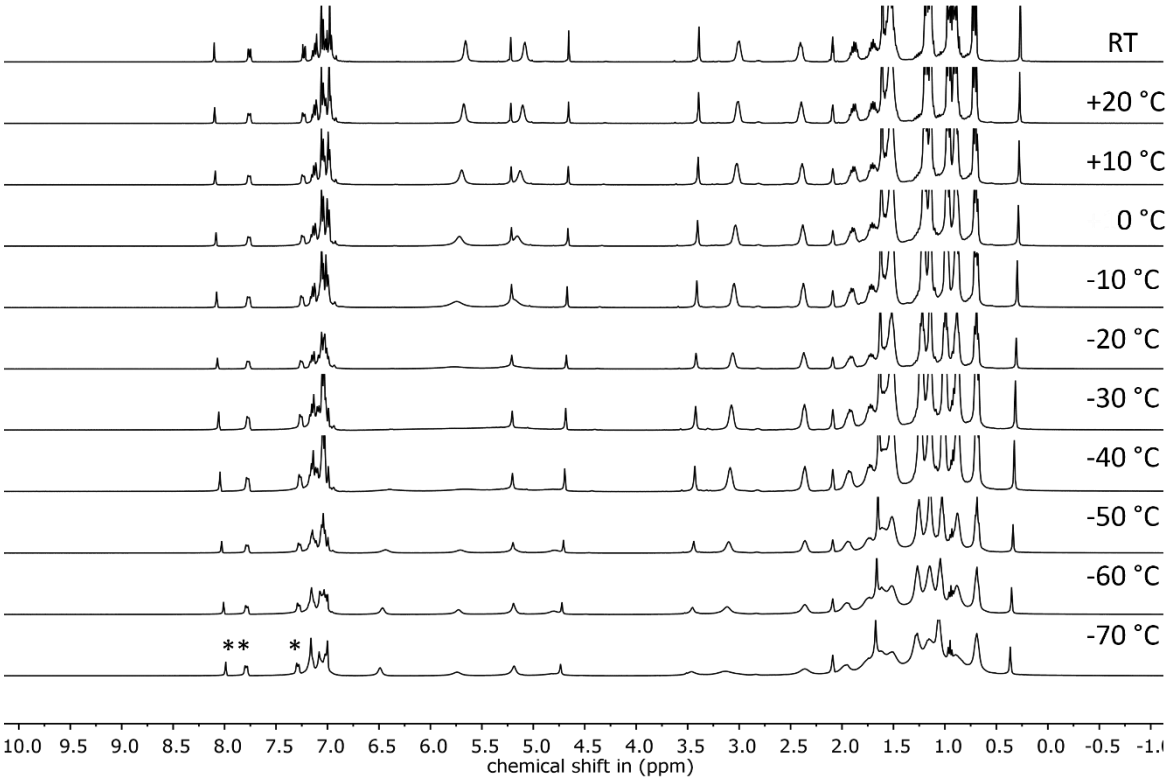


Figure S41. Temperature dependent ^{1}H NMR (400.15 MHz, toluene-d$_8$) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**). Residual anthracene is marked with a *.

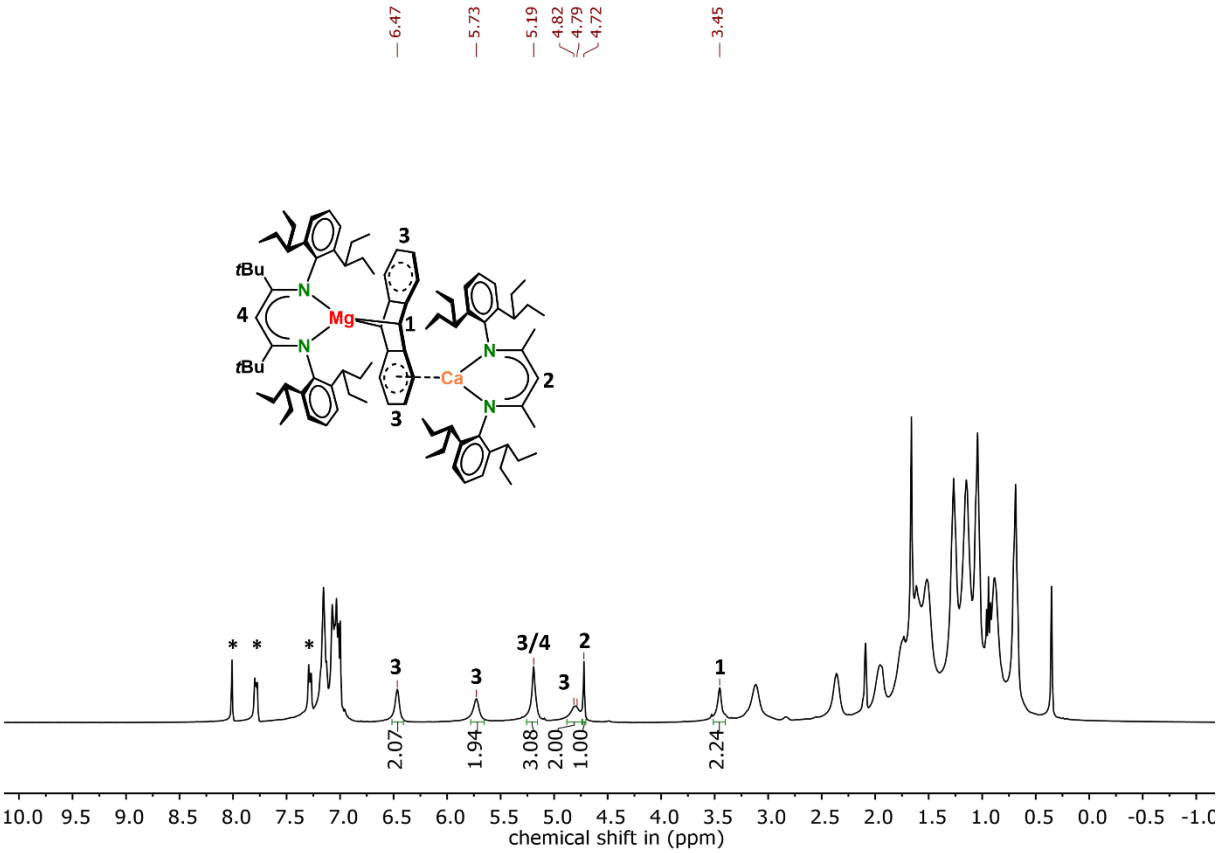


Figure S42. ^{1}H NMR (400.15 MHz, toluene-d$_8$) of (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) at -60 °C. Now five instead of previously three signals for the anthracene are visible. Signals of 3 and 4 are overlapping. Residual anthracene is marked with a *.

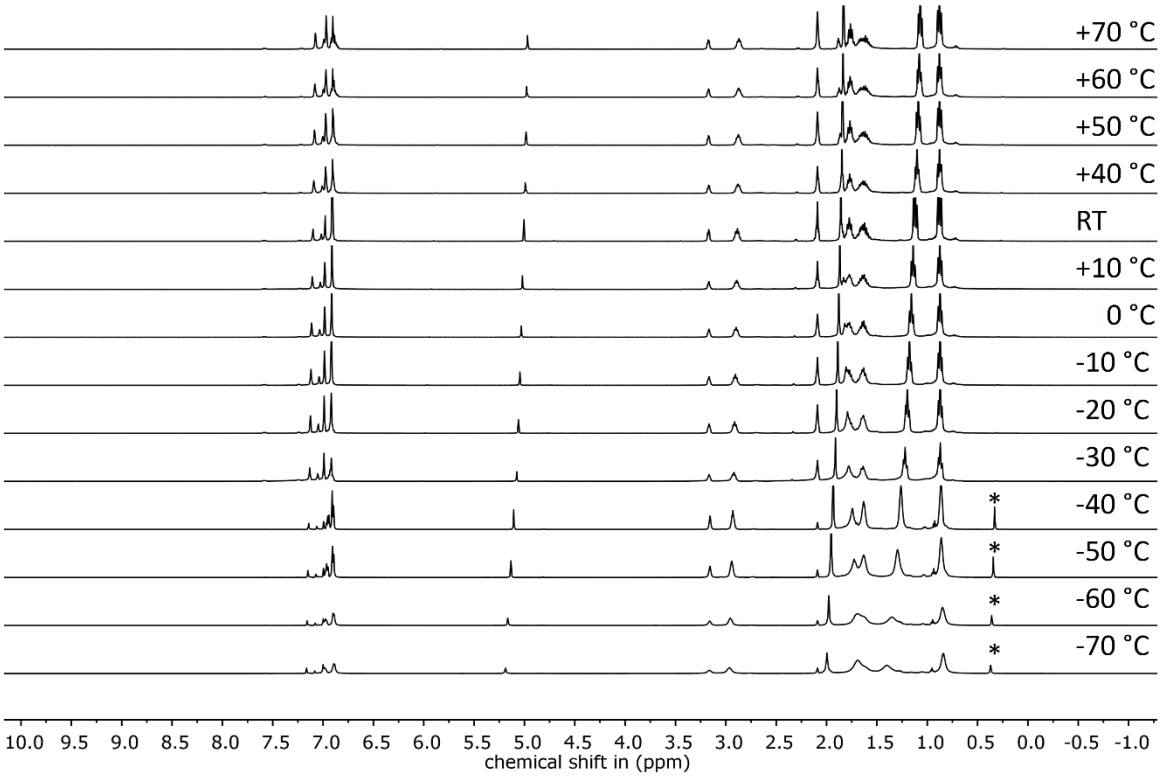


Figure S43. Temperature dependent ^{1}H NMR (600.15 MHz, toluene-d_8) of (^{DIPeP}BDI)Ca(μ^4,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**6**). This demonstrates there is exchange of the calcium atoms between the naphthalene rings.

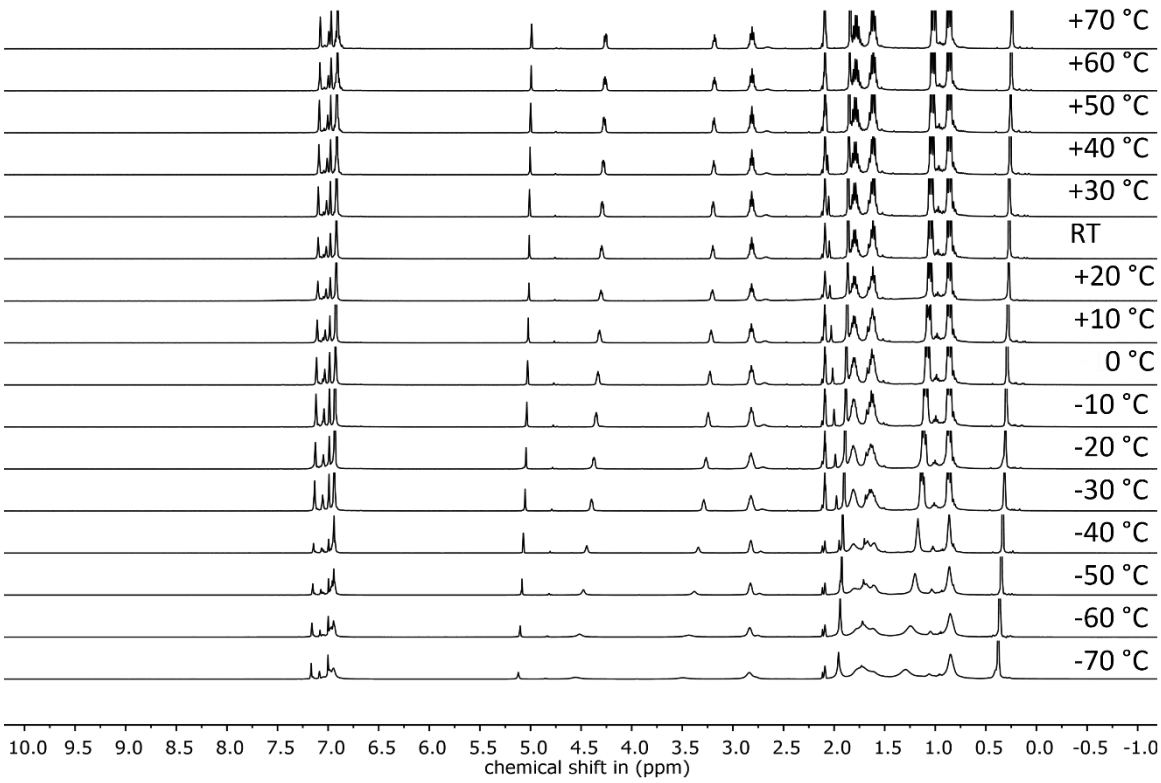


Figure S44. Temperature dependent ^{1}H NMR (600.15 MHz, toluene-d_8) of (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**). This demonstrates there is exchange of the calcium atoms between the anthracene rings.

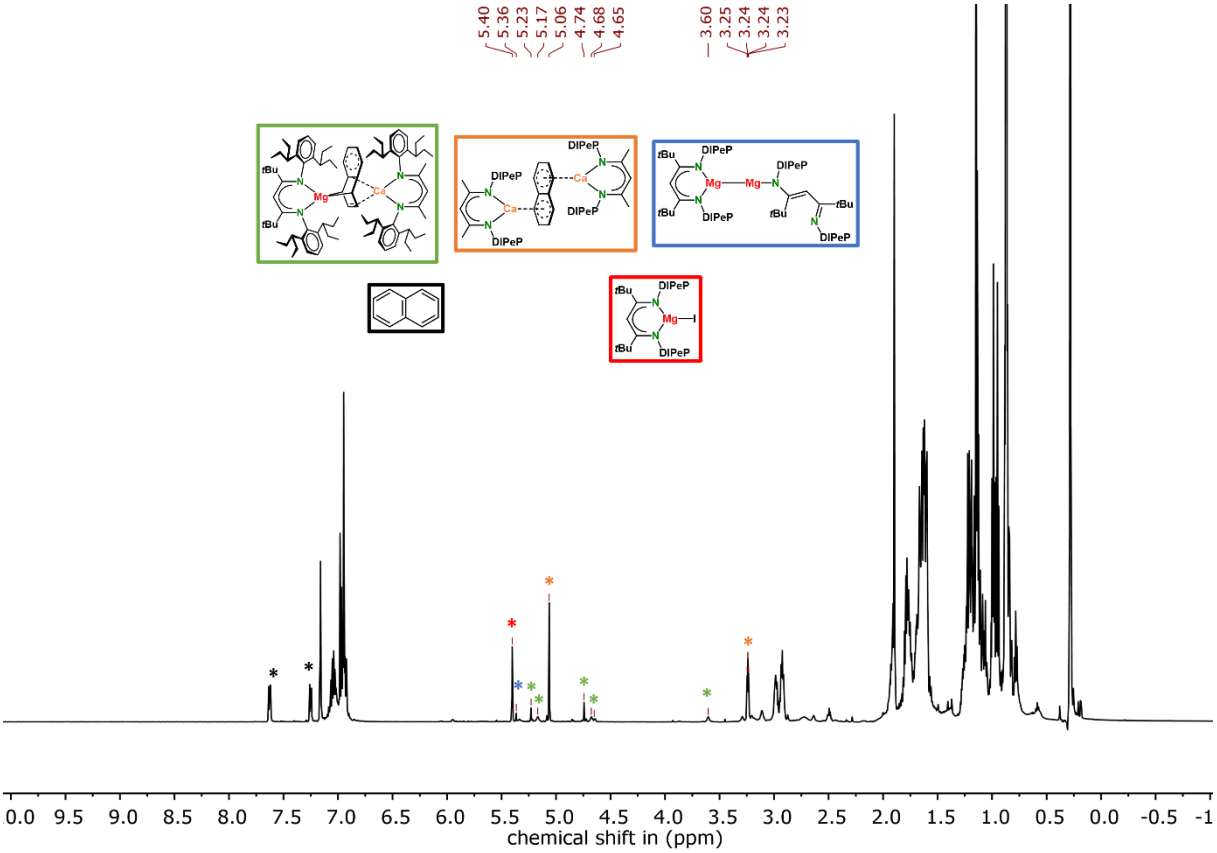


Figure S45. ^{1}H NMR (600.15 MHz, C_6D_6) of the reaction between of (^{DIPeP}BDI*)MgI, (^{DIPeP}BDI)CaI (**XI**) and naphthalene in the presence of reducing agent KC_8 in C_6D_6.

3. Crystal structure determinations

In each case, a crystal of compound **2, 4-7** was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The selected crystal 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 an Agilent SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data were processed with the CrysAlisPro software package.[S1] Using Olex2,[S2] the structures were solved with the ShelXT[S3] structure solution program using Intrinsic Phasing and refined with the ShelXL[S4] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. Most hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

In case of compound [(^{DIPeP}BDI)CaH·(THF)]$_2$ 2Hexane (**2**) the position of the hydride H1 was observed from difference Fourier maps and refined. Additionally, the position of H3 in the ligand backbone deviated noticeably from the idealized position and was also refined freely. The co-crystallized hexanes (an isomeric mixture was used for crystallization) were found to be disordered. One of the hexanes was clearly an *n*-hexane with two alternative orientations. This disorder with modeled with the help of similarity restraints (SADI) and rigid bond restraints (RIGU).[S5] The relative occupancies of the alternative orientations were refined to 0.855(6) and 0.145(6). The other solvent molecule was more severely disordered and different hexane isomers seem to be involved. A suitable disorder model for this solvent molecule could not be built. Therefore, its contribution to the structure factors was secured by back-Fourier transformation using the solvent mask routine[S6,S7] of the program Olex2.[S2] The solvent accessible voids treated this way had a size of 245.6 Å^3 (11.1% of the unit cell) and contained 52.4 electrons/unit cell, which is in good agreement with the 50 electrons calculated for a hexane.

Disorder was also present in case of derivative (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) One dipep moiety and two additional 3-pentyl groups were affected. The disorder was modeled with the help of similarity restraints (SADI, SIMU). The relative occupancies of the two alternative orientations of each group were refined to 0.821(5)/0.179(5) (dipep), 0.835(8)/0.165(8) (3-pentyl) and 0.640(9)/0.360(9) (3-pentyl), respectively. Nevertheless, it was possible to observe and refine the positions of the hydrogen atoms of the reduced anthracene ligand.

The positions of the hydrogen atoms of the reduced naphthalene ligands in (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) and (^{DIPeP}BDI)Ca(μ^4,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**6**) were likewise observed from difference Fourier maps and refined. The latter compound also showed disorder of a 3-pentyl moiety, which was treated using similarity restraints (SADI, SIMU). The relative occupancies of the two alternative orientations of this group were refined to 0.917(3) and 0.083(3).

Substantially disordered solvent was also observed (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) 0.81(*n*-Hexane) (**7**). In this case, an infinitive channel filled with a non-stoichiometric amount of *n*-hexane seems to be present. A disorder model, which included three alternative positions for the *n*-hexane was built with the help of similarity restraints (SADI, SIMU). From this model, it was deduced that approximately 0.8 *n*-hexane per metal complex is incorporated in the crystal. Additionally, extensive disorder of one of the 3-pentyl groups was noticed and modeled with the help of similarity restraints (SADI, SIMU) restraints. The relative occupancies of the three alternative orientations of this group were refined to 0.452(2), 0.395(3) and 0.153(3).

Crystallographic and refinement data are summarized in Table S1.

The crystal structure data of the compounds have been deposited with the Cambridge Crystallographic Data Centre. CCDC 2240705 (compound **2**), 2240706 (compound **4**), 2240707 (compound **5**), 2240708 (compound **6**), and 2240709 (compound **7**) contain the supplementary crystallographic data for the compounds. 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 compounds **2**, **4**-**7**.

Compound	$[(^{DIPeP}BDI)CaH\cdot(THF)]_2$ 2Hexane (**2**)	$(^{DIPeP}BDI)Ca(\mu^6,\mu^6$-anthracene)$Ca(^{DIPeP}BDI)$ 0.81(*n*-Hexane) (**7**)	$(^{DIPeP}BDI)Ca(\mu^4,\mu^4$-naphthalene)$Ca(^{DIPeP}BDI)$ (**6**)
Identification code	hasj180320a	hasj210311a	hasj210304a
Empirical formula	$C_{94}Ca_2H_{160}N_4O_2$	$C_{92.84}H_{135.3}Ca_2N_4$	$C_{84}H_{122}Ca_2N_4$
Formula weight	1458.41	1387.65	1268.01
Temperature/K	100.0(2)	100.0(2)	100.0(1)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	C2/c	C2/c
a/Å	12.4506(6)	47.9193(6)	29.7787(3)
b/Å	12.9760(6)	12.7914(2)	16.8207(2)
c/Å	16.2431(6)	27.3845(4)	14.94992(17)
α/°	74.198(4)	90	90
β/°	73.222(4)	98.7696(12)	90.0659(10)
γ/°	63.566(4)	90	90
Volume/Å^3	2217.94(19)	16589.3(4)	7488.40(15)
Z	1	8	4
ρ_{calc}g/cm^3	1.092	1.111	1.125
μ/mm^{-1}	1.463	1.530	1.652
F(000)	808.0	6083.0	2776.0
Crystal size/mm^3	0.175 × 0.128 × 0.089	0.227 × 0.092 × 0.057	0.403 × 0.345 × 0.225
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.764 to 145.668	6.532 to 145.82	5.936 to 145.41
Index ranges	-15 ≤ h ≤ 10, -15 ≤ k ≤ 11, -20 ≤ l ≤ 19	-56 ≤ h ≤ 59, -15 ≤ k ≤ 14, -33 ≤ l ≤ 28	-36 ≤ h ≤ 34, -11 ≤ k ≤ 20, -18 ≤ l ≤ 18
Reflections collected	16717	64408	13885
Independent reflections	8583 [R_{int} = 0.0343, R_{sigma} = 0.0470]	16214 [R_{int} = 0.0315, R_{sigma} = 0.0247]	7238 [R_{int} = 0.0208, R_{sigma} = 0.0281]
Data/restraints/parameters	8583/25/481	16214/1121/1097	7238/0/435
Goodness-of-fit on F^2	1.036	1.041	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0439, wR_2 = 0.1163	R_1 = 0.0392, wR_2 = 0.0974	R_1 = 0.0350, wR_2 = 0.0890
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.1194	R_1 = 0.0457, wR_2 = 0.1023	R_1 = 0.0377, wR_2 = 0.0917
Largest diff. peak/hole / e Å^{-3}	0.47/-0.29	0.36/-0.33	0.69/-0.38

Table S1. Crystal data and structure refinement for compounds **2**, **4**-**7** (continued).

Compound	(^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**)	(^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**)
Identification code	hasj210728b	hasj201117b
Empirical formula	$C_{94}H_{136}CaMgN_4$	$C_{90}H_{134}CaMgN_4$
Formula weight	1386.45	1336.39
Temperature/K	100.0(3)	100.0(2)
Crystal system	orthorhombic	monoclinic
Space group	$Pca2_1$	$P2_1/n$
a/Å	21.5514(3)	12.38232(18)
b/Å	13.0869(2)	28.8484(3)
c/Å	29.0951(4)	21.8547(2)
α/°	90	90
β/°	90	93.1984(12)
γ/°	90	90
Volume/Å^3	8206.0(2)	7794.57(16)
Z	4	4
ρ_{calc}g/cm^3	1.122	1.139
μ/mm^{-1}	1.079	1.118
F(000)	3040.0	2936.0
Crystal size/mm^3	0.186 × 0.135 × 0.086	0.181 × 0.081 × 0.058
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.076 to 144.654	6.128 to 145.528
Index ranges	-26 ≤ h ≤ 25, -15 ≤ k ≤ 16, -34 ≤ l ≤ 35	-14 ≤ h ≤ 15, -33 ≤ k ≤ 35, -25 ≤ l ≤ 26
Reflections collected	38240	44605
Independent reflections	14603 [R_{int} = 0.0532, R_{sigma} = 0.0550]	15115 [R_{int} = 0.0269, R_{sigma} = 0.0284]
Data/restraints/parameters	14603/2124/1201	15115/331/954
Goodness-of-fit on F^2	1.020	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0523, wR_2 = 0.1356	R_1 = 0.0362, wR_2 = 0.0879
Final R indexes [all data]	R_1 = 0.0591, wR_2 = 0.1425	R_1 = 0.0440, wR_2 = 0.0928
Largest diff. peak/hole / e Å^{-3}	0.35/-0.17	0.25/-0.32
Flack parameter	-0.003(10)	-

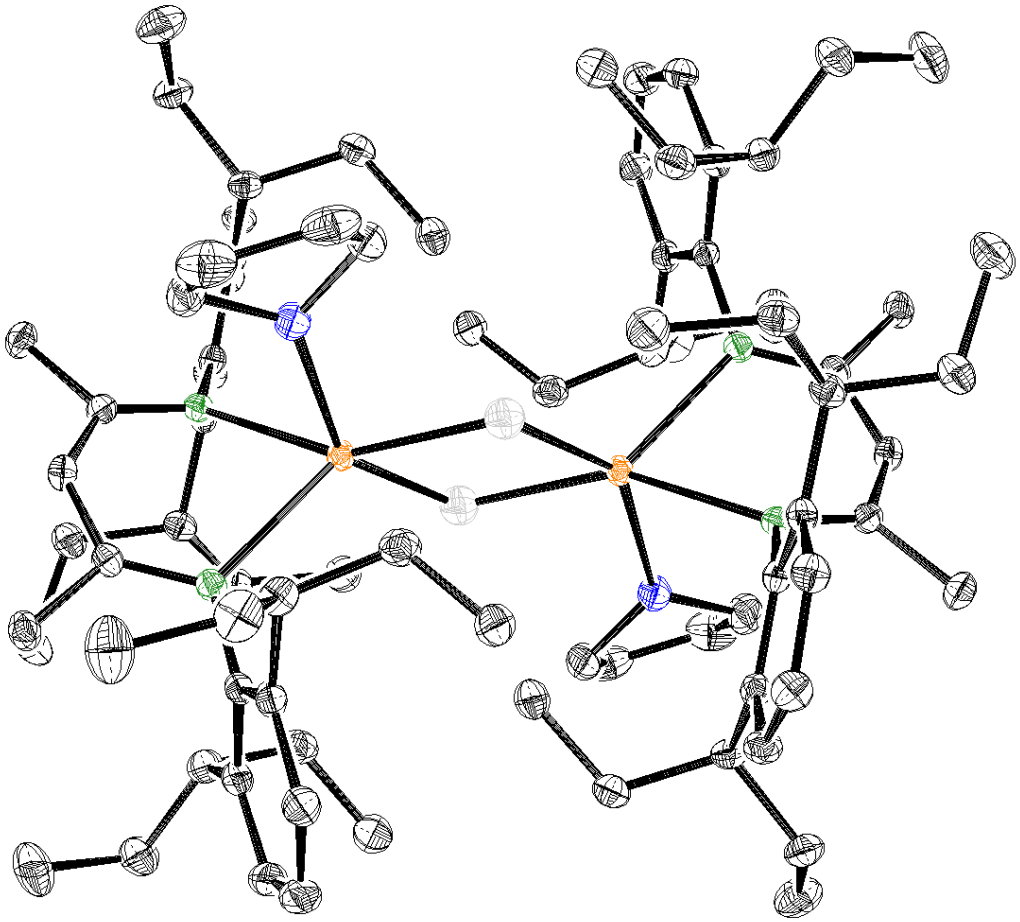


Figure S46. ORTEP representation of [(^{DIPeP}BDI)CaH·(THF)]$_2$ (**2**) with atomic displacement ellipsoids set at 50% probability. Hydrogen atoms except hydrides are omitted for clarity.

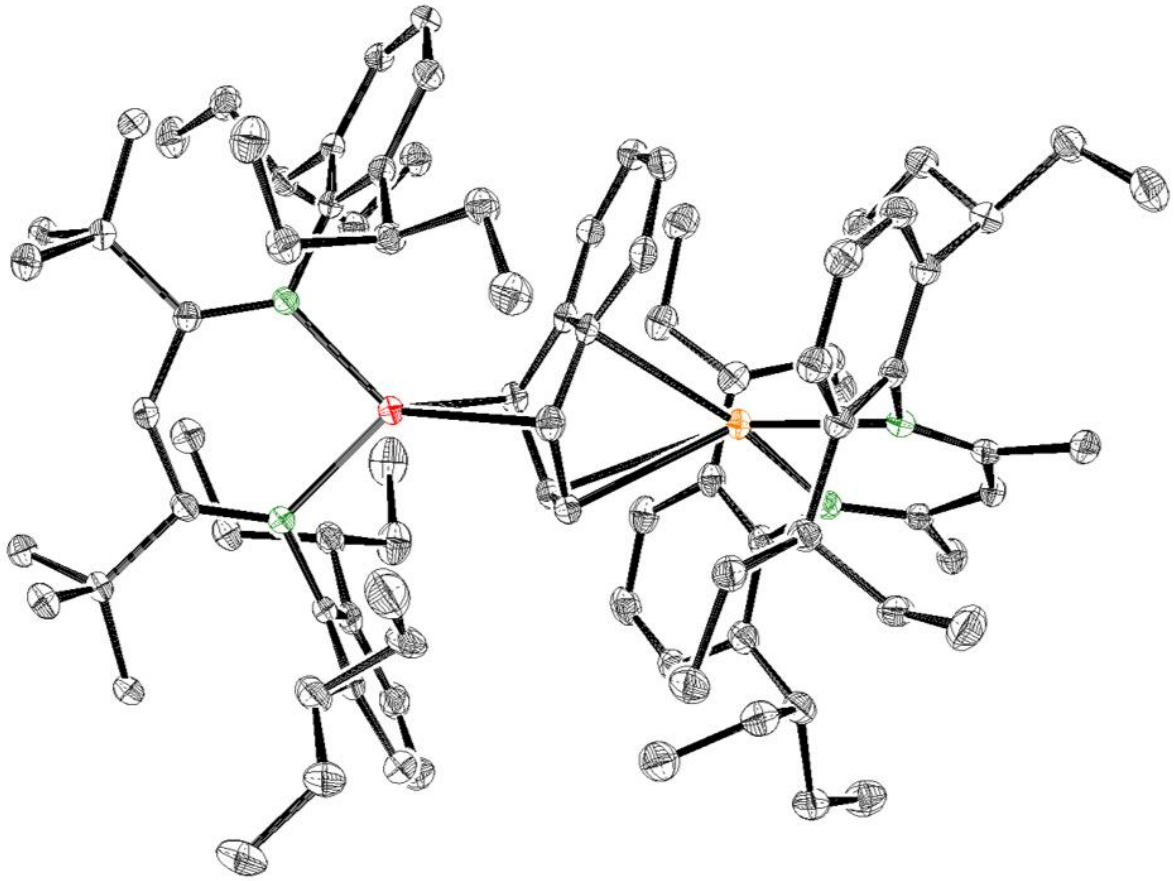


Figure S47. ORTEP representation of (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) with atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

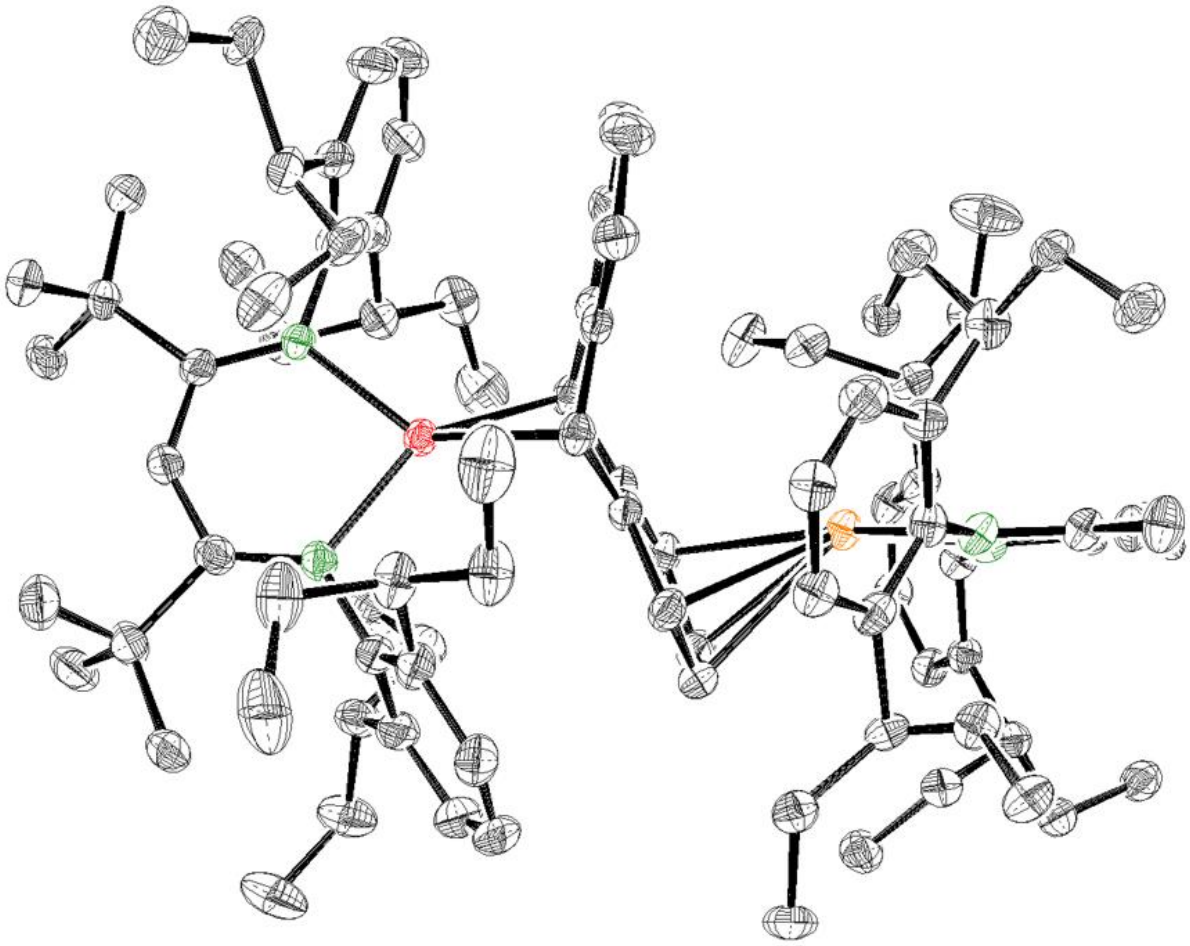


Figure S48. ORTEP representation of (^{DIPeP}BDI*)Mg(μ^2,μ^A-anthracene)Ca(^{DIPeP}BDI) (**5**) with atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

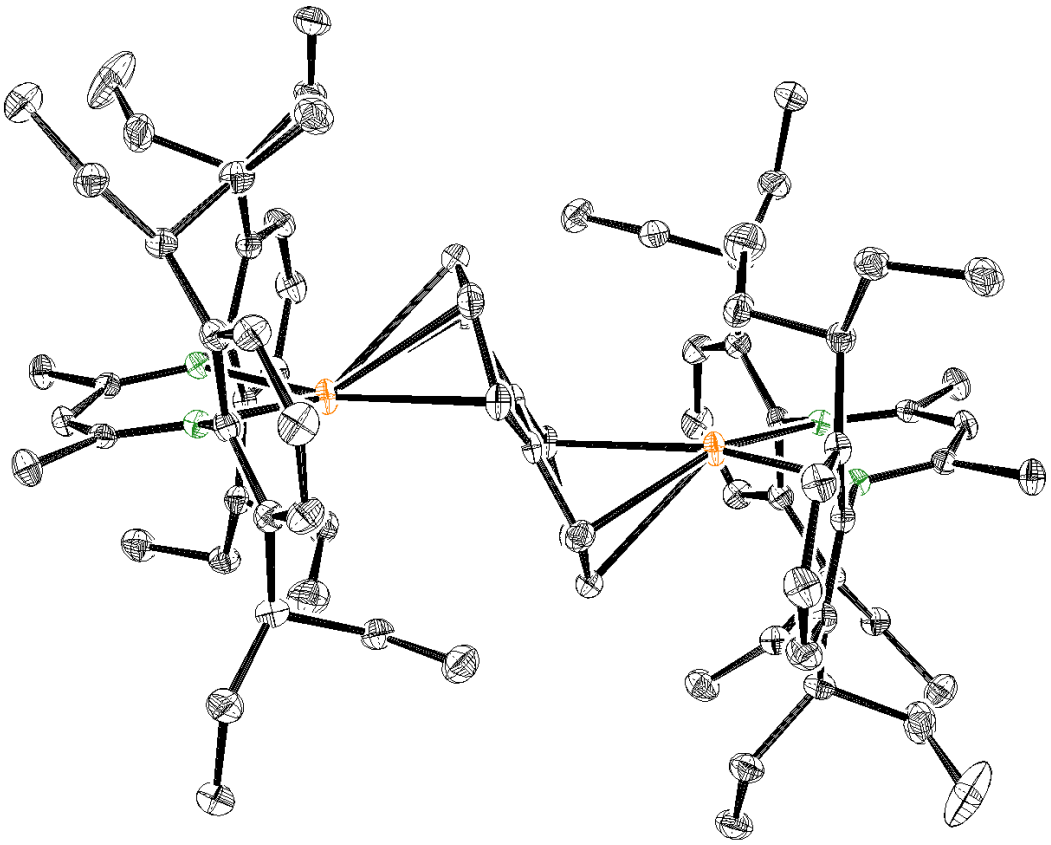


Figure S49. ORTEP representation of (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**) with atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

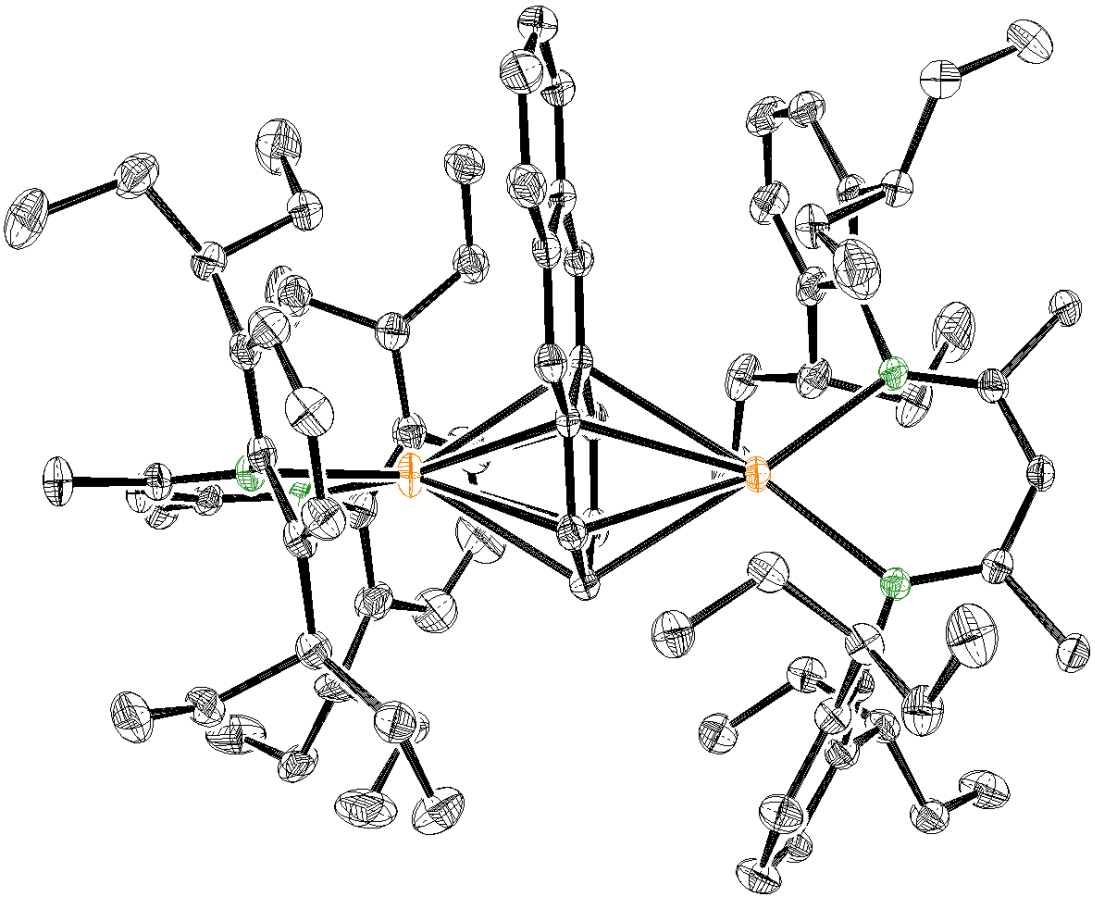


Figure S50. ORTEP representation of (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**) with atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity.

4. DFT calculations

All calculations were carried out using Gaussian 16A.[S8] All methods were used as implemented. All structures were fully optimized at a B3PW91/def2SVP level of theory.[S9–S12] All structures were characterized as true minima (NImag=0) or as transition states (NImag=1) by frequency calculations on the same level of theory. Energies were determined at a B3PW91/def2TZVP level of theory. Grimme's third dispersion correction with Becke-Johnson damping (GD3BJ) was applied, unless stated otherwise.[S13] Charges were calculated via NBO7 Analyses.[S14] All structures were evaluated using Molecule 2.3.[S15] Topological analyses were carried out using the wavefunction of the calculation of B3PW91/def2TZVP level of theory with AIMAll (v17).[S16,S17]

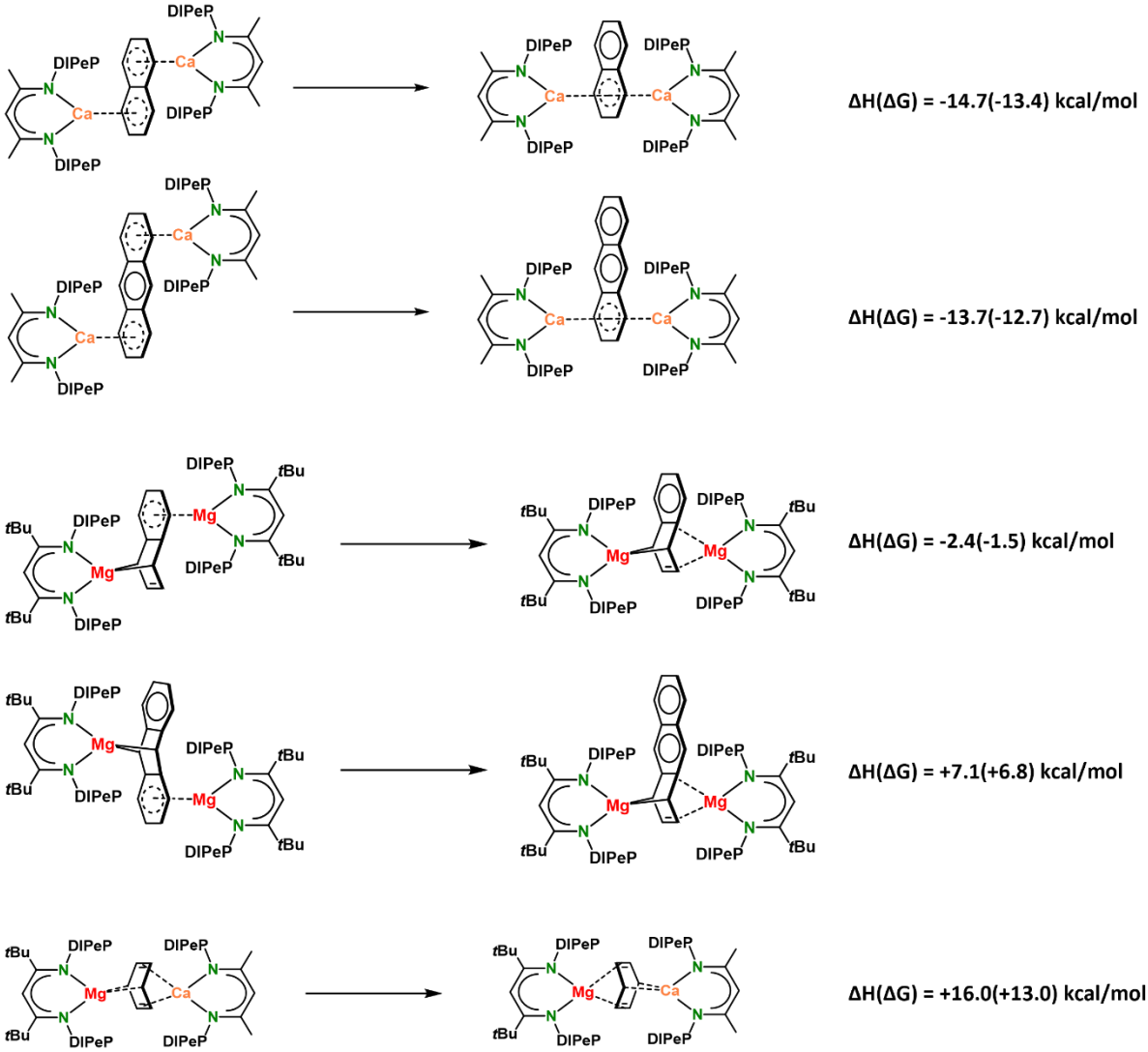


Figure S51. Calculated isomerization energy of (BDI)M(arom)M(BDI), (M = Ca, Mg; arom = benzene, naphthalene, anthracene).

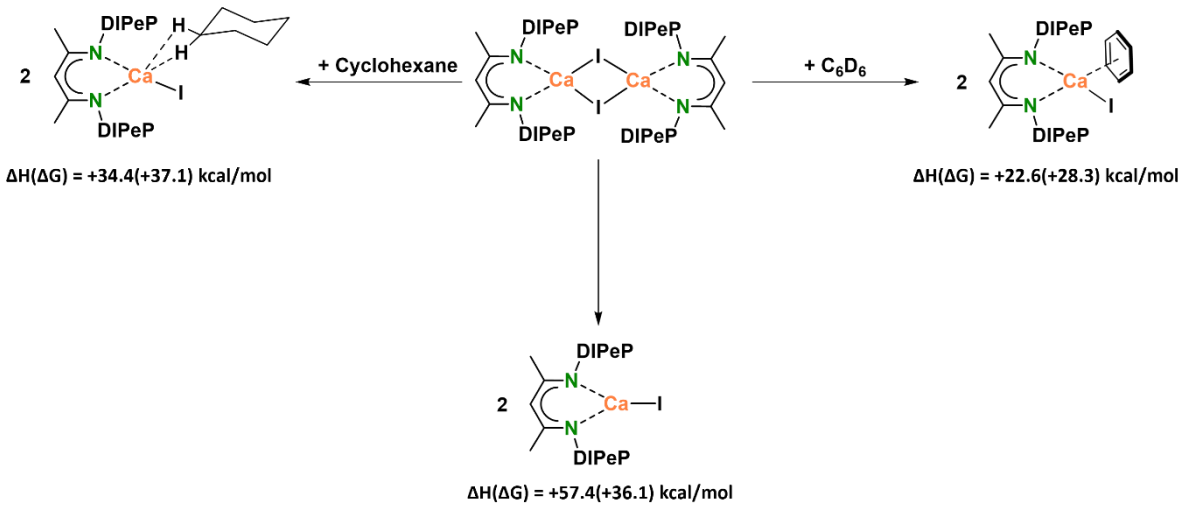


Figure S52. Calculated monomerization energy of $[(^{DIPeP}BDI)CaI]_2$ (**IX**) in the presence of cyclohexane and benzene.

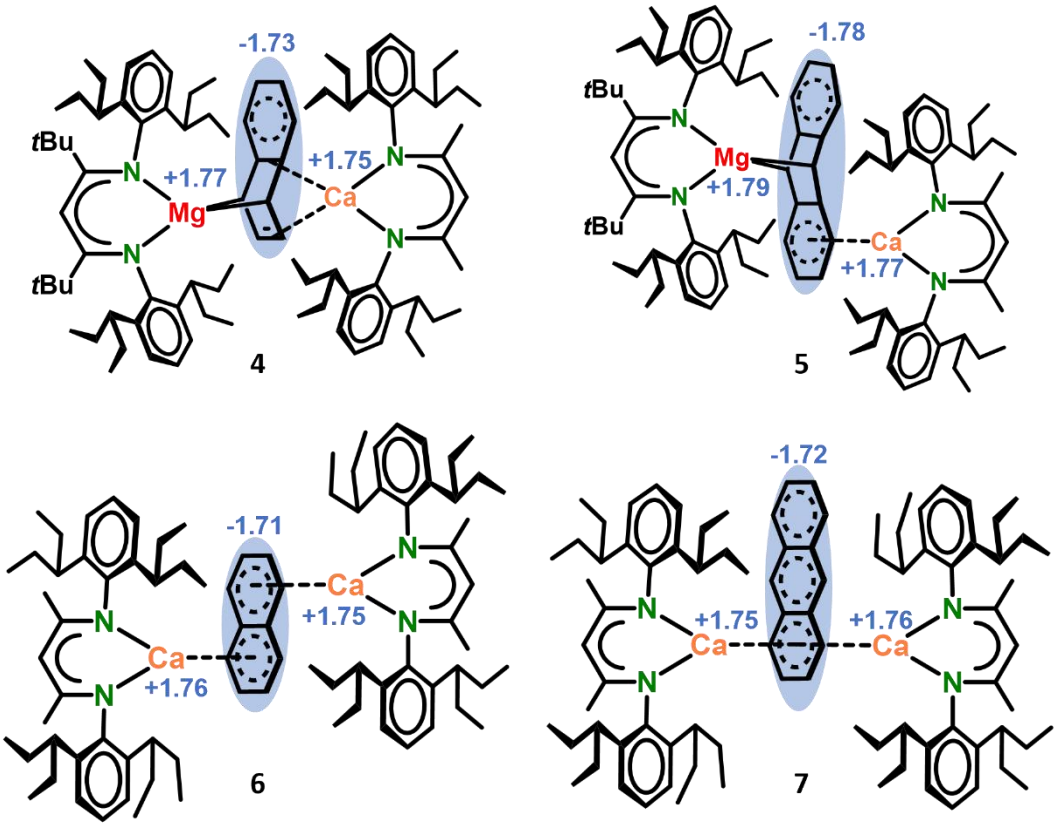
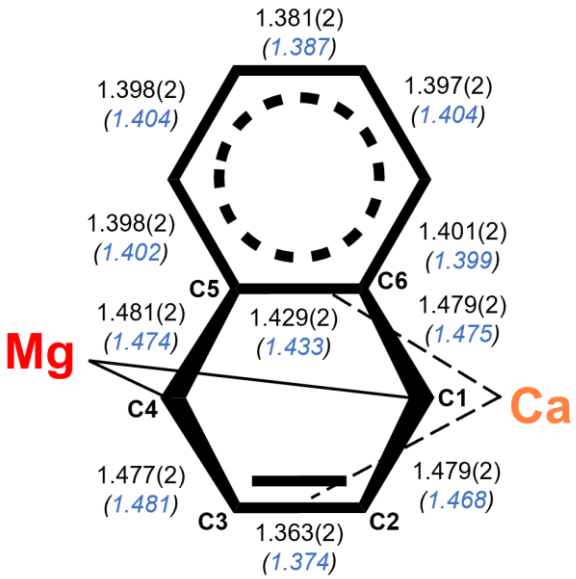
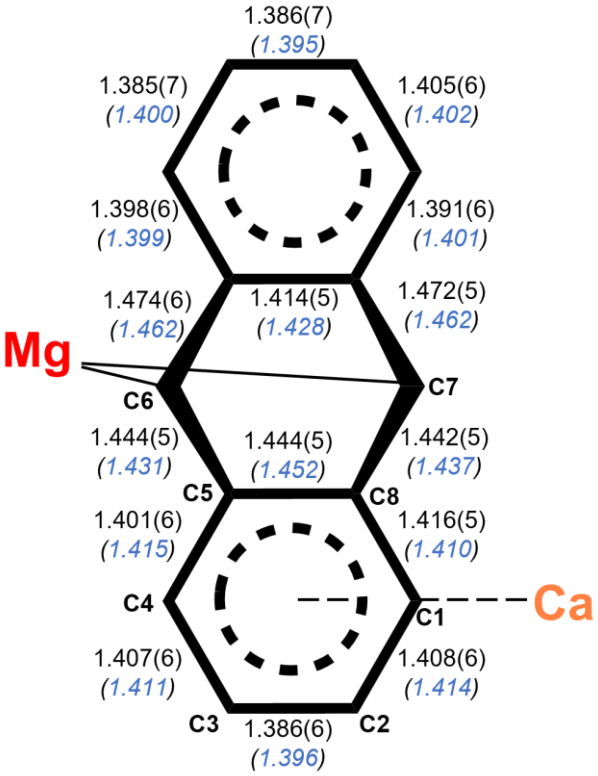


Figure S53. Selected calculated NPA charges of complexes (**4**-**7**).



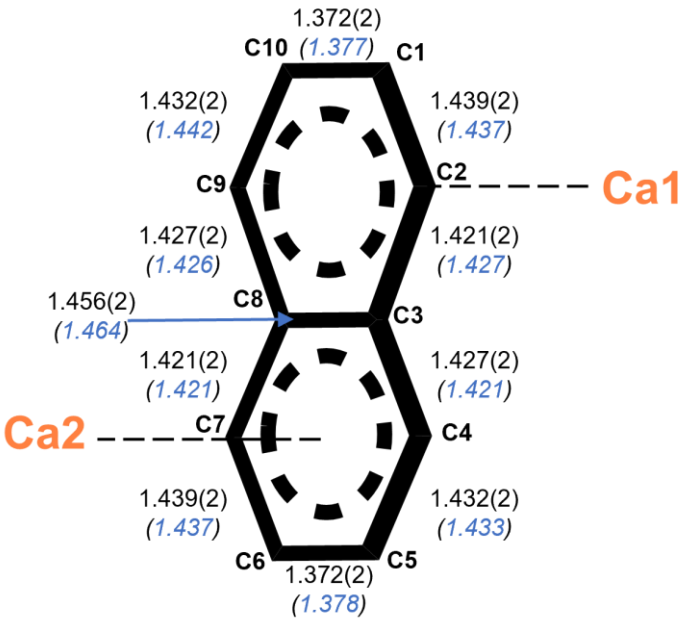
bond	X-Ray (*DFT*) distance [Å]
Mg-C1	2.376(1) (*2.347*)
Mg-C4	2.344(1) (*2.341*)
Ca-C1	3.070(1) (*2.960*)
Ca-C2	2.732(1) (*2.606*)
Ca-C3	2.839(2) (*2.741*)
Ca-C4	3.268(1) (*3.150*)
Ca-C5	2.825(1) (*2.764*)
Ca-C6	2.676(1) (*2.645*)

Figure S54. Comparison of experimentally determined metal-C distances (X-ray) with calculated values *(*in *italic)* for the heterometallic complex (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**).



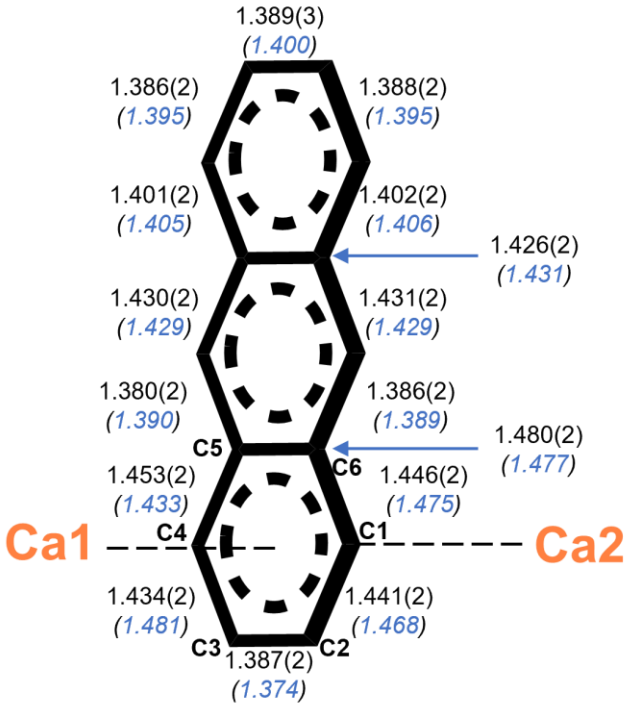
bond	X-Ray (*DFT*) distance [Å]
Mg-C6	2.426(4) (*2.455*)
Mg-C7	2.374(4) (*2.405*)
Ca-C1	2.777(4) (*2.695*)
Ca-C2	2.724(4) (*2.676*)
Ca-C3	2.745(4) (*2.682*)
Ca-C4	2.821(4) (*2.727*)
Ca-C5	3.015(4) (*2.890*)
Ca-C8	2.964(4) (*2.845*)

Figure S55. Comparison of experimentally determined metal-C distances (X-ray) with calculated values *(*in *italic)* for the heterometallic complex (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**).



bond	X-Ray (*DFT*) distance [Å]
Ca1-C1	2.654(1) (*2.683*)
Ca1-C2	2.642(1) (*2.640*)
Ca1-C3	2.951(1) (*2.800*)
Ca1-C8	2.964(1) (*2.858*)
Ca1-C9	2.674(1) (*2.617*)
Ca1-C10	2.673(1) (*2.660*)
Ca2-C3	2.964(1) (*2.716*)
Ca2-C4	2.674(1) (*2.604*)
Ca2-C5	2.673(1) (*2.652*)
Ca2-C6	2.654(1) (*2.638*)
Ca2-C7	2.642(1) (*2.611*)
Ca2-C8	2.951(1) (*2.782*)

Figure S56. Comparison of experimentally determined metal-C distances (X-ray) with calculated values *(*in *italic)* for the homometallic complex (^{DIPeP}BDI)Ca(μ^4,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**6**).



bond	X-Ray (*DFT*) distance [Å]
Ca1-C1	2.709(1) (*2.625*)
Ca1-C2	2.726(1) (*2.705*)
Ca1-C3	2.717(1) (*2.695*)
Ca1-C4	2.702(1) (*2.665*)
Ca1-C5	2.715(1) (*2.715*)
Ca1-C6	2.706(1) (*2.678*)
Ca2-C1	2.715(1) (*2.682*)
Ca2-C2	2.705(1) (*2.691*)
Ca2-C3	2.696(2) (*2.695*)
Ca2-C4	2.681(1) (*2.668*)
Ca2-C5	2.745(1) (*2.627*)
Ca2-C6	2.776(1) (*2.653*)

Figure S57. Comparison of experimentally determined metal-C distances (X-ray) with calculated values *(*in *italic)* for the homometallic complex (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**).

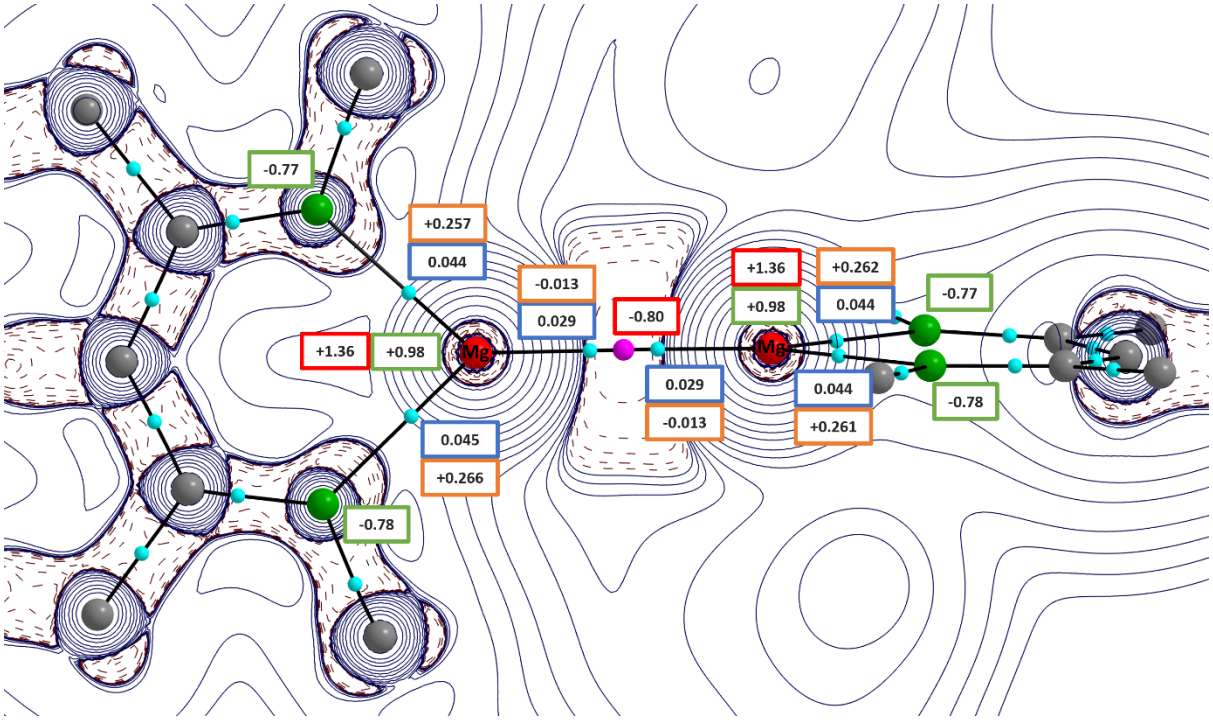


Figure S58. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Mg-Mg(^{DIPP}BDI) (calculated with Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); purple dots, non-nuclear attractor (NNA); green boxes, NPA charges; red boxes, AIM charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

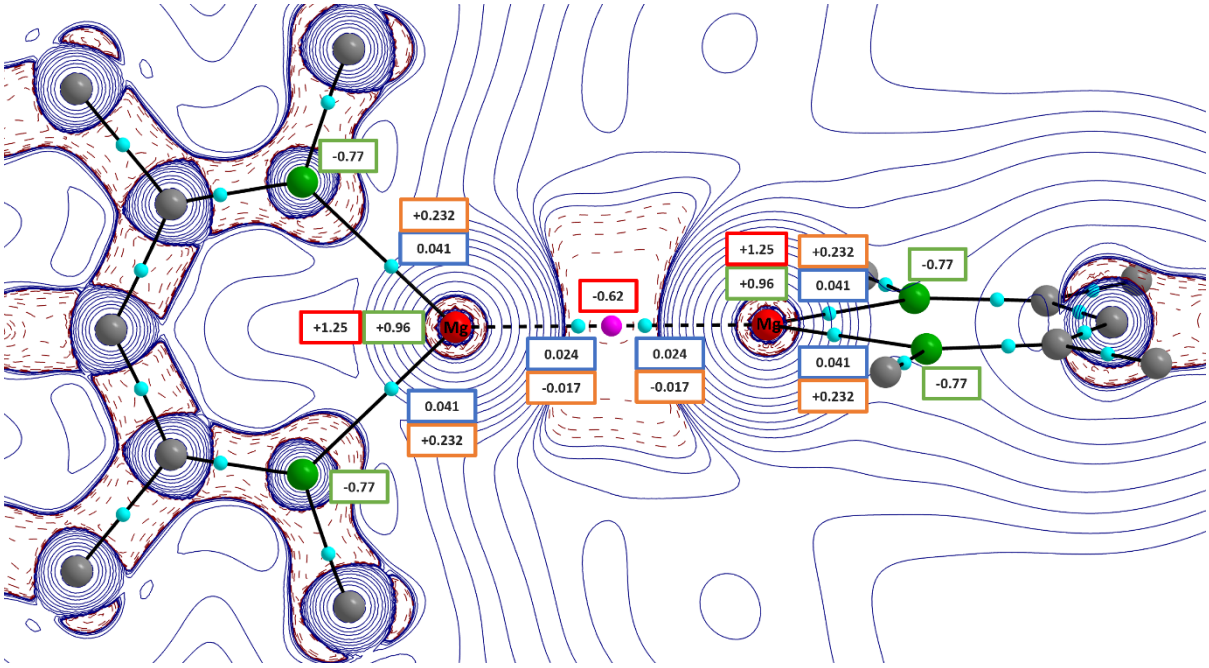


Figure S59. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Mg-Mg(^{DIPP}BDI) (calculated without Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); purple dots, non-nuclear attractor (NNA); green boxes, NPA charges; red boxes, AIM charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

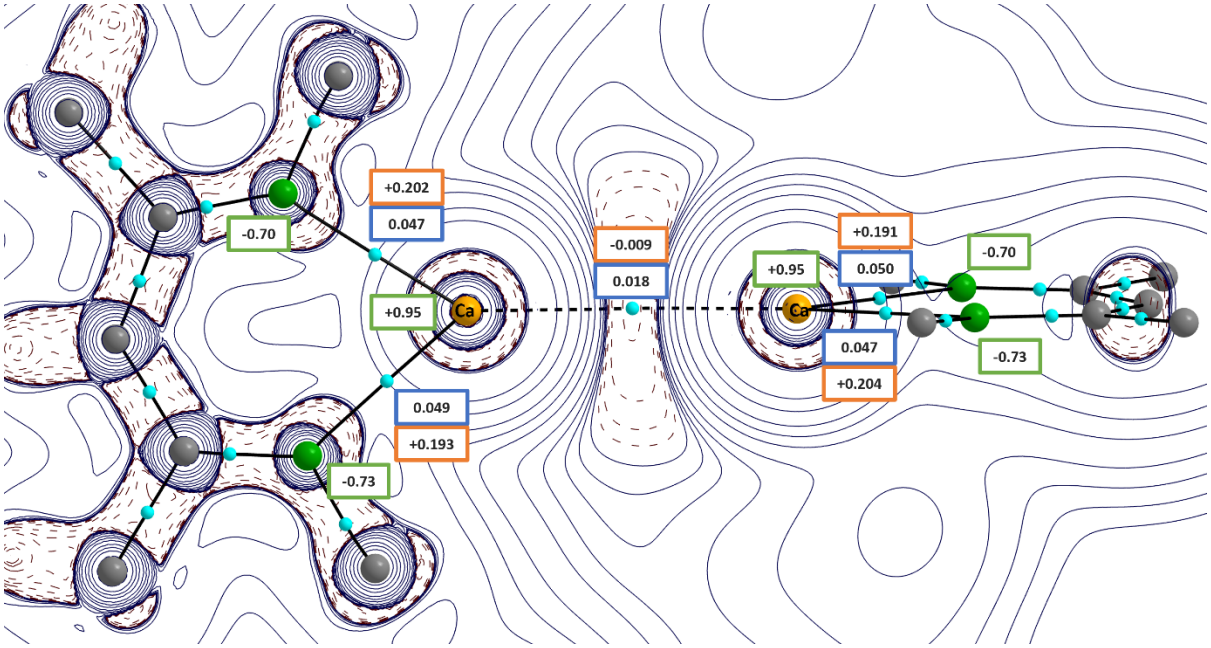


Figure S60. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Ca-Ca(^{DIPP}BDI) (calculated with Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); green boxes, NPA charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

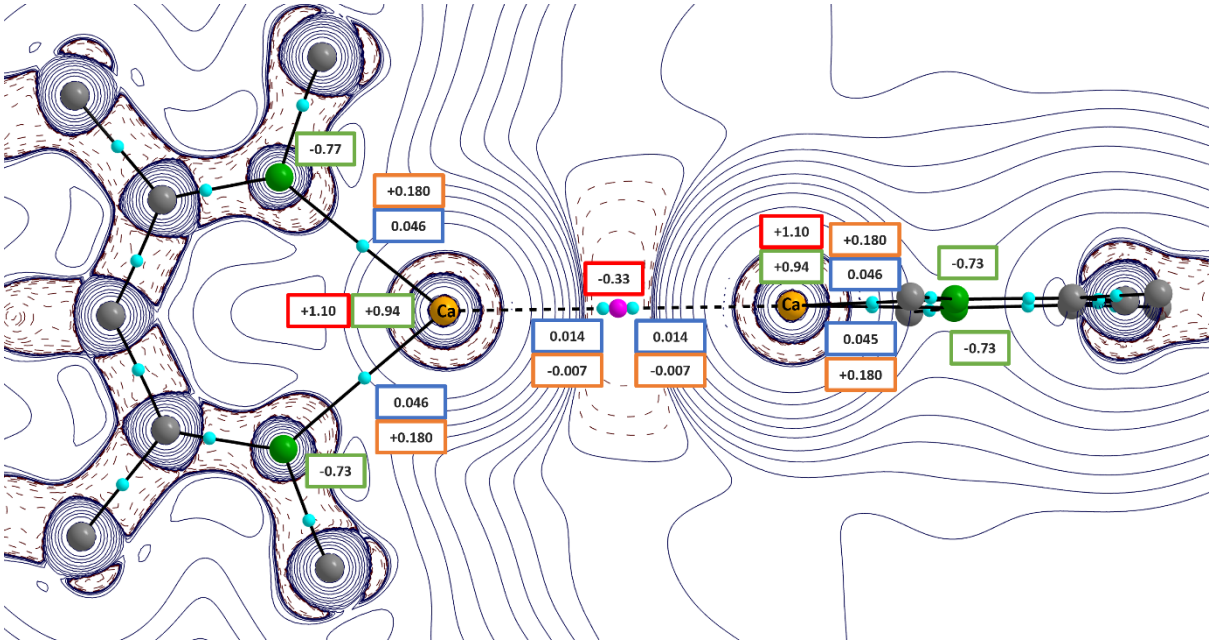


Figure S61. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Ca-Ca(^{DIPP}BDI) (calculated without Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); purple dots, non-nuclear attractor (NNA); green boxes, NPA charges; red boxes, AIM charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

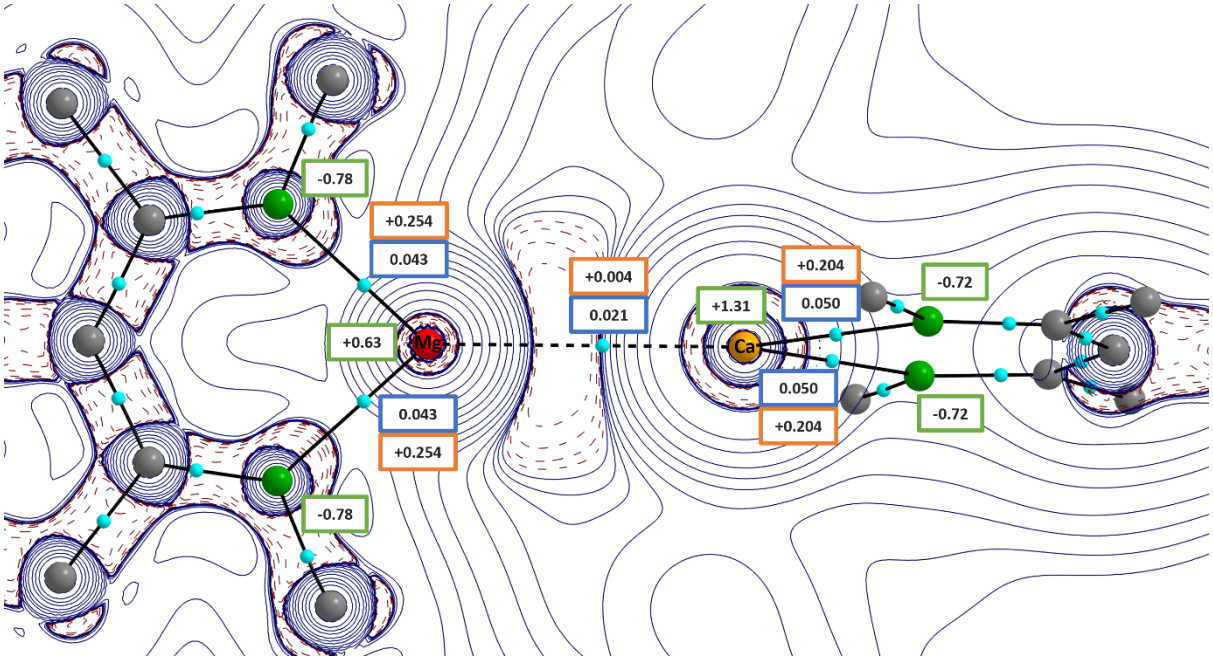


Figure S62. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Mg-Ca(^{DIPP}BDI) (calculated with Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); green boxes, NPA charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

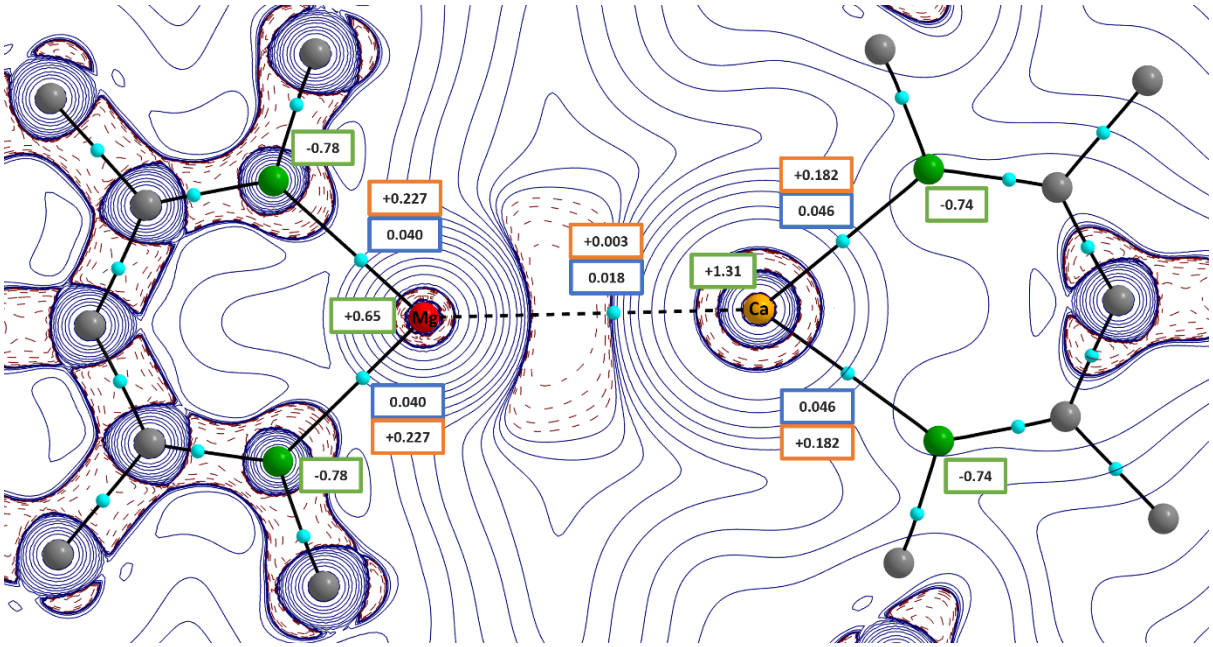


Figure S63. Atoms-In-Molecules: Contour plots of the Laplacian, $\nabla^2\rho(r)$, of (^{DIPP}BDI)Mg-Ca(^{DIPP}BDI) (calculated without Dispersion) through the plane formed by the Mg and the two N atoms bound to Mg. Light-blue dots, bond critical point (BCP); green boxes, NPA charges; blue boxes, electron densities in the BCPs; orange boxes, Laplacian $\nabla^2\rho$ in BCPs. Red dashed lines indicate areas of charge concentration, while blue solid lines show areas of charge depletion. DIPP-groups and hydrogen atoms were omitted for clarity.

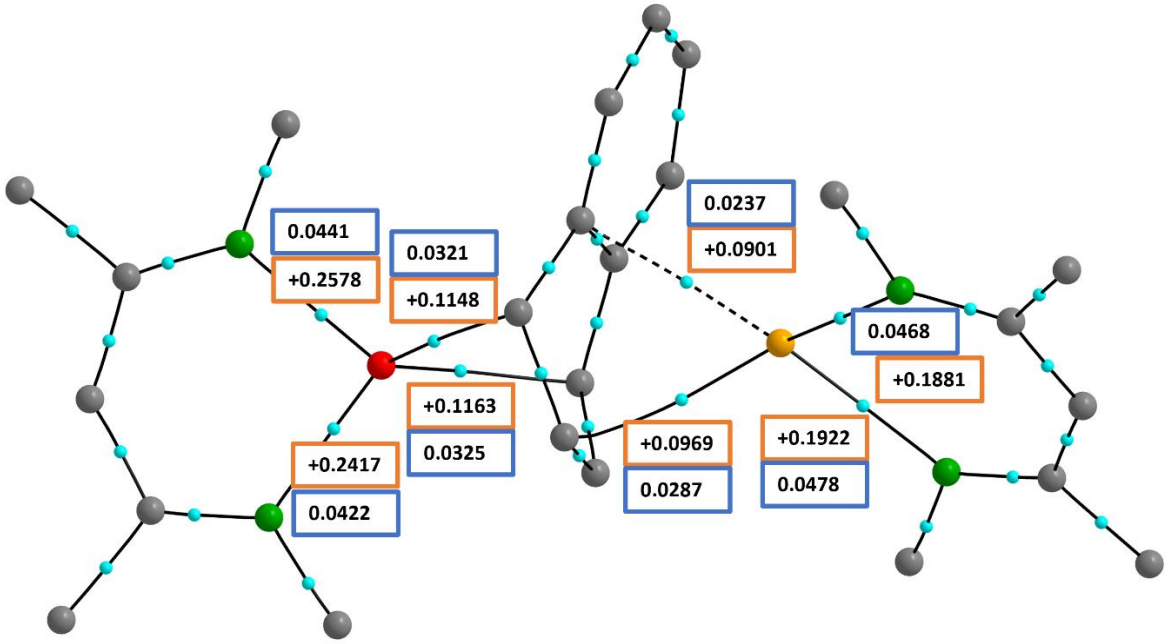


Figure S64. AIM analysis of the (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) complex given the electron densities ρ(r) (blue boxes) and the Laplacian of the electron densities $\nabla^2\rho$(r) (orange boxes) in the BCPs (bond critical points, light blue dots) (Magnesium: red; Calcium: orange). DIPeP-groups, *t*Bu-groups and hydrogen atoms were omitted for clarity.

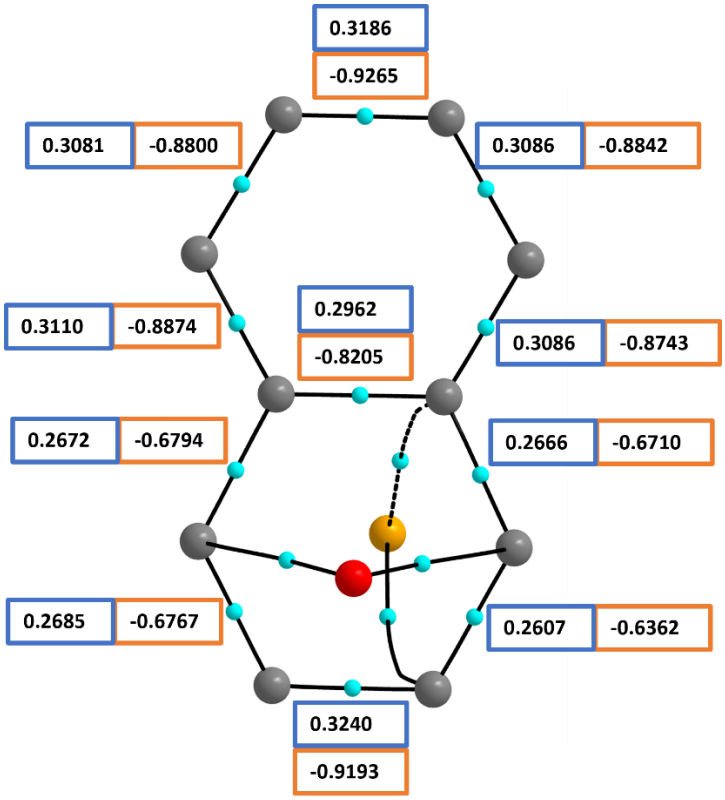


Figure S65. AIM analysis of the (^{DIPeP}BDI*)Mg(μ^2,μ^4-naphthalene)Ca(^{DIPeP}BDI) (**4**) complex given the electron densities ρ(r) (blue boxes) and the Laplacian of the electron densities $\nabla^2\rho$(r) (orange boxes) in the BCPs (bond critical points, light blue dots) of the bridged naphthalene (Magnesium: red; Calcium: orange). Ligand systems and hydrogen atoms were omitted for clarity.

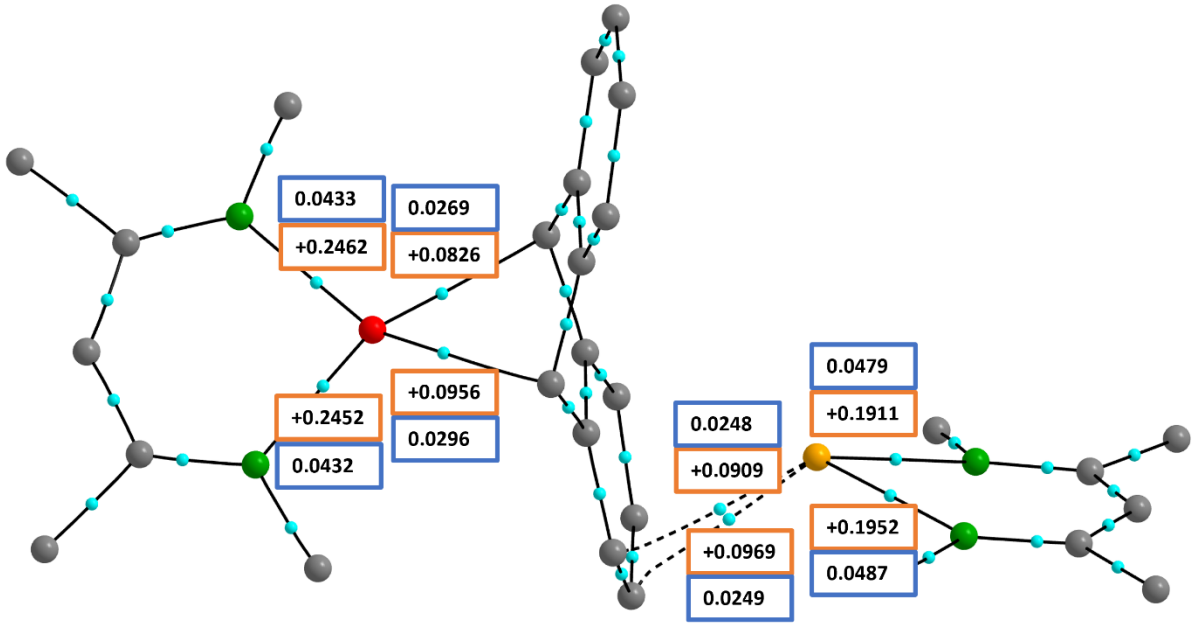


Figure S66. AIM analysis of the (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) complex given the electron densities ρ(r) (blue boxes) and the Laplacian of the electron densities $\nabla^2\rho$(r) (orange boxes) in the BCPs (bond critical points, light blue dots) (Magnesium: red; Calcium: orange). DIPeP-groups, *t*Bu-groups and hydrogen atoms were omitted for clarity.

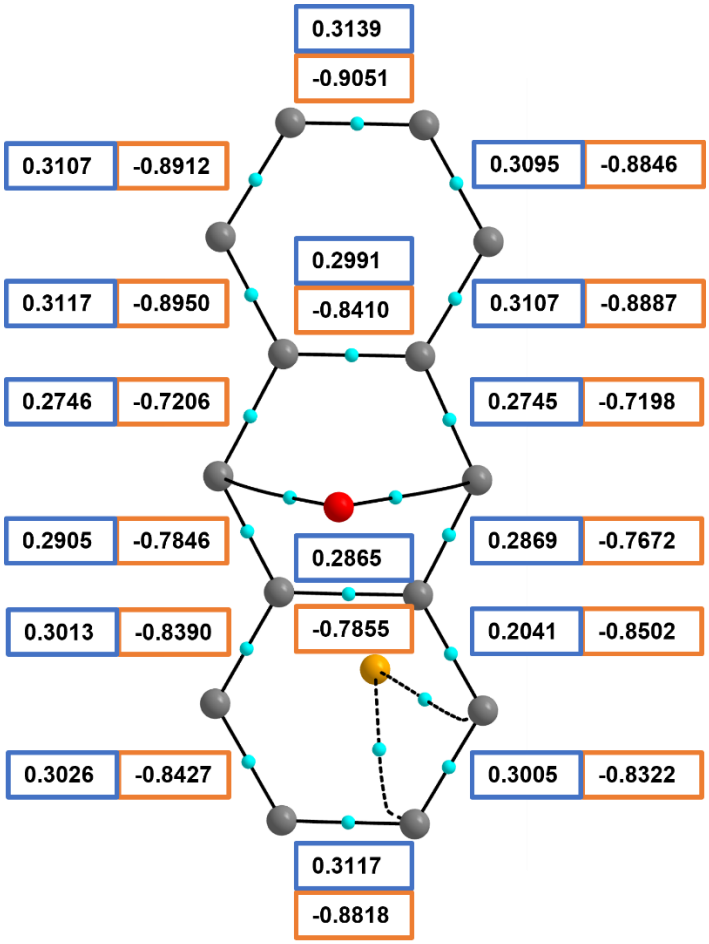


Figure S67. AIM analysis of the (^{DIPeP}BDI*)Mg(μ^2,μ^4-anthracene)Ca(^{DIPeP}BDI) (**5**) complex given the electron densities ρ(r) (blue boxes) and the Laplacian of the electron densities $\nabla^2\rho$(r) (orange boxes) in the BCPs (bond critical points, light blue dots) of the bridged anthracene (Magnesium: red; Calcium: orange). Ligand systems and hydrogen atoms were omitted for clarity.

XYZ-coordinates

73
(^{DIPP}BDI)Mg$^{\bullet}$ Dispersion
Mg -0.000034 -0.000031 -1.010978
N -1.476080 -0.000067 0.434643
N 1.476055 0.000010 0.434599
C -2.467110 -0.000564 2.667988
H -3.099945 -0.880105 2.475450
H -2.167690 -0.000197 3.722834
H -3.100924 0.878170 2.475057
C -1.271225 -0.000181 1.750115
C 0.000016 -0.000054 2.354228
H 0.000033 -0.000063 3.443542
C 1.271238 0.000094 1.750076
C 2.467157 0.000485 2.667904
H 3.100991 -0.878224 2.474918
H 3.099957 0.880051 2.475365
H 2.167779 0.000078 3.722760
C -2.806918 -0.000074 -0.066058
C -3.444586 -1.228282 -0.348099
C -4.716313 -1.204304 -0.929398
H -5.219370 -2.146301 -1.159868
C -5.350844 0.000035 -1.221120
H -6.343784 0.000099 -1.677152
C -4.716455 1.204326 -0.928828
H -5.219657 2.146350 -1.158872
C -3.444747 1.228205 -0.347516
C -2.745469 -2.546181 -0.067275
H -1.918500 -2.333494 0.627095
C -3.655990 -3.573021 0.605766
H -3.081913 -4.469259 0.888161
H -4.467623 -3.904038 -0.061039
C -2.126336 -3.106940 -1.351002
H -2.904692 -3.337903 -2.095636
H -1.557290 -4.028510 -1.150096
C -2.745761 2.546023 -0.066001
H -1.919198 2.333156 0.628795
C -3.656602 3.572771 0.606745
H -3.082640 4.468965 0.889521
H -4.119852 3.163371 1.517559
C -2.125901 3.107070 -1.349244
H -2.903876 3.338398 -2.094162
H -1.439189 2.379504 -1.815810

C 2.806883 0.000071 -0.066132
C 3.444784 -1.228177 -0.347573
C 4.716505 -1.204230 -0.928855
H 5.219766 -2.146226 -1.158880
C 5.350834 0.000096 -1.221135
H 6.343787 0.000084 -1.677139
C 4.716243 1.204402 -0.929405
H 5.219266 2.146425 -1.159841
C 3.444503 1.228311 -0.348132
C 2.745885 -2.546037 -0.066023
H 1.919285 -2.333202 0.628740
C 2.126110 -3.107190 -1.349261
H 2.904129 -3.338501 -2.094138
H 1.439366 -2.379696 -1.815894
C 3.656778 -3.572690 0.606795
H 3.082871 -4.468911 0.889595
H 4.119975 -3.163217 1.517601
C 2.745330 2.546170 -0.067253
H 1.918340 2.333405 0.627068
C 2.126230 3.106993 -1.350968
H 2.904608 3.338041 -2.095551
H 1.557138 4.028527 -1.150019
C 3.655784 3.573000 0.605891
H 3.081661 4.469198 0.888321
H 4.467430 3.904092 -0.060861
H 4.118601 3.163661 1.516952
H 1.439651 2.379399 -1.817688
H -4.467924 3.903890 -0.060384
H -1.556774 4.028465 -1.147775
H 4.468140 -3.903784 -0.060299
H 1.557039 -4.028615 -1.147767
H -4.118827 -3.163722 1.516834
H -1.439709 -2.379337 -1.817637

73

(^{DIPP}BDI)Mg$^{\bullet}$ no Dispersion

Mg 0.000000 0.000020 -1.000497
N 1.504273 -0.000023 0.426503
N -1.504273 0.000008 0.426503
C 2.458458 -0.000059 2.686456
H 3.096717 0.879529 2.513353
H 2.134628 -0.000094 3.734456
H 3.096743 -0.879617 2.513302
C 1.280761 -0.000046 1.740502
C 0.000000 -0.000046 2.332579
H 0.000000 -0.000070 3.422278
C -1.280761 -0.000019 1.740502
C -2.458458 -0.000058 2.686457
H -3.096748 0.879504 2.513344
H -3.096711 -0.879642 2.513313
H -2.134627 -0.000070 3.734457
C 2.839187 -0.000023 -0.077213
C 3.481916 1.229596 -0.368597
C 4.757383 1.201698 -0.944982
H 5.260454 2.144231 -1.177289
C 5.396913 -0.000012 -1.232571
H 6.392396 -0.000008 -1.683962
C 4.757354 -1.201729 -0.945069
H 5.260401 -2.144257 -1.177448
C 3.481888 -1.229638 -0.368683
C 2.809252 2.569928 -0.103658
H 1.896165 2.368360 0.477349
C 3.680266 3.515021 0.731976
H 3.125058 4.434141 0.978666
H 4.591407 3.819983 0.192797
C 2.376792 3.237559 -1.415960
H 3.246246 3.470138 -2.052006
H 1.840762 4.180522 -1.220617
C 2.809185 -2.569974 -0.103860
H 1.896118 -2.368434 0.477189
C 3.680187 -3.515183 0.731655
H 3.124951 -4.434308 0.978267
H 3.996449 -3.048992 1.677588
C 2.376670 -3.237455 -1.416219
H 3.246101 -3.470000 -2.052309
H 1.709461 -2.583058 -2.001461
C -2.839188 0.000031 -0.077213
C -3.481878 1.229656 -0.368662
C -4.757343 1.201765 -0.945052
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C -5.396913 0.000059 -1.232571
H -6.392395 0.000070 -1.683962
C -4.757394 -1.201661 -0.944999
H -5.260473 -2.144186 -1.177318
C -3.481926 -1.229578 -0.368616
C -2.809161 2.569982 -0.103829
H -1.896101 2.368430 0.477225
C -2.376630 3.237465 -1.416182
H -3.246054 3.470022 -2.052277
H -1.709424 2.583064 -2.001421
C -3.680160 3.515198 0.731684
H -3.124915 4.434315 0.978304
H -3.996434 3.049007 1.677613
C -2.809275 -2.569919 -0.103690
H -1.896183 -2.368364 0.477315
C -2.376830 -3.237548 -1.415998
H -3.246290 -3.470114 -2.052040
H -1.840808 -4.180517 -1.220663
C -3.680295 -3.515008 0.731945
H -3.125095 -4.434135 0.978627
H -4.591442 -3.819957 0.192770
H -3.996503 -3.048710 1.677843
H -1.709607 -2.583238 -2.001322
H 4.591302 -3.820125 0.192421
H 1.840610 -4.180419 -1.220960
H -4.591267 3.820152 0.192445
H -1.840562 4.180422 -1.220915
H 3.996485 3.048722 1.677870
H 1.709573 2.583246 -2.001284

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(^{DIPP}BDI)Mg-Mg(^{DIPP}BDI) dispersion

Mg -1.434392 0.125374 -0.093277
Mg 1.428171 -0.167684 0.071355
N -2.994934 -0.845781 -1.112582
N 2.789681 -1.249831 1.243939
N -2.891815 1.378706 0.730931
N 3.083243 0.589607 -0.967441
C -5.244205 -1.468382 -1.848682
C 4.894281 -2.102499 2.156612
H -4.919946 -1.601841 -2.890658
H 4.486512 -3.117229 2.268037
H -6.265764 -1.069406 -1.838178
H 5.954593 -2.167925 1.883861
H -5.256916 -2.474199 -1.400444
H 4.817258 -1.630314 3.148406

C -4.294483 -0.579416 -1.083854
C 4.111744 -1.298853 1.147362
C -4.858252 0.478114 -0.347916
C 4.849018 -0.607683 0.168842
H -5.938266 0.594569 -0.428760
H 5.928141 -0.754459 0.190988
C -4.201756 1.388563 0.497001
C 4.367745 0.278667 -0.808707
C -5.054176 2.435706 1.170053
C 5.388625 0.909265 -1.723538
H -4.721721 3.444080 0.881106
H 5.174446 0.655261 -2.772536
H -4.949574 2.382558 2.264042
H 5.345032 2.006979 -1.661323
H -6.112945 2.322918 0.907517
H 6.405759 0.579581 -1.479823
C -2.514026 -1.904450 -1.918896
C 2.132795 -1.998033 2.249780
C -2.145952 -1.640741 -3.260103
C 1.720064 -3.322453 1.967421
C -1.555810 -2.678802 -3.988472
C 0.970795 -3.991399 2.940707
H -1.259098 -2.513581 -5.024250
H 0.633033 -5.011699 2.758691
C -1.325442 -3.928857 -3.415925
C 0.639135 -3.380295 4.149151
H -0.844454 -4.715105 -4.002782
H 0.042445 -3.922544 4.886580
C -1.728343 -4.180352 -2.108872
C 1.084659 -2.091694 4.422593
H -1.569326 -5.170612 -1.674886
H 0.845466 -1.629722 5.383817
C -2.344524 -3.182702 -1.346461
C 1.843060 -1.382440 3.485739
C -2.459619 -0.287239 -3.895531
C 2.152473 -4.006786 0.671724
H -3.531922 -0.104370 -3.703827
H 3.248968 -3.885061 0.616376
C -2.284090 -0.283329 -5.412852
C 1.882767 -5.510175 0.669864
H -2.646494 0.668219 -5.829814
H 2.327329 -5.969782 -0.225512
H -1.225779 -0.382404 -5.702593
H 0.803836 -5.731654 0.646718
C -1.712292 0.904437 -3.276707
C 1.590997 -3.370670 -0.609526
H -1.832665 1.797401 -3.908174
H 1.762345 -4.032670 -1.471453
H -2.123437 1.165909 -2.292523
H 2.099020 -2.424988 -0.841891
C -2.839261 -3.467551 0.060993
C 2.361161 0.012105 3.794435
H -3.469746 -2.616510 0.357900
H 3.065475 0.276471 2.991926
C -3.704525 -4.727478 0.121980
C 3.129339 0.058065 5.116701
H -4.140300 -4.847407 1.126302
H 3.580572 1.051460 5.267003
H -4.529097 -4.687789 -0.606248
H 3.935528 -0.690885 5.143525
C -1.688879 -3.542780 1.061564
C 1.244863 1.055301 3.772428
H -1.021906 -4.386192 0.831722
H 0.528887 0.888637 4.590886
H -1.070909 -2.630862 1.050873
H 0.673137 1.029900 2.831555
C -2.343420 2.327207 1.630284
C 2.718858 1.535305 -1.957956
C -1.856530 3.554792 1.133509
C 2.369333 1.088703 -3.249919
C -1.190294 4.411062 2.016521
C 1.857028 2.019772 -4.159874
H -0.796075 5.362210 1.650034
H 1.557380 1.689606 -5.157560
C -1.036006 4.076679 3.359281
C 1.741857 3.364602 -3.818409
H -0.508962 4.754688 4.034911
H 1.341229 4.080280 -4.540401
C -1.579970 2.890090 3.848643
C 2.167028 3.803873 -2.565618
H -1.486422 2.657511 4.911151
H 2.111014 4.867269 -2.325444
C -2.244322 1.998783 3.001922
C 2.658414 2.905561 -1.614742
C -2.086886 3.938029 -0.318574
C 2.585661 -0.362944 -3.641445
H -2.833804 3.235534 -0.716624
H 3.238792 -0.804852 -2.874576
C -0.827507 3.776868 -1.167177
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H -0.059330 4.507129 -0.876020
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H -0.377591 2.776645 -1.060968
H 0.762074 -1.094005 -2.665596
C -2.664038 5.347515 -0.458440
C 3.301051 -0.496556 -4.986723
H -2.924726 5.554211 -1.508322
H 3.551671 -1.550322 -5.185829
H -3.571835 5.476319 0.150850
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C 3.154452 3.360214 -0.250685
H -3.724749 0.497989 2.841233
H 3.928248 2.639412 0.053939
C -1.941186 -0.484651 3.437758
C 2.068040 3.304666 0.825193
H -1.139262 -0.414224 4.183293
H 1.318527 4.093915 0.683584
H -2.485152 -1.424522 3.616685
H 2.503046 3.430327 1.828097
C -3.456899 0.859844 4.924161
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H 4.266897 4.966907 0.693202
H -2.664687 0.986179 5.679204
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H 2.469149 -0.135413 5.977154
H -2.057748 -3.679371 2.089316
H 1.648692 2.072146 3.890226
H -1.941385 6.117285 -0.144186
H 2.671377 -0.148058 -5.820669

H -1.043492 3.932819 -2.234745
H 1.470782 -2.229515 -3.830650
H -2.844932 -1.097762 -5.895361
H 2.311899 -6.007861 1.552379
H -0.634956 0.722243 -3.170149
H 0.510733 -3.184509 -0.551909

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(^{DIPP}BDI)Mg-Mg(^{DIPP}BDI) no dispersion
Mg -1.562963 0.002295 0.002365
Mg 1.563420 -0.000596 -0.001311
N -3.095763 -1.052978 1.047310
N 3.099344 1.042453 1.051483
N -3.096554 1.059858 -1.039535
N 3.093665 -1.048703 -1.057310
C -5.358769 -1.737475 1.728198
C 5.364315 1.720663 1.731726
H -5.194084 -2.810461 1.550303
H 5.199278 1.548800 2.805577
H -6.405233 -1.501259 1.499267
H 6.410108 1.487709 1.496476
H -5.189549 -1.576289 2.803039
H 5.198062 2.795167 1.565032
C -4.411910 -0.899429 0.898787
C 4.414970 0.890215 0.897489
C -5.014123 0.005403 0.006635
C 5.014433 -0.005940 -0.005260
H -6.103499 0.006469 0.008099
H 6.103806 -0.007428 -0.006718
C -4.412555 0.908892 -0.887336
C 4.410093 -0.900244 -0.906633
C -5.360016 1.748423 -1.714641
C 5.354927 -1.732479 -1.744158
H -5.194606 1.585435 -2.789842
H 5.185324 -2.806761 -1.579419
H -5.192130 2.821207 -1.538742
H 5.188345 -1.557726 -2.817332
H -6.406337 1.515059 -1.482144
H 6.401956 -1.503502 -1.510535
C -2.629076 -2.010966 1.992522
C 2.635528 1.991309 2.007233
C -2.385504 -3.343829 1.576121
C 2.392096 1.579014 3.341391
C -1.777900 -4.222338 2.480970
C 1.786630 2.487300 4.217865
H -1.568585 -5.250505 2.173849
H 1.576889 2.183142 5.246811
C -1.448405 -3.816550 3.772027
C 1.459941 3.778100 3.809045
H -0.966520 -4.515415 4.460747
H 0.979998 4.469658 4.506443
C -1.770721 -2.529062 4.194366
C 1.782353 4.196364 2.520248
H -1.555739 -2.234836 5.225173
H 1.569517 5.226893 2.223522
C -2.379045 -1.611702 3.329349
C 2.387595 3.327471 1.604523
C -2.830811 -3.831513 0.201053
C 2.834602 0.204093 3.832122
H -3.493557 -3.056499 -0.211591
H 3.500633 -0.209196 3.060222
C -3.646664 -5.127451 0.284876
C 3.644631 0.288069 5.131705
H -4.058236 -5.386566 -0.703801
H 4.055639 -0.700482 5.392168
H -3.031797 -5.980642 0.613586
H 3.025671 0.615955 5.982243
C -1.673841 -3.988823 -0.788770
C 1.676733 -0.785360 3.984786
H -2.052401 -4.231951 -1.794460
H 2.053897 -1.790473 4.232535
H -1.069302 -3.071735 -0.870288
H 1.077971 -0.869090 3.064148
C -2.818204 -0.241417 3.835517
C 2.825573 3.828989 0.232168
H -3.482285 0.182496 3.067732
H 3.484228 3.056980 -0.192644
C -3.629699 -0.338589 5.133341
C 3.644446 5.122497 0.325144
H -4.038159 0.647957 5.405216
H 4.050421 5.391533 -0.663210
H -4.473804 -1.039360 5.038813
H 4.490822 5.023941 1.022613
C -1.657941 0.742971 4.000861
C 1.663223 3.999577 -0.748943
H -0.976811 0.425275 4.804624
H 0.988210 4.808445 -0.431099
H -1.058591 0.836144 3.081607
H 1.057533 3.084141 -0.838250
C -2.630659 2.016017 -1.986992
C 2.625070 -1.995742 -2.012546
C -2.385122 1.615156 -3.324221
C 2.374913 -3.331479 -1.609760
C -1.777163 2.530507 -4.191624
C 1.765254 -4.198538 -2.524256
H -1.565762 2.235083 -5.222804
H 1.550697 -5.228670 -2.227427
C -1.450500 3.817500 -3.771123
C 1.440307 -3.778903 -3.811981
H -0.968733 4.514695 -4.461618
H 0.957004 -4.469047 -4.508460
C -1.775352 4.224922 -2.479464
C 1.768640 -2.488584 -4.220939
H -1.562574 5.252741 -2.173624
H 1.556788 -2.183381 -5.249177
C -2.382789 3.348579 -1.572367
C 2.378733 -1.582164 -3.345745
C -2.828501 0.245447 -3.828348
C 2.815077 -3.834523 -0.238600
H -3.491984 -0.176510 -3.058943
H 3.478036 -3.064971 0.183926
C -1.670919 -0.741853 -3.995262
C 1.655304 -4.000442 0.746358
H -0.990861 -0.426663 -4.800861
H 0.975714 -4.806310 0.430696
H -1.069548 -0.835504 -3.077430
H 1.053849 -3.082493 0.838155
C -3.642538 0.343138 -5.124477
C 3.628720 -5.131174 -0.333886
H -4.053383 -0.642872 -5.394685
H 4.037383 -5.401181 0.653087
H -4.485132 1.045552 -5.028569
H 4.472839 -5.036289 -1.034606
C -2.823320 3.838296 -0.196486
C 2.823349 -0.208463 -3.837831
H -3.488878 3.066117 0.217059

H 3.488457 0.205514 -3.065534
C -1.664019 3.990341 0.791393
C 1.666653 0.781712 -3.994580
H -0.981613 4.797115 0.484540
H 0.984764 0.473943 -4.801551
H -2.039733 4.237997 1.797051
H 2.045232 1.785627 -4.244966
C -3.633414 5.137999 -0.278499
C 3.635564 -0.295830 -5.135898
H -4.042433 5.398279 0.710933
H 4.047483 0.691884 -5.398150
H -3.014955 5.988515 -0.607365
H 3.017662 -0.625616 -5.986473
H -4.477008 5.052784 -0.981104
H 4.477323 -1.000212 -5.047444
H -1.065414 3.069564 0.874208
H 1.067195 0.868890 -3.074802
H -3.012277 -0.678370 5.980351
H 3.032952 5.973009 0.666853
H -2.032595 1.746028 4.260409
H 2.036408 4.254488 -1.753724
H -3.026414 0.681056 -5.973160
H 3.012675 -5.979537 -0.672763
H -2.048577 -1.744301 -4.252765
H 2.030936 -4.257324 1.749729
H -4.488890 -5.037773 0.988578
H 4.486823 0.992309 5.046123
H -0.996274 -4.800646 -0.484582
H 0.994254 -0.479151 4.791685

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(^{DIPP}BDI)Ca$^{\bullet}$ Dispersion

Ca 0.013304 -0.411637 -1.294944
N -1.433872 -0.312691 0.515385
N 1.452851 -0.114456 0.493716
C -2.427224 -0.154663 2.757423
H -3.330592 -0.611666 2.332449
H -2.656488 0.908120 2.936556
H -2.208879 -0.612737 3.731328
C -1.242638 -0.271275 1.827522
C 0.029536 -0.272484 2.431964
H 0.037201 -0.285534 3.522201
C 1.286619 -0.152849 1.810149
C 2.490579 -0.073850 2.718276
H 3.261034 0.594741 2.310010
H 2.951759 -1.069914 2.813890
H 2.211894 0.264310 3.724443
C -2.720747 -0.156798 -0.041968
C -3.292783 1.133289 -0.162525
C -4.532620 1.259804 -0.794684
H -4.986124 2.249324 -0.892643
C -5.195174 0.150405 -1.312232
H -6.164195 0.269548 -1.802588
C -4.611153 -1.109979 -1.218018
H -5.129976 -1.972750 -1.639969
C -3.372632 -1.288238 -0.594518
C -2.552060 2.367464 0.320761
H -1.703338 2.028771 0.932580
C -3.420308 3.275551 1.192424
H -2.821278 4.101574 1.606485
H -4.245450 3.726002 0.618546
C -1.967231 3.137841 -0.866963
H -1.370559 3.998094 -0.525113
H -1.312903 2.495945 -1.481375
C -2.748025 -2.666394 -0.467262
H -1.651373 -2.521631 -0.431609
C -3.131294 -3.327971 0.859487
H -2.663322 -4.320910 0.950490
H -2.806832 -2.723772 1.717452
C -3.046505 -3.581745 -1.651499
H -4.107264 -3.875893 -1.688015
H -2.793193 -3.096367 -2.606749
C 2.715050 0.136867 -0.085933
C 2.967370 1.437084 -0.596874
C 4.181062 1.679010 -1.245864
H 4.394004 2.675937 -1.636164
C 5.124033 0.666923 -1.408406
H 6.067179 0.874346 -1.919393
C 4.853749 -0.612188 -0.932339
H 5.589500 -1.406525 -1.081056
C 3.655125 -0.903468 -0.273880
C 1.942645 2.542251 -0.404114
H 0.948821 2.058312 -0.381969
C 1.929252 3.565231 -1.536290
H 2.844210 4.178096 -1.548756
H 1.833100 3.076882 -2.518360
C 2.104697 3.222987 0.957989
H 1.347186 4.011605 1.091194
H 1.989013 2.505974 1.781826
C 3.360656 -2.320735 0.181321
H 2.452318 -2.283848 0.801110
C 3.050871 -3.219505 -1.019685
H 3.916227 -3.290800 -1.697789
H 2.786418 -4.238061 -0.693837
C 4.486699 -2.908185 1.033927
H 4.195973 -3.891746 1.434793
H 5.407585 -3.053432 0.447412
H 4.735174 -2.252312 1.881930
H 2.205867 -2.825123 -1.609945
H -4.223473 -3.456577 0.927415
H -2.456279 -4.507529 -1.573581
H 3.100551 3.686238 1.045206
H 1.080435 4.254711 -1.415182
H -3.865330 2.721398 2.032539
H -2.762836 3.513681 -1.529700

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(^{DIPP}BDI)Ca$^{\bullet}$ noDispersion

Ca 0.000018 -0.000582 -1.292124
N -1.505920 -0.000126 0.483820
N 1.505919 -0.000190 0.483842
C -2.456921 -0.000095 2.744803
H -3.095186 -0.879883 2.573377
H -3.095335 0.879532 2.573120
H -2.133088 0.000074 3.792879
C -1.280992 -0.000155 1.794830
C -0.000009 -0.000244 2.387077
H -0.000015 -0.000305 3.476960
C 1.280982 -0.000220 1.794850
C 2.456888 -0.000264 2.744851
H 3.095300 0.879387 2.573289
H 3.095158 -0.880029 2.573337
H 2.133029 -0.000212 3.792919
C -2.829430 0.000024 -0.034126
C -3.468044 1.230646 -0.348127
C -4.724216 1.201590 -0.965067

H -5.221167 2.144298 -1.210326
C -5.354142 0.000359 -1.274585
H -6.334182 0.000492 -1.758430
C -4.724543 -1.201029 -0.965055
H -5.221746 -2.143610 -1.210295
C -3.468369 -1.230419 -0.348109
C -2.823652 2.575820 -0.037271
H -1.881286 2.370773 0.494467
C -3.692879 3.436063 0.888696
H -3.165662 4.363858 1.162896
H -4.639488 3.726737 0.405429
C -2.471734 3.343222 -1.318187
H -1.955008 4.287279 -1.081233
H -1.810323 2.754884 -1.977196
C -2.824385 -2.575786 -0.037218
H -1.881912 -2.371004 0.494439
C -3.693835 -3.435670 0.888875
H -3.166905 -4.363613 1.163129
H -3.947766 -2.905708 1.819561
C -2.472827 -3.343407 -1.318097
H -3.374315 -3.591576 -1.901365
H -1.811226 -2.755365 -1.977181
C 2.829421 0.000010 -0.034125
C 3.468015 1.230647 -0.348062
C 4.724188 1.201635 -0.965023
H 5.221124 2.144364 -1.210232
C 5.354115 0.000434 -1.274622
H 6.334153 0.000596 -1.758473
C 4.724521 -1.200982 -0.965162
H 5.221726 -2.143544 -1.210473
C 3.468360 -1.230416 -0.348208
C 2.823644 2.575819 -0.037130
H 1.881226 2.370756 0.494513
C 2.471854 3.343362 -1.317993
H 3.373264 3.591857 -1.901241
H 1.810457 2.755112 -1.977091
C 3.692843 3.435921 0.888995
H 3.165667 4.363726 1.163242
H 3.946875 2.906017 1.819686
C 2.824378 -2.575791 -0.037373
H 1.881866 -2.371027 0.494227
C 2.472910 -3.343429 -1.318268
H 3.374442 -3.591637 -1.901452
H 1.956488 -4.287647 -1.081293
C 3.693781 -3.435672 0.888774
H 3.166854 -4.363634 1.162966
H 4.640550 -3.726035 0.405632
H 3.947633 -2.905725 1.819490
H 1.811377 -2.755393 -1.977422
H -4.640563 -3.726073 0.405680
H -1.956444 -4.287641 -1.081102
H 4.639513 3.726567 0.405831
H 1.955159 4.287419 -1.080970
H -3.947021 2.906259 1.819415
H -3.373099 3.591686 -1.901520

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(^{DIPP}BDI)Ca-Ca(^{DIPP}BDI) dispersion
Ca 1.767358 -0.090234 0.035513
Ca -1.774711 0.054201 -0.123382
N 3.478352 -1.279227 1.102776
N -3.734536 -0.805513 -1.063235
N 3.724941 0.777848 -0.840464
N -3.493642 1.148704 0.982927
C 5.595611 -2.161238 1.988790
C -6.029398 -1.438855 -1.673611
H 4.946263 -2.813440 2.587374
H -5.535783 -2.137483 -2.361897
H 6.242153 -1.584745 2.668246
H -6.706433 -2.005406 -1.016198
H 6.258021 -2.790876 1.375054
H -6.655851 -0.750806 -2.262256
C 4.795108 -1.232495 1.104468
C -5.026638 -0.654900 -0.858563
C 5.529606 -0.346789 0.283598
C -5.544245 0.248650 0.096405
H 6.615888 -0.409858 0.360355
H -6.631379 0.304051 0.166238
C 5.021026 0.580259 -0.644300
C -4.818680 1.107688 0.942693
C 6.005411 1.379922 -1.459654
C -5.597603 2.034239 1.841949
H 5.822403 2.457380 -1.330694
H -5.309696 1.879201 2.892656
H 5.868719 1.170424 -2.531589
H -5.355712 3.082236 1.608249
H 7.044467 1.158304 -1.186010
H -6.680750 1.890713 1.743228
C 2.681582 -2.085418 1.925583
C -3.130561 -1.728076 -1.924615
C 2.400760 -1.690570 3.260885
C -2.963737 -3.080080 -1.519939
C 1.462387 -2.428938 3.985627
C -2.191541 -3.919722 -2.325850
H 1.237446 -2.152170 5.016077
H -2.053459 -4.963315 -2.041022
C 0.786797 -3.506726 3.415627
C -1.569536 -3.449965 -3.482082
H 0.050026 -4.060370 4.002084
H -0.962324 -4.126539 -4.087658
C 1.039342 -3.862397 2.095677
C -1.706385 -2.116478 -3.849496
H 0.497405 -4.698785 1.649751
H -1.202906 -1.749919 -4.746122
C 1.976931 -3.163383 1.329279
C -2.475267 -1.235220 -3.083260
C 3.085355 -0.468186 3.855805
C -3.584345 -3.569361 -0.218514
H 4.157154 -0.542799 3.609725
H -4.627925 -3.214727 -0.201946
C 2.979413 -0.391438 5.376569
C -3.626184 -5.090440 -0.099499
H 3.594634 0.438264 5.756187
H -4.193037 -5.383238 0.797134
H 1.944175 -0.204215 5.703736
H -2.615816 -5.518306 0.000472
C 2.574680 0.835263 3.223262
C -2.891597 -2.961796 1.010628
H 2.973050 1.712169 3.756561
H -3.259969 -3.427743 1.937604
H 2.920665 0.929265 2.182627
H -3.114963 -1.887830 1.099967
C 2.284562 -3.566422 -0.102094
C -2.660259 0.215112 -3.494720
H 2.674973 -2.666436 -0.612046
H -2.937556 0.774094 -2.582024

C 3.419890 -4.594232 -0.135454
C -3.852754 0.349131 -4.447203
H 3.694763 -4.844121 -1.172532
H -4.040003 1.405037 -4.699228
H 4.316214 -4.212702 0.373997
H -4.767156 -0.063797 -3.997206
C 1.062259 -4.042272 -0.881001
C -1.398819 0.858161 -4.065167
H 0.663643 -4.992066 -0.490327
H -1.103907 0.409165 -5.026832
H 0.256390 -3.291554 -0.851649
H -0.552031 0.761253 -3.366687
C 3.204475 1.658627 -1.806682
C -2.772232 2.051768 1.787188
C 2.812568 2.966332 -1.423312
C -2.289499 1.635138 3.053008
C 2.105804 3.754272 -2.336203
C -1.410588 2.470201 3.749173
H 1.795288 4.761272 -2.045450
H -1.030256 2.152192 4.723660
C 1.782097 3.277247 -3.603241
C -1.008374 3.694857 3.223519
H 1.222289 3.904847 -4.300560
H -0.317766 4.332643 3.780164
C 2.165777 1.990749 -3.972416
C -1.482465 4.096574 1.977870
H 1.900153 1.614989 -4.964022
H -1.156354 5.053440 1.562314
C 2.870822 1.163386 -3.094119
C -2.354694 3.292488 1.239559
C 3.134103 3.499304 -0.038678
C -2.699265 0.297731 3.641740
H 3.704029 2.713668 0.480796
H -3.408788 -0.158913 2.934779
C 1.864032 3.764532 0.773202
C -1.503570 -0.647973 3.773626
H 1.268720 4.577390 0.329174
H -0.762162 -0.259854 4.489909
H 1.203665 2.880680 0.815535
H -0.973993 -0.782770 2.814030
C 4.020080 4.745719 -0.101234
C -3.424336 0.463856 4.979322
H 4.304413 5.073097 0.911337
H -3.780929 -0.509277 5.352452
H 4.943063 4.555187 -0.669548
H -4.293671 1.132320 4.886288
C 3.248725 -0.247859 -3.510155
C -2.820588 3.735420 -0.136796
H 3.818965 -0.686751 -2.677091
H -3.513540 2.963270 -0.504990
C 2.011894 -1.123311 -3.733296
C -1.655061 3.819521 -1.127620
H 1.410870 -0.757930 -4.580648
H -0.944701 4.612002 -0.844783
H 2.300021 -2.164567 -3.947917
H -2.016931 4.039750 -2.144355
C 4.155563 -0.252493 -4.743039
C -3.591609 5.056142 -0.080439
H 4.483335 -1.276477 -4.982450
H -3.985200 5.320582 -1.074635
H 3.633205 0.144509 -5.628182
H -2.946693 5.885101 0.252426
H 5.053263 0.363993 -4.584569
H -4.440885 4.996822 0.616866
H 1.344464 -1.130324 -2.853419
H -1.075074 2.880616 -1.167980
H 3.115436 -5.523731 0.371961
H -3.663506 -0.198576 -5.384430
H 1.321678 -4.208753 -1.937372
H -1.564242 1.931542 -4.243815
H 3.498918 5.585825 -0.587590
H -2.759532 0.890378 5.747492
H 2.107758 4.052763 1.807634
H -1.819742 -1.642290 4.125244
H 3.325791 -1.318235 5.858443
H -4.108155 -5.556764 -0.972075
H 1.474874 0.895656 3.245047
H -1.799620 -3.101204 0.973482

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(^{DIPP}BDI)Ca-Ca(^{DIPP}BDI) no dispersion

Ca -1.938186 0.013208 0.008460
Ca 1.937549 -0.008919 0.000606
N -3.746188 1.080363 -1.070164
N 3.738092 -1.105857 -1.060684
N -3.754462 -1.036905 1.090358
N 3.763663 1.061398 1.049530
C -6.009940 1.754646 -1.734709
C 5.996213 -1.798323 -1.725765
H -5.848761 1.568571 -2.807274
H 5.820558 -2.868840 -1.541974
H -5.834236 2.829664 -1.579670
H 5.825619 -1.640430 -2.801213
H -7.056764 1.531960 -1.493929
H 7.045255 -1.570719 -1.499643
C -5.056254 0.929253 -0.899626
C 5.049686 -0.952061 -0.903814
C -5.650709 0.037684 0.018401
C 5.651290 -0.040885 -0.010383
H -6.740561 0.047041 0.023152
H 6.741134 -0.050634 -0.013808
C -5.063662 -0.865036 0.929841
C 5.071474 0.882633 0.885193
C -6.023195 -1.679064 1.769259
C 6.038907 1.713575 1.698610
H -5.850439 -1.500385 2.841195
H 5.880273 2.786780 1.515008
H -5.863723 -2.755932 1.609189
H 5.874360 1.560113 2.775626
H -7.068577 -1.440657 1.537530
H 7.082036 1.467890 1.464234
C -3.246459 2.005583 -2.024601
C 3.229119 -2.050699 -1.991209
C -2.937706 3.334740 -1.628430
C 2.931573 -1.646748 -3.320553
C -2.329966 4.191020 -2.553955
C 2.314341 -2.561259 -4.181821
H -2.086612 5.214686 -2.256027
H 2.078265 -2.256764 -5.205296
C -2.029769 3.768670 -3.845418
C 1.994891 -3.849789 -3.764326
H -1.552371 4.452609 -4.551901
H 1.510298 -4.547597 -4.452105
C -2.345589 2.469425 -4.231179
C 2.300953 -4.243787 -2.465083
H -2.113868 2.142519 -5.248728

H 2.055121 -5.259347 -2.142295
C -2.954308 1.572302 -3.345883
C 2.918328 -3.369246 -1.563226
C -3.254116 3.847968 -0.229368
C 3.268958 -0.250571 -3.828197
H -3.807400 3.051236 0.291493
H 3.822971 0.261415 -3.026210
C -4.157489 5.087263 -0.255540
C 4.180264 -0.285454 -5.061572
H -4.443304 5.379064 0.767833
H 4.477971 0.735193 -5.350956
H -3.651130 5.952219 -0.713557
H 3.675249 -0.738144 -5.930165
C -1.979258 4.124450 0.576182
C 2.006145 0.571711 -4.111459
H -2.222688 4.424799 1.608148
H 2.264257 1.600813 -4.409343
H -1.325623 3.237333 0.628164
H 1.346760 0.630882 -3.228849
C -3.287791 0.163482 -3.820073
C 3.243200 -3.851195 -0.154932
H -3.829072 -0.334500 -3.000673
H 3.797886 -3.041714 0.344504
C -4.213826 0.167234 -5.042927
C 4.148728 -5.089320 -0.159293
H -4.509383 -0.860788 -5.307528
H 4.439252 -5.359641 0.868641
H -5.132658 0.744701 -4.858713
H 5.070882 -4.919899 -0.735992
C -2.023245 -0.657416 -4.101101
C 1.973833 -4.111632 0.664897
H -1.442241 -0.226941 -4.932530
H 1.378948 -4.932900 0.233742
H -1.352766 -0.695063 -3.225908
H 1.318790 -3.224824 0.702269
C -3.262854 -1.976059 2.035617
C 3.279397 2.020566 1.978712
C -2.957924 -1.556885 3.358648
C 2.992149 3.343631 1.547582
C -2.359254 -2.469643 4.234869
C 2.400553 4.234656 2.450495
H -2.118994 -2.154013 5.253985
H 2.173754 5.253757 2.125087
C -2.064612 -3.770572 3.838062
C 2.095762 3.852678 3.753606
H -1.595246 -4.467116 4.537584
H 1.631455 4.563469 4.442064
C -2.376709 -4.178693 2.544789
C 2.390601 2.559283 4.173741
H -2.150330 -5.203694 2.238230
H 2.156086 2.263834 5.200197
C -2.976183 -3.306708 1.628518
C 2.982326 1.628645 3.311719
C -3.270556 -0.147205 3.844700
C 3.315100 3.814719 0.135207
H -3.814402 0.361990 3.033907
H 3.842632 2.990213 -0.369151
C -1.993375 0.656700 4.116087
C 2.044630 4.108895 -0.671205
H -1.407557 0.214009 4.937624
H 1.474841 4.943524 -0.231946
H -1.333642 0.690899 3.232761
H 1.367488 3.238995 -0.704387
C -4.183704 -0.145896 5.077031
C 4.253023 5.028575 0.128178
H -4.463999 0.884280 5.349529
H 4.536421 5.292406 -0.903431
H -5.111363 -0.711146 4.899182
H 5.178291 4.834339 0.691894
C -3.308228 -3.805047 0.227500
C 3.295021 0.227944 3.823534
H -3.841022 -2.990990 -0.288242
H 3.829811 -0.299821 3.018695
C -2.043572 -4.112946 -0.583275
C 2.018389 -0.566479 4.124691
H -1.469780 -4.939015 -0.133237
H 1.442099 -0.104011 4.942110
H -2.299715 -4.407183 -1.613924
H 2.259160 -1.598308 4.427725
C -4.245231 -5.019610 0.250320
C 4.219656 0.249876 5.047344
H -4.537960 -5.301829 -0.773772
H 4.497773 -0.775300 5.340204
H -3.762292 -5.898350 0.707286
H 3.733280 0.718868 5.917842
H -5.165554 -4.816405 0.818981
H 5.148398 0.806588 4.849181
H -1.367116 -3.243475 -0.638901
H 1.349353 -0.619087 3.249189
H -3.720969 0.604384 -5.926259
H 3.641670 -5.964014 -0.597485
H -2.279696 -1.693818 -4.374225
H 2.225095 -4.389210 1.701388
H -3.687418 -0.593208 5.953315
H 3.775194 5.915776 0.574075
H -2.233765 1.694603 4.397983
H 2.292543 4.383331 -1.709311
H -5.082367 4.906943 -0.824499
H 5.098354 -0.863584 -4.875628
H -1.385744 4.934759 0.122988
H 1.412389 0.126598 -4.926126

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(^{DIPP}BDI)Mg-Ca(^{DIPP}BDI) dispersion

Mg 1.743521 0.000266 -0.000111
Ca -1.499252 -0.000735 0.000048
N 3.274328 1.444321 -0.010373
N -3.332449 0.007205 1.412513
N 3.275252 -1.442816 0.009911
N -3.332815 -0.008149 -1.411920
C 5.487927 2.476824 0.000609
C -5.522756 0.007128 2.487973
H 5.291375 3.106481 -0.880298
H -5.313949 0.894283 3.105358
H 6.548453 2.196846 0.007985
H -6.589355 -0.004348 2.232330
H 5.278865 3.105900 0.878958
H -5.297282 -0.866124 3.118853
C 4.589405 1.265506 -0.003811
C -4.648654 0.004519 1.260167
C 5.207392 0.001356 -0.000354
C -5.277488 -0.000428 0.000544
H 6.296915 0.001701 -0.000452
H -6.367202 -0.000433 0.000684
C 4.590208 -1.263187 0.003169
C -4.648979 -0.005472 -1.259239

C 5.489479 -2.473949 -0.001450
C -5.523384 -0.008392 -2.486825
H 5.280519 -3.103220 -0.879682
H -5.297890 0.864509 -3.118180
H 5.293599 -3.103654 0.879574
H -5.314911 -0.895892 -3.103835
H 6.549830 -2.193318 -0.009180
H -6.589919 0.003406 -2.230925
C 2.720546 2.746196 -0.024172
C -2.720164 0.021336 2.680997
C 2.417846 3.357666 -1.262272
C -2.371923 1.261574 3.270987
C 1.699054 4.556638 -1.256003
C -1.602366 1.253685 4.436628
H 1.447328 5.037409 -2.204547
H -1.319911 2.201787 4.900149
C 1.298124 5.149344 -0.060176
C -1.181797 0.057796 5.014323
H 0.728641 6.081890 -0.074899
H -0.570399 0.072613 5.919434
C 1.643238 4.560174 1.153985
C -1.542713 -1.156008 4.435606
H 1.349882 5.043826 2.089386
H -1.216168 -2.090284 4.898819
C 2.362571 3.361688 1.196279
C -2.312876 -1.200423 3.270202
C 2.865202 2.714043 -2.564029
C -2.816248 2.564181 2.628707
H 3.603069 1.942672 -2.299578
H -3.559177 2.303416 1.860690
C 3.554364 3.710040 -3.497399
C -3.495950 3.502798 3.626503
H 3.960171 3.193208 -4.381308
H -3.887395 4.394938 3.113084
H 2.855772 4.479989 -3.862056
H -2.794471 3.851710 4.400785
C 1.714074 1.998829 -3.272533
C -1.659164 3.269875 1.916910
H 2.077448 1.426067 -4.140173
H -2.017464 4.125261 1.324211
H 1.191273 1.298625 -2.599347
H -1.101740 2.603080 1.236235
C 2.761425 2.734419 2.521165
C -2.706468 -2.525843 2.641766
H 3.440829 1.902007 2.285940
H -3.388854 -2.292835 1.810533
C 3.524178 3.717390 3.411426
C -3.466979 -3.419875 3.623340
H 3.886968 3.214549 4.321849
H -3.813068 -4.338328 3.123692
H 4.393387 4.145143 2.888704
H -4.346758 -2.905111 4.038197
C 1.563526 2.136791 3.259193
C -1.501275 -3.262561 2.052721
H 0.867765 2.923428 3.587782
H -0.822170 -3.612544 2.843581
H 0.996476 1.442023 2.617995
H -0.892161 -2.625488 1.388486
C 2.722221 -2.745008 0.023734
C -2.720827 -0.022484 -2.680542
C 2.364271 -3.360588 -1.196679
C -2.314405 1.199249 -3.270421
C 1.645581 -4.559459 -1.154313
C -1.544462 1.154747 -4.435951
H 1.352230 -5.043168 -2.089686
H -1.218557 2.088996 -4.899663
C 1.301102 -5.148929 0.059880
C -1.182887 -0.059124 -5.014155
H 0.732122 -6.081781 0.074667
H -0.571640 -0.073991 -5.919367
C 1.702029 -4.556120 1.255660
C -1.602599 -1.254983 -4.435809
H 1.450797 -5.037108 2.204223
H -1.319659 -2.203143 -4.898922
C 2.420167 -3.356758 1.261855
C -2.371955 -1.262778 -3.270020
C 2.762507 -2.733039 -2.521617
C -2.708490 2.524678 -2.642333
H 3.441257 -1.900069 -2.286472
H -3.391274 2.291687 -1.811434
C 1.564074 -2.136437 -3.259593
C -1.503641 3.261455 -2.052650
H 0.868838 -2.923645 -3.587919
H -0.824218 3.611571 -2.843174
H 0.996627 -1.441950 -2.618447
H -0.894728 2.624378 -1.388235
C 3.526002 -3.715456 -3.411863
C -3.468491 3.418665 -3.624327
H 3.888329 -3.212389 -4.322346
H -3.814965 4.337053 -3.124830
H 4.395590 -4.142469 -2.889167
H -4.347978 2.903834 -4.039732
C 2.867429 -2.712963 2.563559
C -2.815532 -2.565393 -2.627236
H 3.604910 -1.941252 2.299028
H -3.557643 -2.304621 -1.858422
C 1.716041 -1.998289 3.272183
C -1.657693 -3.271180 -1.916764
H 0.968363 -2.718636 3.634769
H -0.918018 -3.647428 -2.637276
H 2.079203 -1.425450 4.139863
H -2.015370 -4.126735 -1.323931
C 3.557152 -3.708651 3.496838
C -3.496355 -3.503908 -3.624385
H 3.962874 -3.191631 4.380675
H -3.887179 -4.396149 -3.110663
H 2.858944 -4.478890 3.861620
H -2.795727 -3.852627 -4.399525
H 4.387887 -4.225894 2.992493
H -4.336453 -3.007938 -4.133932
H 1.192909 -1.298245 2.599083
H -1.099636 -2.604520 -1.236465
H 2.885054 4.555815 3.731627
H -2.830260 -3.723861 4.469347
H 1.886410 1.582394 4.154217
H -1.817599 -4.142749 1.472723
H 2.887534 -4.554424 -3.731951
H -2.831321 3.722803 -4.469939
H 1.886433 -1.581980 -4.154771
H -1.820295 4.141541 -1.472676
H 4.384957 4.227626 -2.993173
H -4.335451 3.006871 4.137082
H 0.966074 2.718818 -3.635183
H -0.918794 3.646316 2.636594

(^{DIPP}BDI)Mg-Ca(^{DIPP}BDI) no dispersion

Mg -1.864158 -0.000318 -0.000233
Ca 1.574075 0.000313 -0.000266
N -3.384171 -1.408900 0.534153
N 3.369785 1.429230 0.536181
N -3.384499 1.407909 -0.534560
N 3.370139 -1.428316 -0.536419
C -5.656624 -2.294816 0.851448
C 5.645978 2.301676 0.831437
H -5.504416 -3.192984 0.234083
H 5.483764 2.615783 1.873401
H -6.700256 -1.972443 0.749588
H 6.688721 1.980678 0.718811
H -5.483243 -2.607421 1.891701
H 5.485405 3.198757 0.214219
C -4.696940 -1.196529 0.449314
C 4.679502 1.204517 0.442968
C -5.290116 -0.000718 -0.000243
C 5.265286 0.000783 -0.000371
H -6.379712 -0.000852 -0.000275
H 6.354995 0.000958 -0.000494
C -4.697211 1.195260 -0.449725
C 4.679793 -1.203189 -0.443462
C -5.657149 2.293410 -0.851626
C 5.646532 -2.300113 -0.831940
H -5.483110 2.607129 -1.891420
H 5.486291 -3.197171 -0.214606
H -5.505902 3.191047 -0.233243
H 5.484267 -2.614374 -1.873851
H -6.700694 1.970414 -0.750848
H 6.689200 -1.978812 -0.719486
C -2.933435 -2.678285 0.997929
C 2.915046 2.698218 0.991751
C -2.707897 -3.726929 0.069723
C 2.661724 2.908742 2.372417
C -2.199891 -4.943945 0.538229
C 2.141656 4.142233 2.781414
H -2.016881 -5.755820 -0.170440
H 1.942993 4.314523 3.842675
C -1.931637 -5.145784 1.889275
C 1.874022 5.155212 1.865649
H -1.542952 -6.106982 2.236298
H 1.468114 6.111396 2.205766
C -2.173292 -4.117981 2.795710
C 2.129659 4.943785 0.513937
H -1.972208 -4.282755 3.858023
H 1.919066 5.742724 -0.201453
C -2.674682 -2.879263 2.377399
C 2.654574 3.731285 0.053270
C -3.004325 -3.552650 -1.414145
C 2.940670 1.828660 3.409404
H -3.610516 -2.640073 -1.518695
H 3.484734 1.019898 2.897376
C -3.821956 -4.710360 -1.997956
C 3.834417 2.324127 4.552502
H -4.111865 -4.488446 -3.037528
H 4.091899 1.493111 5.228502
H -3.251228 -5.652737 -2.016037
H 3.334861 3.095624 5.159984
C -1.716388 -3.332495 -2.214945
C 1.638840 1.231178 3.957195
H -1.939904 -3.161149 -3.280829
H 1.845683 0.407338 4.659150
H -1.157730 -2.459105 -1.839748
H 0.997287 0.835627 3.152041
C -2.936863 -1.791390 3.410790
C 2.927796 3.538688 -1.432526
H -3.434965 -0.960801 2.887872
H 3.541568 2.630452 -1.534385
C -3.876392 -2.259247 4.529091
C 3.727132 4.693822 -2.045894
H -4.119043 -1.423074 5.204521
H 3.995184 4.463278 -3.089304
H -4.823514 -2.653843 4.130171
H 4.659757 4.883516 -1.492325
C -1.629234 -1.242034 3.991735
C 1.627558 3.304554 -2.210502
H -1.067194 -2.024384 4.527644
H 0.961706 4.179568 -2.156043
H -0.979123 -0.848030 3.194529
H 1.045850 2.456717 -1.808971
C -2.933997 2.677468 -0.998072
C 2.915689 -2.697546 -0.991586
C -2.674667 2.878584 -2.377415
C 2.655624 -3.730436 -0.052807
C -2.173874 4.117621 -2.795508
C 2.131011 -4.943217 -0.513096
H -1.972461 4.282519 -3.857744
H 1.920707 -5.742014 0.202539
C -1.933199 5.145558 -1.888969
C 1.875318 -5.155095 -1.864722
H -1.544978 6.107005 -2.235821
H 1.469675 -6.111497 -2.204543
C -2.201762 4.943489 -0.538018
C 2.142522 -4.142265 -2.780783
H -2.019396 5.755418 0.170756
H 1.943782 -4.314891 -3.841975
C -2.709271 3.726180 -0.069735
C 2.662232 -2.908503 -2.372167
C -2.935718 1.790627 -3.411004
C 2.928946 -3.537410 1.432916
H -3.431823 0.958914 -2.887966
H 3.542177 -2.628778 1.534515
C -1.627659 1.243948 -3.993491
C 1.628691 -3.303929 2.211056
H -1.067653 2.027446 -4.529853
H 0.963326 -4.179328 2.156834
H -0.975955 0.850935 -3.197118
H 1.046512 -2.456446 1.809478
C -3.877149 2.257321 -4.528213
C 3.729112 -4.691968 2.046301
H -4.118572 1.421174 -5.204119
H 3.997148 -4.461162 3.089657
H -4.824795 2.649587 -4.128257
H 4.661788 -4.881113 1.492633
C -3.005904 3.551664 1.414071
C 2.940562 -1.828537 -3.409439
H -3.611771 2.638854 1.518459
H 3.484630 -1.019562 -2.897746
C -1.718005 3.331875 2.215042
C 1.638381 -1.231445 -3.956814
H -1.046726 4.201932 2.142802
H 1.044298 -1.989277 -4.492468
H -1.941628 3.160448 3.280891
H 1.844746 -0.407616 -4.658921
C -3.824029 4.709038 1.997853

C 3.833989 -2.323974 -4.552800
H -4.114070 4.486924 3.037344
H 4.090991 -1.493013 -5.229048
H -3.253614 5.651600 2.016136
H 3.334388 -3.095705 -5.159949
H -4.745380 4.890632 1.422647
H 4.774628 -2.755688 -4.177828
H -1.159070 2.458637 1.839904
H 0.997012 -0.835998 -3.151453
H -3.420657 -3.053049 5.142736
H 3.151634 5.633076 -2.059454
H -1.827909 -0.424122 4.703356
H 1.833085 3.097841 -3.273259
H -3.423548 3.052604 -5.141525
H 3.154217 -5.631590 2.059992
H -1.825579 0.425865 -4.705123
H 1.834283 -3.096970 3.273753
H -4.743362 -4.892185 -1.422913
H 4.774801 2.756144 4.177239
H -1.044878 -4.202365 -2.142582
H 1.044762 1.988806 4.493144

164
(^{DIPP}BDI*)Mg-Ca(^{DIPP}BDI)
Ca 1.784830 -0.014056 0.152549
Mg -1.397588 0.037060 0.054720
N -2.850928 1.431177 -0.594889
N -2.896611 -1.383609 0.530166
N 3.525458 -1.429760 -0.534340
N 3.664133 1.239389 0.737574
C -4.164958 1.221265 -0.598354
C -4.736244 0.010544 -0.146480
H -5.808812 0.002328 -0.211941
C -4.205076 -1.191154 0.373338
C -5.181465 2.294102 -1.106119
C -4.871980 2.669226 -2.560589
H -3.912050 3.187854 -2.648440
H -5.651449 3.348124 -2.940735
H -4.854278 1.779697 -3.207533
C -5.114097 3.558778 -0.238997
H -5.284770 3.325410 0.822304
H -5.897044 4.264352 -0.559028
H -4.150122 4.069359 -0.336683
C -6.641498 1.815536 -1.075562
H -6.805496 0.931084 -1.708015
H -7.281381 2.621911 -1.464974
H -6.988386 1.586922 -0.057542
C -5.262053 -2.277084 0.757055
C -5.072118 -3.544397 -0.088058
H -5.111048 -3.316320 -1.163400
H -5.881445 -4.257595 0.134617
H -4.122792 -4.044295 0.131233
C -6.713779 -1.820159 0.542490
H -6.968395 -0.937017 1.146089
H -7.385230 -2.635232 0.852502
H -6.934424 -1.599095 -0.511735
C -5.132301 -2.639327 2.241912
H -4.186609 -3.148087 2.453781
H -5.947399 -3.322550 2.527969
H -5.202948 -1.744578 2.878033
C -2.146342 2.608522 -0.947451
C -1.574333 2.741322 -2.240225
C -0.760761 3.846756 -2.511479
H -0.332745 3.959378 -3.510509
C -0.473638 4.793870 -1.534571
H 0.159881 5.652792 -1.767214
C -0.991669 4.630896 -0.254013
H -0.738932 5.354353 0.523222
C -1.821654 3.552438 0.063250
C -2.234903 -2.555967 0.972201
C -1.784879 -3.505606 0.016376
C -1.021986 -4.595459 0.445477
H -0.680426 -5.325819 -0.289849
C -0.689637 -4.764517 1.785948
H -0.111687 -5.634845 2.106232
C -1.088400 -3.806124 2.711459
H -0.802652 -3.920406 3.759891
C -1.838051 -2.688796 2.329002
C 5.734792 -2.433989 -0.908120
H 5.572520 -2.623469 -1.978443
H 5.492654 -3.374759 -0.396554
H 6.795023 -2.205085 -0.746039
C 4.846192 -1.309498 -0.423799
C 5.505807 -0.182599 0.107001
H 6.594420 -0.236408 0.105658
C 4.962710 1.018661 0.607426
C 5.952537 2.097534 0.985765
H 5.576066 2.726018 1.803774
H 6.133666 2.763461 0.126387
H 6.918465 1.663258 1.275142
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C 2.690971 -3.717820 -0.264071
C 2.296825 -4.916350 -0.871239
H 2.064577 -5.775096 -0.235322
C 2.190575 -5.028401 -2.253242
H 1.897324 -5.977439 -2.707956
C 2.395498 -3.904345 -3.051035
H 2.230665 -3.979666 -4.126763
C 2.770231 -2.679526 -2.491861
C 3.170506 2.484417 1.172408
C 2.705052 2.607599 2.503656
C 2.194739 3.840529 2.921127
H 1.851455 3.962827 3.949487
C 2.098978 4.911211 2.038480
H 1.691134 5.865946 2.378777
C 2.495962 4.757487 0.712487
H 2.381269 5.596408 0.026189
C 3.033219 3.553162 0.251324
C -1.782564 1.692792 -3.321461
C 2.772472 1.417849 3.446640
C 3.444180 3.368810 -1.203287
C 2.838755 -1.413498 -3.336854
C 2.727689 -3.670793 1.257701
C -2.157380 -1.623337 3.365033
C -2.071317 -3.333070 -1.465792
C -2.308169 3.380065 1.493022
C -2.808029 4.680615 2.124598
C -1.206556 2.770772 2.360904
H -3.144180 2.666721 1.470456
H -3.269673 4.474893 3.103000
H -1.981463 5.386756 2.301373
H -3.553767 5.188245 1.496419
H -1.569533 2.579695 3.383421
H -0.836733 1.819626 1.939964
H -0.337088 3.441451 2.415695
C -2.180265 2.286889 -4.675172

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H -2.593879 1.032883 -2.979700
H -2.437073 1.483199 -5.382975
H -3.043831 2.961438 -4.598822
H -1.350474 2.856830 -5.122350
H -0.707989 0.016600 -4.209636
H 0.314823 1.432707 -3.860994
H -0.222130 0.382085 -2.530014
C -0.858359 -2.726530 -2.171480
C -2.478503 -4.632789 -2.162263
H -2.902315 -2.619053 -1.557202
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H -0.551807 -1.774154 -1.704662
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H -1.631967 -5.333806 -2.232093
H -3.298897 -5.145885 -1.640436
C -0.913504 -0.783532 3.665919
H -2.910299 -0.954841 2.920976
C -2.722461 -2.188067 4.670601
H -1.153747 0.043259 4.351516
H -0.130301 -1.398547 4.137398
H -0.487441 -0.354458 2.742007
H -3.044293 -1.368217 5.331684
H -3.584688 -2.847490 4.502686
H -1.962754 -2.765452 5.220900
C 1.980159 -1.499992 -4.596828
H 2.404602 -0.613175 -2.709234
C 4.255025 -0.960527 -3.702934
H 1.903942 -0.509521 -5.068930
H 2.420290 -2.181909 -5.341751
H 0.963003 -1.848805 -4.372110
H 4.209480 -0.085927 -4.370939
H 4.839673 -0.669288 -2.821634
H 4.795816 -1.759285 -4.235414
C 4.125445 -3.817459 1.865353
C 2.006453 -2.471596 1.875551
H 2.150469 -4.555924 1.567945
H 1.749325 -2.674086 2.924663
H 2.666413 -1.586974 1.886745
H 1.049239 -2.255269 1.366067
H 4.050041 -3.965866 2.954537
H 4.659233 -4.683029 1.444985
H 4.734515 -2.917070 1.698106
C 3.494222 4.674072 -1.992398
H 4.464430 2.951918 -1.204974
C 2.551322 2.346685 -1.925050
H 3.905524 4.490305 -2.996336
H 2.489864 5.104403 -2.123364
H 4.129273 5.426387 -1.500918
H 2.654731 2.433894 -3.016984
H 2.867140 1.320506 -1.682760
H 1.486679 2.490422 -1.681912
C 1.736609 1.475282 4.565385
H 2.548909 0.520113 2.840214
C 4.176404 1.207496 4.020871
H 4.184476 0.354314 4.717491
H 4.912406 1.001178 3.233729
H 4.504670 2.101624 4.574353
H 1.709145 0.517644 5.105987
H 1.978070 2.257117 5.302701
H 0.729958 1.673169 4.173632

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C6H6

C 1.395789 -0.031957 0.000000
C 0.725522 1.192755 0.000000
C -0.670196 1.224738 0.000000
C -1.395749 0.031956 0.000000
C 0.670174 -1.224710 0.000000
C -0.725546 -1.192782 0.000000
H 1.293513 2.126543 0.000000
H -1.194832 2.183531 0.000001
H -2.488415 0.056972 0.000000
H 1.194830 -2.183515 -0.000001
H -1.293515 -2.126558 0.000000
H 2.488459 -0.056973 0.000000

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(^{DIPP}BDI*)Mg(C_6H_6)Ca(^{DIPP}BDI)

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C -5.283747 0.225829 -0.327302
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C -4.854811 -0.977224 0.290397
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C -5.106069 2.622767 -2.948439
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H -5.806147 3.318673 -3.436869
H -5.153108 1.664759 -3.485985
C -5.341088 3.821925 -0.784813
H -5.590180 3.767045 0.284739
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C -6.994393 2.120820 -1.442362
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H -7.549907 2.940993 -1.922103
H -7.377893 2.019595 -0.416644
C -6.041168 -1.956293 0.580562
C -5.708483 -3.186349 1.434760
H -4.998722 -3.864484 0.954704
H -6.640367 -3.747552 1.606431
H -5.294690 -2.920846 2.414007
C -6.577460 -2.449744 -0.777411
H -6.949704 -1.619576 -1.393574
H -7.406897 -3.157257 -0.617390
H -5.798237 -2.968773 -1.350936
C -7.182540 -1.219249 1.312821
H -6.837447 -0.770243 2.255098
H -7.978189 -1.940000 1.557209
H -7.639557 -0.422951 0.711607
C -2.433600 2.509977 -1.158801
C -1.767011 2.397908 -2.414397
C -0.749714 3.328144 -2.683740
H -0.224498 3.283806 -3.636514
C -0.359774 4.299972 -1.770498
H 0.452301 4.987574 -2.018087
C -1.012642 4.390232 -0.547529
H -0.705270 5.148252 0.175739
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C -2.996707 -2.369685 1.140540

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C -1.934617 -4.537838 0.968575
H -1.664889 -5.415191 0.375086
C -1.567070 -4.478417 2.308101
H -1.020721 -5.305861 2.767521
C -1.883993 -3.347065 3.055997
H -1.568450 -3.293562 4.099209
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C -0.214759 0.306394 1.466253
H -0.226440 0.711937 2.480128
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C -0.001842 -0.705949 -1.017452
H 0.139912 -1.110861 -2.023260
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C 0.394696 1.198402 0.444377
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H 7.689058 -1.946988 -1.080120
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H 7.426675 0.223132 -0.168373
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H 7.170632 2.695500 0.403314
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H 1.528003 -5.203557 -2.609583
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H -1.815626 1.953353 2.111412
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C -3.825413 -4.892980 -1.398376
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H -2.087501 -3.615975 -3.068233
H -1.254143 -2.609405 -1.858656
H -1.099546 -4.376795 -1.795869
H -4.173289 -4.895907 -2.443476
H -3.205724 -5.792594 -1.257433
H -4.706467 -4.993788 -0.749064
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H -2.631124 -0.166137 2.574931
C -4.245620 -0.848759 3.783542
H -1.921885 0.216482 4.841489
H -2.031434 -1.500240 5.268044
H -0.788777 -0.947384 4.120095
H -4.361184 0.087996 4.351416
H -4.956681 -0.818001 2.950892
H -4.523803 -1.684158 4.446336
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H 4.429366 -0.514546 -2.852061
C 4.556244 -1.656468 -4.658308
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H 5.430525 -2.255814 -4.364677
H 3.930691 -2.282271 -5.314515
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C 3.731009 -2.630822 2.018968
H 3.564420 -4.649078 1.383000
H 3.972481 -2.948347 3.044966
H 4.323571 -1.724147 1.819453
H 2.653191 -2.395335 2.007506
H 5.887026 -4.368145 2.034369
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H 6.154113 -3.124721 0.798651
C 4.139094 4.970879 -1.268983
H 5.125642 3.188114 -0.667884
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H 4.744531 5.028317 -2.186258
H 3.137570 5.354999 -1.518985
H 4.585405 5.646275 -0.523365
H 3.899940 2.747853 -2.793554
H 3.523882 1.567436 -1.533620
H 2.352064 2.862266 -1.910851
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H 3.446969 0.001043 2.797810
C 4.638728 1.010592 4.219406
H 4.885250 0.100899 4.789393
H 5.457854 1.204265 3.514730

H 4.590021 1.855417 4.924425
H 2.408714 -0.499859 4.925048
H 2.077714 1.206425 5.264449
H 1.220993 0.386054 3.936062

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TS bridged C_6H_6

Ca -2.454215 -0.239846 -0.253621
Mg 1.989694 -0.078554 -0.325628
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N -4.375206 -0.890340 0.962532
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H 6.361352 3.540445 2.234738
H 5.698629 1.941453 2.643161
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H 6.077349 4.445929 -0.188838
H 4.334444 4.176909 -0.067851
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H 7.673362 2.993572 0.417776
H 7.210243 1.830981 -0.837802
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C 5.570812 -3.646696 -1.141696
H 4.997521 -4.207841 -0.397846
H 6.503863 -4.200685 -1.328955
H 4.991719 -3.646347 -2.071642
C 6.700007 -2.371261 0.663036
H 7.100779 -1.410067 1.012809
H 7.544214 -3.067805 0.539444
H 6.050318 -2.772188 1.452761
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H 6.434658 -1.516762 -2.696799
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C 2.386530 2.733721 2.184779
C 1.838619 3.930268 2.657749
H 1.686589 4.063649 3.730360
C 1.465711 4.945311 1.781798
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C 2.891217 -2.781174 -0.768876
C 2.750366 -3.658761 0.329440
C 2.080372 -4.870838 0.142912
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C 1.552179 -5.213127 -1.096634
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H 1.205949 -4.583910 -3.115894
C 2.305330 -3.090869 -2.019868
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C -2.164777 -2.361731 -1.943875
H -2.982221 -2.959002 -2.345364
C -1.436640 -2.798746 -0.808769
H -1.729406 -3.724911 -0.308833
C -0.350819 -2.090630 -0.333526
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C -0.578260 -0.513268 -2.144596
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H -2.446644 -4.510193 3.007206
C -3.401776 -2.766728 2.168924
C -3.106872 2.821143 -0.827675
C -2.996184 2.860338 -2.238008
C -2.334854 3.941679 -2.831225
H -2.257274 3.997412 -3.918323
C -1.774079 4.952524 -2.055957
H -1.269928 5.794757 -2.536055
C -1.841582 4.877327 -0.665894
H -1.378788 5.661057 -0.065083
C -2.493809 3.819760 -0.028176
H -0.229013 0.320880 -2.757328
H -0.426778 0.293485 0.228032
C 2.634830 1.571449 3.126303
C -3.637395 1.770963 -3.079478
C -2.527673 3.713905 1.487311
C -2.879639 -1.813778 3.228411
C -5.749595 -2.766752 -0.941576
C 2.338488 -2.095239 -3.168196
C 3.263177 -3.280234 1.706605
C 2.199738 3.312971 -1.593110
C 2.361076 4.567989 -2.444555
C 0.953224 2.532346 -2.014434
H 3.075664 2.670361 -1.768714
H 2.503916 4.293566 -3.501053
H 1.466277 5.207307 -2.397157
H 3.228042 5.166878 -2.127943
H 1.044255 2.156702 -3.045407
H 0.744696 1.680578 -1.348737
H 0.055472 3.162341 -1.955719
C 3.126665 1.970385 4.515422
C 1.338400 0.762212 3.232242
H 3.399000 0.927798 2.665177
H 3.379622 1.072549 5.100207
H 4.021311 2.607558 4.467519
H 2.354333 2.514374 5.081490

H 1.482693 -0.150509 3.827583
H 0.551508 1.363961 3.711013
H 0.938036 0.476876 2.244461
C 2.124159 -2.713593 2.553527
C 3.963374 -4.428812 2.431874
H 3.995935 -2.472101 1.577749
H 2.482855 -2.393855 3.544390
H 1.658766 -1.842342 2.071246
H 1.333421 -3.465511 2.701031
H 4.423600 -4.069676 3.365637
H 3.260064 -5.230782 2.704906
H 4.755149 -4.876776 1.813163
C 1.320568 -2.398612 -4.263176
H 2.051112 -1.121664 -2.729421
C 3.728328 -1.922176 -3.781680
H 1.269949 -1.556340 -4.969814
H 1.605769 -3.292347 -4.841783
H 0.315404 -2.552103 -3.849703
H 3.697179 -1.184301 -4.598853
H 4.455284 -1.567974 -3.042934
H 4.095170 -2.872391 -4.201467
C -1.411857 -1.453431 3.001246
H -3.458083 -0.883184 3.134066
C -3.098023 -2.348721 4.644400
H -1.051780 -0.772829 3.786718
H -0.778283 -2.352242 3.008471
H -1.232123 -0.943652 2.038508
H -2.824242 -1.586735 5.391005
H -4.150485 -2.626264 4.806751
H -2.482309 -3.239572 4.846620
C -7.190535 -2.877388 -0.425218
C -5.561872 -1.432029 -1.668509
H -5.634027 -3.553127 -1.707997
H -6.217183 -1.414451 -2.554057
H -5.820539 -0.565404 -1.046798
H -4.531192 -1.304869 -2.025095
H -7.906188 -2.785850 -1.257945
H -7.366811 -3.841126 0.075751
H -7.415132 -2.074877 0.291486
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H -3.485778 3.254991 1.769307
C -1.432384 2.770529 1.983393
H -2.602458 4.932892 3.277361
H -1.459044 5.532716 2.067692
H -3.208011 5.767160 1.823644
H -1.482960 2.655050 3.077812
H -1.512663 1.772057 1.529142
H -0.436782 3.150151 1.721700
C -2.962809 1.575190 -4.433570
H -3.527475 0.825520 -2.520288
C -5.143394 1.989268 -3.247545
H -5.583379 1.193303 -3.868675
H -5.659677 1.978001 -2.279234
H -5.343524 2.956115 -3.736321
H -3.364576 0.680449 -4.933274
H -3.145716 2.426809 -5.107607
H -1.874230 1.453243 -4.330641

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(^{DIPP}BDI)Mg(H)(Ph)Ca(^{DIPP}BDI)

Ca -1.718846 -0.232599 0.115251
Mg 1.387817 0.189791 0.278797
C 0.096956 0.936838 1.880610
C 0.238827 0.459845 3.206004
C -0.436140 1.028913 4.287114
C -1.304134 2.104755 4.082187
C -0.776351 2.036429 1.726991
C -1.474792 2.611781 2.796806
H 0.902738 -0.387488 3.409903
H -0.289593 0.627338 5.294129
H -1.849846 2.545314 4.920528
H -0.904221 2.497344 0.735755
H -2.156285 3.445771 2.626444
H 0.116231 -0.506531 -0.802278
N 2.889513 -1.152252 0.709566
N 2.507099 1.404511 -0.980119
C 4.743844 -2.601645 -0.235805
C 5.824676 -2.550548 0.854658
C 5.463579 -2.791704 -1.581929
C 3.874660 -3.848458 -0.028407
C 3.850439 -1.322145 -0.209370
C 4.104481 -0.381478 -1.221266
H 4.918665 -0.668650 -1.867934
C 3.606684 0.918052 -1.530278
C 4.524317 1.666966 -2.548371
C 4.063444 3.053796 -3.015114
C 4.692106 0.808560 -3.819171
C 5.896815 1.854004 -1.870427
C 2.823462 -1.764512 1.982119
C 1.806394 -2.701717 2.292410
C 1.706710 -3.198436 3.596709
H 0.928076 -3.929648 3.828020
C 2.572675 -2.780722 4.600152
H 2.483919 -3.183568 5.611785
C 3.542546 -1.826363 4.304341
H 4.201256 -1.468570 5.098272
C 3.676456 -1.297949 3.017959
C 1.891211 2.652325 -1.250767
C 0.890551 2.743261 -2.250156
C 0.340424 3.996915 -2.537867
H -0.399155 4.080771 -3.337994
C 0.718773 5.135006 -1.833900
H 0.301166 6.110684 -2.092947
C 1.608772 5.010949 -0.772548
H 1.867347 5.892435 -0.180686
C 2.191808 3.781881 -0.452873
C 0.399698 1.534642 -3.026975
C 3.129942 3.696300 0.734555
C 4.626812 -0.140154 2.775502
C 0.780643 -3.142235 1.266160
C 0.841880 1.551925 -4.491011
C -1.122369 1.416747 -2.939333
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H 0.452512 2.438894 -5.016226
H 1.935663 1.563810 -4.585920
H -1.478213 0.461278 -3.347912
H -1.479983 1.491143 -1.901497
H -1.633719 2.220345 -3.490644
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H 1.535490 3.292348 2.174111
H 4.051731 5.676669 0.597562

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H 4.899362 4.426276 -0.335253
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H 1.080242 -2.720327 0.296003
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H 0.293113 -5.126393 2.037943
H -1.304332 -2.766725 0.806019
H -0.997104 -3.020733 2.534250
H -0.503715 -1.487716 1.841989
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H 4.868044 -0.116537 1.704012
C 3.899152 1.165049 3.099207
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H 2.972071 1.259302 2.518156
H 3.619217 1.205487 4.163622
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C -3.540397 -1.334478 -2.434225
C -3.809885 -2.251562 -3.606748
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C -5.066523 3.510109 2.741928
H -5.451282 4.166807 3.525768
C -5.162659 2.128067 2.876490
H -5.608860 1.703032 3.778478
C -4.702681 1.279358 1.866679
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C -0.966758 -3.344442 -2.401316
C -0.605703 -4.695673 -2.485205
H 0.253833 -4.976815 -3.098888
C -1.314842 -5.684636 -1.813306
H -1.021870 -6.732884 -1.907237
C -2.374768 -5.324342 -0.983701
H -2.898022 -6.096720 -0.416665
C -2.767239 -3.989600 -0.858377
C -0.135237 -2.314946 -3.147435
C -3.884665 -3.596293 0.095870
C -4.729903 -0.227996 2.034308
C -3.130982 3.834083 -0.544545
C -0.196513 -2.492461 -4.667420
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H 0.407051 -1.718942 -5.167027
H 0.206493 -3.471596 -4.971715
H -1.220155 -2.421527 -5.061091
H 1.895348 -1.520392 -3.153379
H 1.395106 -2.197141 -1.601100
H 1.819486 -3.283557 -2.951423
C -3.911114 -4.451299 1.362114
C -5.263729 -3.578561 -0.569781
H -3.677561 -2.555485 0.397883
H -4.609467 -4.021969 2.096959
H -4.254161 -5.477489 1.157416
H -2.917667 -4.517399 1.829371
H -5.504862 -4.566290 -0.994241
H -6.043049 -3.326430 0.167031
H -5.317946 -2.832747 -1.373132
C -2.400251 5.112078 -0.138592
H -2.366153 3.082809 -0.801701
C -3.942020 4.075208 -1.821005
H -3.314339 4.576447 -2.574495
H -4.301511 3.138617 -2.265099
H -4.811689 4.722231 -1.622561
H -1.702618 5.409095 -0.931503
H -3.096749 5.950433 0.020452
H -1.812523 4.975292 0.781144
C -6.020494 -0.767911 2.643759
H -4.646216 -0.662880 1.026061
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H -6.006221 -1.868632 2.660335
H -6.160141 -0.428715 3.682092
H -6.898215 -0.447571 2.062940
H -3.362712 -1.766783 2.804319
H -2.575612 -0.174656 2.530331
H -3.611677 -0.387941 3.903390
H 5.390829 -2.589290 1.860806
H 6.495857 -3.417601 0.746515
H 6.434144 -1.638663 0.768439
H 4.761143 -2.780493 -2.428143
H 6.240184 -2.033974 -1.761313
H 5.969264 -3.769177 -1.575251
H 3.051742 -3.884423 -0.756208
H 4.487416 -4.753262 -0.162125
H 3.450111 -3.885985 0.979554
H 4.816652 3.441055 -3.719033
H 3.100989 3.033866 -3.537229
H 3.976751 3.773993 -2.195790
H 5.261108 1.375664 -4.572035
H 5.232281 -0.130210 -3.640206
H 3.716111 0.551560 -4.255949
H 6.575177 2.403465 -2.542509
H 5.796707 2.433460 -0.940744
H 6.367121 0.894952 -1.615379

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(^{DIPP}BDI)CaH

Ca 0.0001 0.019722 -1.218246
N 1.464387 -0.002907 0.578792
N -1.464327 -0.0022 0.578702
C 2.474475 -0.024144 2.800781
H 2.188619 -0.028287 3.8595
H 3.109558 0.853594 2.605252
H 3.101671 -0.905593 2.596763
C 1.270631 -0.014653 1.892117
C 0.000005 -0.018198 2.501469
H -0.000031 -0.027322 3.591149
C -1.270593 -0.013235 1.892043
C -2.474449 -0.020277 2.800721

H -3.108205 0.858247 2.604406
H -2.188578 -0.023899 3.859438
H -3.102988 -0.900952 2.597512
C 2.770533 -0.000459 0.039
C 3.389774 1.230004 -0.285481
C 4.633156 1.210275 -0.923478
H 5.119939 2.153836 -1.182025
C 5.259068 0.007958 -1.24139
H 6.230032 0.010902 -1.742081
C 4.637363 -1.19821 -0.929461
H 5.127233 -2.138541 -1.193594
C 3.394027 -1.226999 -0.291894
C 2.684505 2.542259 0.003779
H 1.860691 2.319958 0.698789
C 3.589954 3.57196 0.679178
H 3.016455 4.471402 0.952448
H 4.041562 3.164408 1.596158
C 2.065363 3.111282 -1.277923
H 1.462817 4.009014 -1.069264
H 2.844921 3.383014 -2.00673
C 2.693677 -2.543567 -0.011504
H 1.8702 -2.329371 0.686395
C 2.073857 -3.103912 -1.296781
H 1.476193 -4.005833 -1.091837
H 1.420529 -2.374879 -1.806488
C 3.604447 -3.574041 0.655663
H 3.034023 -4.476852 0.924076
H 4.422788 -3.89106 -0.009723
C -2.770549 0.001269 0.03905
C -3.387716 1.232009 -0.288199
C -4.631379 1.21294 -0.925721
H -5.116582 2.156752 -1.186344
C -5.259495 0.010987 -1.240523
H -6.23065 0.014423 -1.740841
C -4.639722 -1.19554 -0.926022
H -5.131289 -2.135622 -1.187846
C -3.396221 -1.224979 -0.288861
C -2.697637 -2.541963 -0.00605
H -1.875001 -2.327941 0.692879
C -2.076256 -3.103894 -1.289879
H -1.421282 -2.375881 -1.798874
H -1.479863 -4.006287 -1.083311
C -3.610319 -3.571116 0.660494
H -4.065082 -3.167733 1.577948
H -4.427587 -3.888433 -0.006068
C -2.680218 2.543822 -0.002402
H -1.854984 2.321413 0.690912
C -2.06374 3.110625 -1.286388
H -2.844942 3.383247 -2.013109
H -1.459023 4.007473 -1.08023
C -3.582875 3.575267 0.674104
H -4.032085 3.169471 1.593033
H -3.007911 4.474706 0.944304
H -2.85568 -3.368941 -2.021491
H -3.04095 -4.473976 0.930969
H -4.404052 3.897909 0.014995
H -1.417011 2.380932 -1.803785
H 1.415635 2.383252 -1.793851
H 4.409427 3.895077 0.018188
H 2.854226 -3.369338 -2.027258
H 4.05772 -3.171935 1.574411
H -0.000859 -0.191849 -3.260959

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(^{DIPP}BDI)MgPh

Mg -0.026024 0.621870 -0.058095
C 0.011532 2.706440 -0.121675
C 1.197357 3.427592 -0.368216
C 1.221062 4.824908 -0.406133
C 0.045940 5.548388 -0.195300
C -1.157123 3.468717 0.083439
C -1.147394 4.865613 0.049789
H 2.139791 2.892122 -0.530834
H 2.160318 5.352088 -0.599232
H 0.059458 6.641657 -0.222566
H -2.113219 2.964566 0.270584
H -2.073363 5.425101 0.214174
N -1.498397 -0.769860 -0.070624
N 1.483325 -0.732043 0.064823
C -2.457997 -3.110298 -0.095059
C -1.984962 -4.569973 -0.165197
C -3.307290 -2.855920 -1.347989
C -3.345815 -2.986668 1.152609
C -1.285076 -2.088582 -0.038789
C 0.013819 -2.628174 0.038571
H 0.039530 -3.707064 0.069081
C 1.305126 -2.043951 0.103694
C 2.446930 -3.091230 0.260336
C 2.391359 -4.088826 -0.911929
C 2.213480 -3.833191 1.591769
C 3.876186 -2.538522 0.302183
C -2.724024 -0.055958 -0.001256
C -3.301288 0.481234 -1.178254
C -4.417520 1.315995 -1.060170
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H -5.820248 2.299359 0.252727
C -4.340856 1.159919 1.337378
H -4.734186 1.450726 2.313735
C -3.222951 0.324182 1.271444
C 2.691004 0.007588 0.008999
C 3.310760 0.221490 -1.245216
C 4.421448 1.064458 -1.309090
H 4.912812 1.233218 -2.269533
C 4.909529 1.700419 -0.168792
H 5.782011 2.354267 -0.236189
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H 4.633603 2.036840 1.936734
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C -2.496859 -0.079995 2.543287
C -2.685197 0.242384 -2.546231
C 3.788100 -0.883923 -3.492061
C 1.751731 0.569120 -3.160542
H 2.151197 -1.286136 -2.188061
H 3.312994 -1.425432 -4.324638
H 4.352050 -0.046472 -3.931476
H 4.511589 -1.562029 -3.014235
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H 1.390188 2.457507 2.319487
H 4.223192 0.329493 3.734108
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H 3.572062 -1.213349 3.142919
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H -1.954184 -0.572974 -2.434032
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H -4.409547 0.637244 -3.833043
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H -3.857864 -2.019026 1.198072
H -4.119020 -3.770534 1.129589
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H -1.430711 -4.876114 0.733993
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H -1.357031 -4.762053 -1.047408
H -3.821407 -1.890368 -1.301166
H -2.691637 -2.883227 -2.259378
H -4.077579 -3.637654 -1.436553

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[(^{DIPP}BDI)CaH]$_2$

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C 4.318104 4.132601 -1.335200
H 5.405880 4.265362 -1.391400
H 3.906904 4.813315 -0.576570
H 3.887349 4.440157 -2.301795
C 3.944966 2.697731 -1.047313
C 4.928550 1.717972 -1.301342
H 5.880387 2.090703 -1.679933
C 4.876341 0.336481 -1.029584
C 6.147304 -0.456729 -1.203502
H 6.461306 -0.880997 -0.237331
H 6.964116 0.158696 -1.599766
H 5.983029 -1.312039 -1.875755
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C 1.743381 3.703242 1.222477
C 0.823581 4.662301 1.653572
H 0.753409 4.898861 2.716781
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H -0.729782 6.058381 1.108653
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C 0.971940 4.065656 -1.084460
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H 4.523710 3.769891 1.408434
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H -0.210805 -5.586153 3.387647
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H 3.844077 4.717873 2.753759
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H 1.971870 5.578027 -3.166142
H -1.414392 3.431756 2.878707
H -4.025613 2.806317 4.616096
H -5.619571 2.154698 -3.458091
H -2.268204 0.466719 -2.694095
H -3.842488 -4.719677 -2.753443
H -1.039255 -2.193955 -3.450924
H 1.166057 -3.430186 2.715158
H -1.973017 -5.576949 3.167114
H 0.200750 0.126168 1.354671
H -0.201048 -0.126430 -1.355709

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TS addition to Mg-Ca bond

Ca -1.888492 -0.282484 0.135815
Mg 1.421269 0.175622 0.211158
C 0.138996 0.971672 2.475067
C 0.170983 0.214493 3.666956
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C -1.644759 1.515400 4.622412
C -0.840369 1.983499 2.396224
C -1.696983 2.285869 3.453754
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H -0.671241 -0.132653 5.627054
H -2.333835 1.719728 5.445946
H -0.938201 2.540930 1.452024
H -2.422284 3.097204 3.360276
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C 4.607454 -2.812033 -0.144377
C 5.681852 -2.795168 0.953359
C 5.326100 -3.063831 -1.482015
C 3.674690 -4.008705 0.076282
C 3.782105 -1.486864 -0.153756
C 4.140141 -0.562609 -1.153437
H 4.975116 -0.895801 -1.748597
C 3.738516 0.761771 -1.488489
C 4.769529 1.475743 -2.420720
C 4.360141 2.836693 -3.000672
C 5.119985 0.581032 -3.628387
C 6.038650 1.695969 -1.572666
C 2.666417 -1.857487 2.000402
C 1.606412 -2.744400 2.315697
C 1.511690 -3.258376 3.614592
H 0.705144 -3.957162 3.849828
C 2.409725 -2.894930 4.609523
H 2.320102 -3.310290 5.615869
C 3.405980 -1.967854 4.315372
H 4.084104 -1.641277 5.105988
C 3.543012 -1.428574 3.034192
C 2.091164 2.580880 -1.323937
C 1.097690 2.673206 -2.329336
C 0.638878 3.940541 -2.702071
H -0.086576 4.026341 -3.513528
C 1.089532 5.091098 -2.062744
H 0.734819 6.073954 -2.381678
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H 2.256635 5.867071 -0.430773
C 2.451249 3.728057 -0.580648
C 0.547362 1.443278 -3.027868
C 3.332615 3.639656 0.648761
C 4.528507 -0.298328 2.797140
C 0.533457 -3.137257 1.316730
C 1.236234 1.183057 -4.366818
C -0.969183 1.508414 -3.195092
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H 2.311532 1.005077 -4.236254
H -1.355819 0.566318 -3.607935

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H 0.789021 -2.668545 0.353853
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H -0.348778 -4.858726 0.340574
H 1.358415 -5.092795 0.771644
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H -1.200989 -3.105370 2.654832
H -0.748173 -1.524293 2.039244
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H 4.783106 -0.284601 1.728538
C 3.834420 1.027869 3.113058
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H 5.670958 -0.284947 4.666362
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H -3.872350 -1.679575 2.515301
H -2.941171 -0.137809 2.423584
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(^{DIPeP}BDI*)Mg-Ca(^{DIPeP}BDI) (1)

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C -3.154884 -3.557657 0.017015
C -2.563581 -4.773354 0.373951
H -2.392696 -5.534931 -0.387231
C -2.205158 -5.043956 1.691467
H -1.761395 -6.008279 1.948600
C -2.403251 -4.084247 2.679324
H -2.124723 -4.312930 3.708538
C -2.933453 -2.829133 2.367678
C -3.664598 -3.288480 -1.394753
H -4.685736 -2.889929 -1.284794
C -3.796192 -4.544699 -2.263061
H -4.017138 -4.214228 -3.291964
H -2.828413 -5.068944 -2.330791
C -4.891203 -5.501418 -1.807634
H -4.953191 -6.382755 -2.464358

H -5.874700 -5.004768 -1.823789
H -4.724744 -5.859416 -0.780775
C -2.877060 -2.187893 -2.124941
H -3.329457 -2.046251 -3.120563
H -3.083465 -1.232587 -1.612357
C -1.391531 -2.453125 -2.262820
H -1.201477 -3.322651 -2.904915
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H -0.859219 -1.599510 -2.703390
C -3.183568 -1.773294 3.429898
H -3.060863 -0.792301 2.934974
C -4.648132 -1.801731 3.911395
H -4.812452 -0.945141 4.584788
H -5.299248 -1.617045 3.047988
C -5.069955 -3.090498 4.601148
H -6.128510 -3.047668 4.900095
H -4.480792 -3.283310 5.511718
H -4.944865 -3.959983 3.937244
C -2.179821 -1.820933 4.585686
H -2.225765 -2.796356 5.096565
H -1.165882 -1.758893 4.160220
C -2.374228 -0.719256 5.618593
H -3.317629 -0.834898 6.172873
H -2.386529 0.276968 5.147240
H -1.560490 -0.724427 6.359027
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C -2.862039 2.818124 -2.241000
C -2.538505 4.066288 -2.780841
H -2.324148 4.150567 -3.846518
C -2.467320 5.202937 -1.980990
H -2.198757 6.166138 -2.420772
C -2.709370 5.100945 -0.615143
H -2.618091 5.990479 0.011888
C -3.096240 3.888226 -0.034803
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H -2.732328 0.712851 -2.433500
C -1.745153 1.539040 -4.126810
H -1.754479 2.446760 -4.750373
H -0.803533 1.579415 -3.555670
C -1.730620 0.322922 -5.041584
H -2.581357 0.317532 -5.739622
H -1.765048 -0.615995 -4.469119
H -0.812833 0.306058 -5.648009
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H -4.244781 0.348886 -4.263599
H -5.005730 1.167436 -2.921701
C -4.770963 2.400532 -4.678639
H -5.755066 2.141258 -5.098242
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H -4.872636 3.368184 -4.163416
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H -3.997831 2.927533 1.640864
C -2.050716 3.612128 2.233823
H -1.391564 4.473010 2.037940
H -2.271425 3.633790 3.314825
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H -0.332042 2.289413 2.434535
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H -3.414000 5.917969 1.953856
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H -5.359078 5.538988 0.335056
H -5.849097 6.297042 1.865559
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C 2.745690 -2.490983 -4.965286
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C 1.641695 -0.630799 -3.603063
H 3.536125 -1.900165 -5.457444
H 3.173751 -3.500547 -4.849252
C 1.542420 -2.543662 -5.903175
C 2.347182 0.549033 -4.250102
H 0.691958 -0.844595 -4.114314
H 1.347368 -0.356700 -2.574407
H 1.701642 1.437881 -4.273355
H 3.255523 0.813971 -3.685462
H 2.648340 0.334818 -5.287516
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H 0.668123 -3.030495 -5.445895
H 1.221633 -1.536088 -6.208031

224

(^{DIPeP}BDI*)Mg(C_6H_6)Ca(^{DIPeP}BDI) (3)

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C 1.571964 -0.522996 -4.370673
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H 4.090377 -0.850781 -4.850594
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H -5.039413 -3.031360 -0.822211
C -3.252453 -3.161590 -1.933931
H -3.016158 -2.101936 -1.731797
C -1.961111 -3.923158 -2.162975
C -4.642109 -5.108925 -1.000358
H -5.236740 -5.395174 -0.116562
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Ca -2.587909 0.080911 -0.093344
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C 2.213339 2.350804 2.539550
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H 2.062204 0.252360 2.573648
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C -5.800288 5.208713 2.232157
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H -2.062774 -1.533377 -4.164052
H -3.031426 -0.977480 -5.545531
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H -2.373607 1.786386 4.100077
H -3.288587 1.118772 5.466682
H -6.005274 -1.789937 5.268704
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H -4.305695 -1.730563 5.770763
H -6.252310 6.206186 2.342299
H -6.618640 4.470214 2.224847
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H -1.590198 3.544438 2.793374
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H 1.062791 -1.240795 4.352535
H 2.183143 -0.693481 5.614763
H 4.666048 -6.617649 2.181593
H 5.345141 -5.029680 1.781400
H 4.113477 -5.169091 3.045494
H 1.872437 -4.965225 3.378746
H 2.677505 -3.404287 3.658505
H 0.910112 -3.525267 3.744898
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C 6.725397 2.583853 -0.146380
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C 6.554440 -2.682776 0.473193
C 5.429379 -3.513538 -1.572981
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H 7.191640 1.730710 -0.657133
H 6.081771 3.095322 -0.874846
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H 6.399102 1.092046 2.973498
H 7.412296 0.581793 1.612413
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H 4.902410 4.099571 1.169172
H 4.862392 3.234864 2.705669
H 7.768425 -2.350549 -1.929605
H 6.567951 -1.309467 -2.720137
H 7.448285 -0.726729 -1.297173
H 7.268223 -3.500310 0.283156
H 7.098806 -1.861042 0.957256
H 5.804298 -3.045814 1.188738
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H 4.793358 -4.148028 -0.950602
H 4.882539 -3.307270 -2.501195
H -7.437126 -1.765944 1.655767
H -6.976329 -2.823706 0.313149
H -6.022038 -2.850795 1.812894
H -7.395681 2.488768 -0.526532
H -6.197837 2.934101 -1.771699
H -7.359282 1.608706 -2.061684

224
(^{DIPeP}BDI*)Mg(C_6H_6)Ca(^{DIPeP}BDI) (3')
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C -3.568005 2.196937 -1.500822
C -3.085258 1.915550 -2.808625
C -2.322955 2.886972 -3.461258
H -1.956052 2.696538 -4.470692
C -2.010738 4.097546 -2.844567
H -1.410862 4.841018 -3.374173
C -2.453924 4.346261 -1.551064
H -2.190431 5.286846 -1.060820
C -3.232877 3.411725 -0.860462
C -3.382318 0.565458 -3.437542
H -3.228256 -0.172786 -2.630885
C -2.386757 0.206411 -4.542810
H -2.559373 0.852769 -5.421613
H -1.376080 0.444844 -4.182241
C -4.856236 0.426553 -3.890214
H -4.906775 0.551283 -4.986682
C -5.510925 -0.885224 -3.475012
C -3.671467 3.707672 0.560788
H -4.365408 2.910362 0.868469
C -2.446024 3.622774 1.490906
H -2.072522 2.584452 1.464677
H -1.633659 4.232733 1.059209
C -4.438542 5.045092 0.641793
H -4.891598 5.243377 -0.342989
C -5.541505 5.080926 1.693612
C 4.644483 1.489444 0.154736
C 5.694582 2.653399 0.116348
C 2.672592 2.818020 -0.379830
C 2.109257 3.723243 0.549206
C 1.316610 4.762865 0.050292
H 0.873804 5.482301 0.737254
C 1.096496 4.920122 -1.314791
H 0.464783 5.734316 -1.674163
C 1.715523 4.063829 -2.219367
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C 2.471677 3.625381 2.025154
H 3.520085 3.285416 2.037151
C 1.695262 2.540846 2.777125
H 0.622339 2.790652 2.798497
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C 2.451180 4.980908 2.761156
C 1.112255 5.431152 3.341685
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H 2.009902 0.419037 -2.389006
C 1.341369 1.273100 -4.233328
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H 2.039077 -0.610875 2.633445
C 1.214140 -1.710396 4.284473
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H 4.463318 -4.060044 3.460096
C 4.619942 -2.617655 5.058575
H -3.728203 5.874146 0.810459
H -5.444803 1.258569 -3.479055
C -2.416445 -1.250587 -4.979105
H -5.567487 -5.252337 -0.175092
H -3.557426 -3.276918 -2.735968
C -5.370232 0.791254 3.565512
C -2.197734 0.827833 4.925840
C 4.790218 -4.193651 -3.644521
C 2.050526 -2.477704 -4.452596
H 3.002705 -3.883390 4.413488
C -2.661600 4.026785 2.940811
H 3.030522 -0.576088 4.071500
C 2.209230 2.271993 4.182883
H 2.841885 5.754794 2.079906
H 3.150839 3.419676 -4.505449
H 3.138547 0.205200 -3.706330
C 6.370218 2.704305 1.501707
C 6.753512 2.355191 -0.964345
C 5.186958 4.071478 -0.181063
C 6.847108 -1.895974 1.570584
C 5.576165 -3.618820 0.356721
C 6.788067 -1.910233 -0.944860
C -0.118328 1.251223 0.285460
C -0.417459 0.279983 1.361323
C -0.071524 -1.088783 0.910480
C -0.126303 -1.433806 -0.427188
C -0.180310 0.891612 -1.048090
C -0.554003 -0.474156 -1.458681
H -0.148552 0.551317 2.382361
H 0.131713 -1.876198 1.637569
H 0.065387 -2.472843 -0.692441
H -0.055172 1.678589 -1.793697
H -0.375682 -0.746300 -2.499516
H 0.059435 2.299684 0.520586
H 0.790117 0.366423 -4.517465
H 0.615860 1.979021 -3.803217
H 1.734030 1.720238 -5.159448
H 5.365826 2.746531 -5.505170
H 5.603175 1.579802 -4.185162
H 4.283923 1.351099 -5.348814
H -6.558925 -0.934065 -3.810182
H -4.987445 -1.757017 -3.893347
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H -1.638077 -1.450799 -5.732178
H -2.234626 -1.918511 -4.123489
H -3.381531 -1.533166 -5.426239
H -6.094206 -6.092092 -2.439812
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H -1.171931 -3.932189 -2.568430
H -1.360023 -4.339276 -0.852817
H -2.184789 -5.309046 -2.096304
H 5.183227 -5.127382 -4.076138
H 4.529455 -3.526533 -4.477748
H 5.612538 -3.717706 -3.088752
H 1.164308 -2.049237 -4.945003
H 2.889657 -1.785333 -4.621883
H 2.284945 -3.419428 -4.971237
H 1.645398 1.454757 4.656021
H 3.270957 1.977957 4.162186
H 2.122280 3.151187 4.838340
H 1.193822 6.447623 3.756249
H 0.301209 5.442163 2.599896
H 0.780287 4.774378 4.159179
H 5.075163 -3.351833 5.740541
H 5.433831 -2.002634 4.641460
H 3.988524 -1.953082 5.667781
H 0.634573 -0.852892 4.653047
H 0.530987 -2.343619 3.699199
H 1.531372 -2.290040 5.164869
H -6.390210 0.924186 3.958952
H -4.745411 1.592029 3.987095
H -5.413041 0.937915 2.474930
H -1.354419 0.941308 5.625285

H -2.025756 1.510666 4.080690
H -3.103795 1.165031 5.451642
H -6.075717 6.043888 1.676125
H -6.283546 4.287326 1.509683
H -5.159295 4.931743 2.712418
H -2.920520 5.091820 3.039025
H -3.463698 3.439061 3.411481
H -1.744703 3.861482 3.526150
H 7.128414 3.502977 1.518043
H 5.633051 2.924138 2.289098
H 6.865592 1.759773 1.763532
H 7.467963 3.190909 -1.018667
H 7.329577 1.442033 -0.768443
H 6.285219 2.250589 -1.953929
H 6.057364 4.745754 -0.162177
H 4.720258 4.161211 -1.168095
H 4.474471 4.442387 0.561155
H 7.678054 -2.618195 1.568069
H 7.284295 -0.889477 1.601224
H 6.280394 -2.044684 2.500809
H 6.507087 -4.206846 0.345184
H 5.013410 -3.906835 1.251003
H 4.990600 -3.916824 -0.517078
H 7.583516 -2.668895 -1.013938
H 6.154879 -1.999756 -1.839607
H 7.260421 -0.919733 -0.971792
H -7.512750 -1.585585 1.642958
H -7.075040 -2.650571 0.295423
H -6.194068 -2.783361 1.832252
H -7.384667 1.912224 -1.506780
H -6.572079 3.012778 -0.376477
H -5.910490 2.802529 -2.004199

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(^{DIPeP}BDI*)Mg(naphthalene)Ca(^{DIPeP}BDI) (4)

Ca 2.580579 -0.150195 0.322968
Mg -2.033434 0.023227 -0.067575
N -3.646169 -1.301890 0.160851
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N 4.215714 1.472057 0.709652
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C -4.907507 -1.008788 -0.145836
C -5.277375 0.232618 -0.706098
H -6.332608 0.289798 -0.929727
C -4.601477 1.442933 -0.963431
C -6.161613 -1.924551 0.102332
C -7.044013 -1.228418 1.157538
H -6.493964 -1.067300 2.092647
H -7.918514 -1.858315 1.385427
H -7.407663 -0.250797 0.814146
C -5.901795 -3.352800 0.598767
H -5.253204 -3.926591 -0.068610
H -6.869954 -3.874841 0.651879
H -5.453903 -3.386155 1.594880
C -6.987862 -2.064036 -1.195163
H -7.392098 -1.109691 -1.556340
H -7.844984 -2.727840 -1.003864
H -6.398977 -2.505886 -2.010717
C -5.583417 2.543889 -1.516541
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H -4.299436 3.961243 -2.625447
C -6.742244 2.751976 -0.518175
H -7.302680 1.831279 -0.313909
H -7.449466 3.486081 -0.934385
H -6.382690 3.141956 0.441654
C -6.192650 2.037122 -2.841178
H -5.419894 1.828051 -3.594174
H -6.862743 2.807363 -3.254449
H -6.777951 1.117751 -2.708501
C -3.193082 -2.495028 0.785330
C -3.256114 -2.621247 2.196214
C -2.773347 -3.794805 2.783774
H -2.843766 -3.920166 3.865407
C -2.224281 -4.813331 2.014036
H -1.856819 -5.724803 2.491084
C -2.121258 -4.656366 0.636119
H -1.659469 -5.449091 0.046938
C -2.580788 -3.502080 -0.004921
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C -4.902943 -2.071664 4.056022
H -5.632218 -2.691187 3.510290
H -4.419206 -2.756750 4.770822
C -5.640170 -0.982199 4.824113
H -4.967584 -0.417646 5.487527
H -6.438115 -1.408809 5.451123
H -6.106523 -0.254539 4.140496
C -2.806971 -0.645458 3.731757
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H -3.297413 0.286976 4.049282
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C -2.443078 -3.337790 -1.512032
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C -1.316367 -4.183068 -2.117233
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H -1.537860 -5.255443 -1.990361
C -1.058754 -3.912834 -3.592459
H -0.801160 -2.857374 -3.768559
H -1.932173 -4.147101 -4.219344
H -0.222093 -4.523826 -3.964339
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H -4.521597 -2.905962 -1.794653
H -3.675903 -3.207623 -3.286038
C -4.268903 -5.003154 -2.248033
H -3.638179 -5.655631 -2.871571
H -5.295442 -5.069043 -2.640452
H -4.272229 -5.428346 -1.231656
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H -1.090905 5.297318 0.808437
C -0.946321 5.026057 -1.312413
H -0.329526 5.916113 -1.456654
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H 0.481225 2.400938 0.120374
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C 0.733274 -2.592589 3.023341
H 0.853908 -3.006791 4.027121
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H 1.140465 -4.455373 2.009886
C 0.748346 -2.849136 0.619608
H 0.926890 -3.471508 -0.255926
C 0.323221 -1.524259 0.443487
C 6.369076 2.633320 1.027126
H 5.753667 3.484454 1.341919
H 7.071587 2.969220 0.251419
H 6.972611 2.308114 1.889443
C 5.531560 1.470143 0.537748
C 6.247845 0.417864 -0.062332
H 7.327372 0.564656 -0.131516
C 5.758827 -0.763473 -0.655023
C 6.789613 -1.615184 -1.363622
H 6.353540 -2.533553 -1.774188
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H 7.235550 -1.041106 -2.190455
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H 2.394652 5.543830 -0.365251
C 1.857530 4.833564 1.588032
H 1.211635 5.687452 1.801331
C 2.014797 3.826625 2.534660
H 1.492928 3.912303 3.486985
C 2.827597 2.716191 2.287430
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C 4.462607 4.925592 -1.865719
H 4.901477 4.733751 -2.860014
H 3.568708 5.540806 -2.059339
C 5.451950 5.712509 -1.017504
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C 3.250140 2.722137 -2.259107
H 3.865359 2.556411 -3.160025
H 3.110047 1.723188 -1.813082
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H 2.000483 4.284972 -3.130203
H 1.257926 3.440652 -1.760685
H 1.360014 2.652283 -3.338279
C 3.022601 1.629364 3.334533
H 2.904504 0.647797 2.834109
C 4.458719 1.636805 3.891818
H 4.578239 0.779216 4.572952
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C 4.845484 2.925082 4.602397
H 5.894015 2.892003 4.935700
H 4.224333 3.108009 5.493381
H 4.731309 3.795332 3.937407
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H 1.992687 2.621846 4.970242
H 0.972754 1.602044 3.969965
C 2.108907 0.538307 5.469782
H 2.985508 0.684087 6.118795
H 2.213507 -0.444483 4.985217
H 1.224367 0.492629 6.123062
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C 3.153267 -2.419241 -2.208146
C 2.503806 -3.621106 -2.500192
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C 2.674683 -4.748403 -1.700842
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C 3.536561 -4.695218 -0.610666
H 3.680735 -5.589413 -0.000585
C 4.231580 -3.527126 -0.283274
C 3.018648 -1.201410 -3.111040
H 2.835504 -0.322178 -2.464254
C 1.835713 -1.287237 -4.080488
H 1.958433 -2.155474 -4.748105
H 0.924622 -1.486378 -3.497656
C 1.622274 -0.042757 -4.928635
H 2.444024 0.124150 -5.640857
H 1.539677 0.858850 -4.303610
H 0.695178 -0.125739 -5.514954
C 4.344527 -0.900372 -3.837487
H 4.223018 0.027395 -4.418774
H 5.106101 -0.668153 -3.083616
C 4.836535 -2.021377 -4.740514
H 5.804975 -1.763871 -5.196058
H 4.133490 -2.229670 -5.562389
H 4.969149 -2.957822 -4.176375
C 5.219941 -3.539465 0.875135
H 5.920593 -2.706138 0.727235
C 4.572584 -3.305679 2.247838
H 3.820902 -4.090196 2.440217
H 5.359132 -3.435698 3.010638
C 3.929220 -1.942327 2.428444
H 2.983111 -1.925469 1.865036
H 4.600877 -1.128881 2.111165
H 3.643114 -1.767969 3.474173
C 6.057349 -4.828333 0.920337
H 6.761560 -4.734226 1.764316
H 5.405653 -5.678848 1.185888
C 6.833791 -5.151804 -0.347782
H 7.569857 -4.367059 -0.577587
H 6.167263 -5.247310 -1.218342
H 7.383662 -6.099577 -0.242169
C -2.506758 2.242725 -3.433761
C -2.332313 2.961807 -4.774320
H -3.585731 2.080980 -3.304609

C -1.869462 0.836638 -3.439940
C -2.937012 2.232865 -5.966350
H -2.783067 3.966174 -4.700622
H -1.256674 3.125099 -4.963276
C -2.857469 -0.295703 -3.677036
H -1.063027 0.809544 -4.191095
H -1.356937 0.665571 -2.486270
H -2.829033 2.828121 -6.886028
H -2.449967 1.262600 -6.146430
H -4.012203 2.042176 -5.818896
H -2.340477 -1.262688 -3.741662
H -3.586644 -0.360611 -2.854164
H -3.427065 -0.162341 -4.608409

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(^{DIPeP}BDI*)Mg(anthracene)Ca(^{DIPeP}BDI) (5)

Ca 2.940780 -0.218553 -0.217899
Mg -2.445559 0.035264 -0.080437
N -3.313845 1.639947 0.987153
N -4.104460 -1.253300 0.143212
N 4.496707 1.226647 -1.174341
N 4.937617 -1.376136 0.143452
C -4.540039 1.554676 1.504536
C -5.360602 0.418626 1.337120
H -6.333114 0.551732 1.789065
C -5.229716 -0.850527 0.729975
C -5.276602 2.669899 2.336533
C -4.502359 3.969237 2.588723
H -3.624809 3.825938 3.224242
H -5.173998 4.670939 3.107290
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C -5.671267 2.105157 3.717352
H -6.379026 1.269174 3.644403
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H -7.090704 3.854231 2.179906
H -7.279750 2.223681 1.507070
C -6.555383 -1.685687 0.864665
C -6.906565 -1.841101 2.360734
H -6.110466 -2.353443 2.917584
H -7.823487 -2.443076 2.457020
H -7.088861 -0.878935 2.856414
C -7.710121 -0.915803 0.190326
H -7.912033 0.049445 0.672932
H -8.630976 -1.517251 0.244922
H -7.503731 -0.717127 -0.870308
C -6.547489 -3.096712 0.264465
H -6.443289 -3.095833 -0.823480
H -7.510564 -3.573947 0.503701
H -5.754771 -3.730435 0.671116
C -2.360232 2.667151 1.226838
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C -2.783740 3.622328 -1.116790
H -2.927182 2.564225 -1.393976
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H -4.717867 3.668686 -0.209944
H -4.751503 4.041358 -1.913309
C -4.218027 5.718767 -0.668632
H -3.848870 6.326036 -1.509599
H -3.593714 5.958863 0.206650
H -5.243345 6.054186 -0.449156
C -1.981494 4.282067 -2.245326
H -1.832565 5.352063 -2.026781
H -0.972912 3.842836 -2.260638
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H -3.576184 4.673332 -3.693400
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H -3.078265 1.624355 3.549853
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H -1.730707 1.195511 5.598528
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C -2.172614 3.294768 5.516539
H -1.989116 4.185056 4.896633
H -1.789031 3.507424 6.526386
H -3.263371 3.170416 5.596902
C -1.528099 0.221117 3.217363
H -1.396183 0.074321 2.133284
H -0.517787 0.066342 3.624861
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H -2.100307 -1.822472 3.705550
H -3.454759 -0.776706 3.216750
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C -4.237691 -5.215678 2.325158
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C -0.752433 -1.572967 -0.837444
H -0.858740 -2.645205 -0.683266
C 0.137910 -0.874890 0.039319
C 0.890426 -1.457409 1.086050
H 0.898128 -2.541202 1.197313
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C -0.784480 0.302902 -2.413947
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H -0.870306 1.901731 -3.855673
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H -1.415030 0.414638 -5.776687
C -1.381383 -1.390286 -4.583871
H -1.631487 -2.048706 -5.419517
C -1.178047 -1.932808 -3.309027
H -1.280447 -3.007687 -3.146494
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H 5.862277 3.003111 -2.490677
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C 5.765393 1.070982 -1.500102
C 6.501836 -0.097712 -1.202720
H 7.520278 -0.117434 -1.592827
C 6.123268 -1.220658 -0.444203
C 7.141415 -2.327023 -0.315465
H 7.317818 -2.581442 0.738119
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H 4.847604 -3.523642 4.211066
C 3.916340 -4.628857 2.621631
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C 3.647674 -4.679773 1.258248
H 3.159448 -5.562748 0.842959
C 4.019517 -3.632355 0.406005
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C 6.815075 -1.700682 3.972250
H 7.264695 -0.774131 4.369707
H 6.323216 -2.176427 4.836552
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C 4.823321 -0.209067 3.455261
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H 4.638776 -0.733077 5.570318
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H -5.380203 -2.050396 -4.550065
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H -7.727062 -2.879240 -4.379729
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H 2.923842 5.403390 -0.076396
C 1.867447 4.460665 -1.691873
H 1.136709 5.265586 -1.785444
C 1.823088 3.371616 -2.553536
H 1.068005 3.329559 -3.341667
C 2.741300 2.320800 -2.455530
C 4.902997 3.599394 0.465900
H 5.732156 2.961658 0.129430
C 5.477984 5.010858 0.633299
H 4.699171 5.703449 0.992542
H 6.227133 4.972702 1.443088
C 6.117337 5.575447 -0.627437
H 6.509852 6.589801 -0.457918
H 5.392334 5.630439 -1.454056
H 6.955516 4.946576 -0.964953
C 4.452026 2.994327 1.805544
H 5.334877 2.929541 2.464224
H 4.148675 1.952765 1.618144
C 3.330395 3.726704 2.523650
H 3.606919 4.763353 2.770309
H 3.081633 3.227058 3.472685
H 2.414568 3.759406 1.916636
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H 1.685589 -0.224857 -2.361378
C 2.153324 -1.130908 -4.228874
H 3.013141 -1.339732 -4.881986
H 1.348380 -0.688637 -4.832047
H 1.770257 -2.087040 -3.854542
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H 4.822039 1.045654 -3.972861
H 3.765872 0.687943 -5.329373
C 4.118332 2.789111 -5.048209
H 4.966738 2.817426 -5.749089
H 4.314331 3.520787 -4.250161
H 3.224024 3.135202 -5.591428
C 3.776752 -3.727850 -1.087614
H 4.303742 -2.874898 -1.544525
C 2.299103 -3.564843 -1.490925
H 1.902295 -2.625047 -1.069356
H 2.262621 -3.427184 -2.580290
C 1.347848 -4.686873 -1.110683
H 1.261784 -4.801345 -0.021419
H 1.670722 -5.654782 -1.524702
H 0.340523 -4.481327 -1.500637
C 4.420937 -4.992358 -1.678272
H 5.465315 -5.036524 -1.327283
H 3.938149 -5.893572 -1.265396
C 4.391176 -5.045210 -3.199444
H 4.836397 -4.136494 -3.636746
H 3.365890 -5.129647 -3.590813
H 4.957451 -5.909802 -3.578020

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(^{DIPeP}BDI)Ca(naphthalene)Ca(^{DIPeP}BDI) (6)

Ca 2.741107 0.180725 0.048870
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N -3.924199 1.251510 -1.624614
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H 8.183190 -0.277114 -0.085804
H 7.294379 -1.385056 -1.170183
C 6.069209 -0.406793 0.347836
C 6.158603 0.279340 1.579360
H 7.155306 0.319913 2.020679
C 5.124328 0.839573 2.348706
C 5.473110 1.357083 3.722151
H 5.089796 2.378716 3.864100
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H 2.648908 -5.154999 1.199128
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H 6.536987 1.280274 -4.632304
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H 7.981256 -0.633169 -3.752408
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H 1.154588 5.611205 1.194568
H 0.420323 3.993534 1.119804
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H 3.644280 4.592023 3.978044
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H -1.760689 5.160876 -0.575553
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H -1.360562 0.085803 -2.568356
C -2.470495 -1.399682 -3.714705
H -2.781766 -1.587951 -4.754252
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H -1.182171 1.748014 -5.679905
H -2.304460 0.476843 -6.123011
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H -2.923149 2.632646 -7.247966
H -3.121539 3.415435 -5.662624
H -4.214903 2.105669 -6.146881
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H -3.064468 5.199165 1.297907
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H -2.844845 4.319306 3.610388
H -3.118678 2.660917 3.038442
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H -5.591305 3.003942 -0.458627
H -5.573955 3.758179 1.122061
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H -6.325887 5.381334 -0.613113
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H -4.785711 5.938000 0.066936
C -4.543986 -2.302130 0.668273
C -3.887323 -3.533972 0.430667
C -3.789591 -4.451407 1.481876
H -3.315291 -5.418798 1.309466
C -4.273945 -4.149476 2.751297
H -4.192618 -4.882101 3.557728
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H -5.146554 -2.645636 4.010790
C -4.953695 -1.946886 1.981242
C -3.258041 -3.820473 -0.920935
H -2.821823 -2.864833 -1.261846
C -2.094729 -4.820673 -0.848500
H -1.534393 -4.655516 0.085118
H -2.487102 -5.849374 -0.779260
C -1.129649 -4.717361 -2.020954
H -1.632199 -4.867994 -2.988749
H -0.331020 -5.470694 -1.946991
H -0.648065 -3.726982 -2.045793
C -4.290977 -4.212125 -1.993701
H -4.903885 -3.329723 -2.223119
H -3.753381 -4.444229 -2.927968
C -5.191262 -5.377937 -1.612435
H -5.899532 -5.611199 -2.422259
H -5.775344 -5.151571 -0.707548
H -4.614691 -6.294051 -1.408476
C -5.434801 -0.533963 2.253731
C -4.907582 0.061757 3.578678
C -6.954304 -0.384148 2.089345
H -4.991721 0.075257 1.446981
H -4.771632 1.144301 3.428270
C -5.754231 -0.127479 4.833373
H -3.896083 -0.338295 3.753390
H -5.239293 0.300494 5.707520
H -6.727802 0.378889 4.751706
H -5.959491 -1.183583 5.062163
C -7.403422 1.061290 1.932126
H -7.464043 -0.864369 2.941615
H -7.271288 -0.951784 1.206051
H -8.495940 1.132779 1.815932
H -7.122141 1.682253 2.797050
H -6.941765 1.508869 1.038209
H 1.660592 1.579495 -2.879828
H 2.058074 -0.884614 -3.066006

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(^{DIPeP}BDI)Ca(naphthalene)Ca(^{DIPeP}BDI) (same ring)

Ca 2.217235 -0.358831 0.056663
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N 3.875260 -1.556790 -1.023706
N -4.236243 -0.772063 0.783005
N -3.785201 1.683541 -0.704241
C 6.576095 1.281667 1.187102
H 7.235964 1.680537 0.401959
H 7.203274 0.668163 1.851179
H 6.173024 2.121208 1.765521
C 5.485523 0.432993 0.566693
C 5.948366 -0.652752 -0.212111
H 7.032064 -0.769293 -0.256414
C 5.201069 -1.561264 -0.977525
C 5.952218 -2.586998 -1.790467
H 5.639720 -3.603482 -1.505334
H 7.037755 -2.499690 -1.658846
H 5.716264 -2.482119 -2.860719
C 3.801800 1.799973 1.575741
C 3.275273 2.976472 0.985095
C 2.752620 3.964927 1.826325
H 2.351005 4.882761 1.396064
C 2.742197 3.806998 3.209786
H 2.324844 4.590487 3.846562
C 3.267135 2.650359 3.778498
H 3.253946 2.533205 4.863664
C 3.806061 1.636485 2.983811
C 3.336088 3.165791 -0.521953
H 3.000329 2.217500 -0.978652
C 2.393912 4.259967 -1.032867
H 1.400905 4.104595 -0.585971
H 2.733278 5.245141 -0.671824
C 2.243449 4.305743 -2.545119
H 1.559234 5.112907 -2.845599

H 1.828983 3.362844 -2.929996
H 3.201086 4.486018 -3.056117
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H 5.352057 2.456313 -0.818354
H 4.772782 3.481264 -2.106020
C 5.498793 4.563837 -0.383113
H 4.997964 5.517042 -0.615087
H 6.533354 4.640260 -0.751591
H 5.538189 4.472806 0.713340
C 4.346867 0.355547 3.589719
H 5.138457 -0.015994 2.923192
C 4.982021 0.542264 4.971108
H 4.219772 0.901603 5.683860
H 5.280374 -0.450083 5.347118
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H 5.934113 2.473011 4.620886
H 6.994381 1.078455 4.340939
H 6.602815 1.573020 6.001631
C 3.260023 -0.731942 3.621291
H 2.605685 -0.558563 4.488733
H 2.584923 -0.605484 2.757481
C 3.804189 -2.150344 3.634134
H 2.988345 -2.882439 3.718930
H 4.488426 -2.319627 4.480066
H 4.361801 -2.367038 2.708312
C 3.142228 -2.372896 -1.904403
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C 2.054141 -4.036690 1.037252
H 2.587210 -4.251756 1.975363
H 1.744065 -2.980479 1.110663
C 0.809000 -4.902800 0.963723
H 0.141300 -4.698830 1.813353
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H 0.233821 -4.711877 0.047354
C 3.559942 -5.615437 -0.314582
H 2.728545 -6.275628 -0.613051
H 4.256111 -5.620254 -1.170153
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C 1.524305 0.762169 -4.342843
H 0.844938 -0.082109 -4.166566
H 1.750256 0.791842 -5.420003
H 0.975021 1.684660 -4.101139
C -0.103201 -0.802779 1.407145
C -0.173723 -1.489049 0.119798
H -0.361286 -2.558280 0.114923
C -0.130339 -0.760982 -1.135636
H -0.212578 -1.314604 -2.072365
C 0.052042 0.611736 -1.131944
H 0.056473 1.180854 -2.061442
C 0.229021 1.317751 0.121401
H 0.365766 2.393920 0.114095
C 0.132561 0.632985 1.410104
C 0.251875 1.286371 2.644115
H 0.478866 2.353016 2.642702
C 0.123264 0.594315 3.866894
C -0.143597 -0.761243 3.864669
C -0.258646 -1.453170 2.640539
H -0.492947 -2.518729 2.636597
C -6.618046 -1.250594 1.217339
H -6.241185 -2.131028 1.752012
H -7.265167 -1.593740 0.395443
H -7.251061 -0.665800 1.901299
C -5.498396 -0.392164 0.667074
C -5.904369 0.786661 0.007202
H -6.981076 0.963032 -0.024758
C -5.110380 1.719763 -0.683940
C -5.855113 2.789344 -1.453709
H -5.202854 3.628639 -1.726283
H -6.702658 3.167353 -0.864652
H -6.268000 2.372194 -2.386219
C -3.844094 -1.903398 1.521622
C -3.824130 -1.843131 2.939193
C -3.302341 -2.926813 3.646036
H -3.270289 -2.894008 4.736580
C -2.812311 -4.049202 2.981326
H -2.410009 -4.890559 3.550731
C -2.833022 -4.097786 1.590122
H -2.451411 -4.985248 1.084675
C -3.336621 -3.033406 0.834559
C -4.326639 -0.587855 3.625054
H -5.198107 -0.238729 3.053442
C -3.287806 0.551562 3.558769
H -2.695254 0.554732 4.486228
H -2.535756 0.333333 2.781973
C -3.912934 1.914552 3.313307
H -4.673696 2.150456 4.074780
H -4.408717 1.947643 2.329700
H -3.158702 2.713788 3.343543
C -4.816386 -0.798477 5.059085
H -3.992036 -1.185703 5.682747
H -5.054624 0.192741 5.480984
C -6.038194 -1.699552 5.173153
H -6.357073 -1.817295 6.220280
H -5.840403 -2.703307 4.767143
H -6.888417 -1.281409 4.611016
C -3.397996 -3.085786 -0.683213
H -3.063004 -2.100583 -1.058447
C -2.457137 -4.127937 -1.295148
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H -2.811781 -5.142845 -1.049699
C -2.279632 -4.005082 -2.800222
H -3.228688 -4.115647 -3.346127

H -1.594115 -4.778257 -3.176191
H -1.851295 -3.028221 -3.068258
C -4.848388 -3.242038 -1.184101
H -5.405713 -2.334259 -0.918727
H -4.838450 -3.263426 -2.285891
C -5.574529 -4.467924 -0.650089
H -6.606019 -4.511637 -1.032164
H -5.623262 -4.454650 0.449610
H -5.076507 -5.404992 -0.945235
C -3.023621 2.480770 -1.575358
C -2.204042 3.507713 -1.038637
C -1.345120 4.189890 -1.905662
H -0.712430 4.989058 -1.518908
C -1.291320 3.880991 -3.262671
H -0.618337 4.432239 -3.922514
C -2.105494 2.876387 -3.780349
H -2.063756 2.652525 -4.847977
C -2.973709 2.155008 -2.956344
C -2.317554 3.874417 0.433151
H -2.351066 2.926739 1.003645
C -1.118274 4.663279 0.968642
H -0.196443 4.134180 0.687063
H -1.059076 5.646662 0.473585
C -1.120767 4.861628 2.477434
H -1.949536 5.502242 2.814707
H -0.184168 5.333823 2.809409
H -1.206350 3.898228 3.003043
C -3.655236 4.582766 0.727311
H -4.472986 3.888132 0.495915
H -3.728177 4.762686 1.811437
C -3.858571 5.887565 -0.028538
H -4.847933 6.318024 0.189575
H -3.791143 5.734194 -1.117094
H -3.105875 6.644606 0.242537
C -3.818262 1.018484 -3.501635
C -3.034527 -0.309137 -3.523613
C -4.480640 1.360627 -4.841083
H -4.634546 0.845565 -2.789317
H -3.748851 -1.143497 -3.610314
C -1.967988 -0.424843 -4.597729
H -2.557075 -0.435629 -2.537278
H -1.389987 -1.354617 -4.485407
H -2.403343 -0.432397 -5.608921
H -1.258822 0.411669 -4.543977
C -5.489067 0.316922 -5.301939
H -3.719448 1.504677 -5.625598
H -4.980902 2.337714 -4.733137
H -6.008393 0.639577 -6.217274
H -5.009830 -0.649870 -5.520671
H -6.254046 0.135474 -4.529183
H -0.267707 -1.309165 4.801333
H 0.234051 1.142837 4.804814

218

(^{DIPeP}BDI)Ca(anthracene)Ca(^{DIPeP}BDI) (7)

Ca -2.257082 0.195225 0.309970
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C -6.542489 -1.112559 -1.342419
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H -7.151067 -1.791357 -0.726560
H -6.109011 -1.687385 -2.168787
C -5.485788 -0.443643 -0.490296
C -5.986608 0.342589 0.573823
H -7.072575 0.357701 0.675232
C -5.272708 1.134118 1.485575
C -6.056200 1.925986 2.502943
H -5.752119 1.643175 3.522686
H -7.137094 1.770302 2.399784
H -5.842230 3.001556 2.405786
C -3.750084 -1.414904 -1.822283
C -3.228686 -0.806824 -2.992384
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H -2.286076 -1.185928 -4.896474
C -2.627655 -3.012220 -3.823604
H -2.189235 -3.636169 -4.605882
C -3.135615 -3.596994 -2.668106
H -3.080860 -4.679738 -2.545606
C -3.706142 -2.821549 -1.656396
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H -3.020074 1.164657 -2.221416
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H -2.721278 0.936556 -5.248688
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H -1.713364 3.062973 -3.268049
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H -4.945839 0.678590 -5.549602
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H -4.095914 -5.543768 -0.954046
H -5.166516 -5.223463 0.392922
C -6.061587 -4.833666 -1.523906
H -5.797806 -4.456231 -2.523781
H -6.867984 -4.194157 -1.132800
H -6.472854 -5.847578 -1.646109
C -3.075390 -3.534943 0.650494
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H -2.479794 -2.607462 0.596836
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H -4.181753 -2.943144 2.428358
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H -0.319013 0.232543 -2.406574
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C -0.170820 -2.286807 -1.327628
H -0.361216 -2.286105 -2.400858
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H 0.449740 -2.294484 2.515461
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H 6.179171 -1.530342 2.234380
H 7.228379 -0.188847 1.707172
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H 2.613292 -4.247462 -0.410887
H 2.537368 -2.521451 -0.287597
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H 4.615991 -4.012459 -2.010722
H 4.430560 -2.247372 -1.901355
H 3.137712 -3.244547 -2.618127
C 4.724058 -4.837708 0.956285
H 3.875768 -5.433048 1.335007
H 4.973627 -5.286611 -0.019823
C 5.924472 -4.957330 1.884868
H 6.218728 -6.008136 2.031011
H 5.715812 -4.526758 2.876251
H 6.795263 -4.422138 1.473263
C 3.339708 0.972378 3.104138
H 3.028479 1.338182 2.107118
C 2.383302 1.610826 4.116742
H 1.398359 1.129822 4.024253
H 2.726608 1.394864 5.142112
C 2.205611 3.111565 3.947873
H 3.152965 3.661379 4.053402
H 1.510300 3.509866 4.700786
H 1.789689 3.350163 2.957976
C 4.791004 1.463989 3.281338
H 5.362369 1.183858 2.386561
H 4.789692 2.566093 3.291372
C 5.490597 0.936267 4.525241
H 6.523117 1.313203 4.585022
H 5.533303 -0.163653 4.521775
H 4.976788 1.241979 5.450298
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C 1.382738 3.424761 -3.956875
H 0.722885 4.072818 -4.537211
C 2.183246 3.965509 -2.953952
H 2.143314 5.038839 -2.759099
C 3.034996 3.156729 -2.196538
C 2.374215 -0.278955 -3.823009
H 2.385005 -0.822336 -2.858318
C 1.180889 -0.823567 -4.615507
H 0.254541 -0.543898 -4.092080
H 1.123765 -0.332478 -5.600888
C 1.192818 -2.332581 -4.813228
H 2.013010 -2.661538 -5.468792
H 0.251091 -2.671132 -5.269854
H 1.300105 -2.859479 -3.853019
C 3.719206 -0.612348 -4.498892
H 4.529028 -0.358748 -3.802834

H 3.785699 -1.703316 -4.631848
C 3.945592 0.087135 -5.830986
H 4.940086 -0.153254 -6.236958
H 3.881369 1.181621 -5.724957
H 3.202913 -0.212607 -6.587143
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C 3.045513 3.771644 0.255189
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H 4.672307 3.022328 -0.852628
H 3.739971 3.906742 1.099714
C 1.945238 4.815542 0.313893
H 2.593658 2.776948 0.410253
H 1.370367 4.733851 1.248636
H 2.348803 5.838862 0.269182
H 1.239841 4.696444 -0.519278
C 5.501348 5.552914 -0.354436
H 3.756201 5.840855 -1.585961
H 5.039873 4.939054 -2.373252
H 6.024862 6.462025 -0.687567
H 4.999891 5.793810 0.595666
H 6.264609 4.787723 -0.137300

218

(^{DIPeP}BDI)Ca(anthracene)Ca(^{DIPeP}BDI) (different rings)

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H -8.496269 -1.291415 -1.003816
H -7.466916 -2.607277 -0.366214
C -6.381659 -0.828058 -1.006171
C -6.502917 0.342782 -1.783886
H -7.432619 0.441786 -2.345556
C -5.544921 1.351190 -1.995288
C -5.864340 2.412486 -3.018259
H -5.684332 3.417921 -2.609914
H -6.902864 2.346002 -3.365327
H -5.198279 2.308813 -3.888387
C -5.268180 -2.226331 0.594809
C -4.358938 -3.279493 0.319284
C -4.216167 -4.297588 1.268462
H -3.532786 -5.124420 1.074584
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H -4.788737 -5.078484 3.195282
C -5.804493 -3.230509 2.731684
H -6.350849 -3.218553 3.676989
C -5.998625 -2.198388 1.812318
C -3.571835 -3.298784 -0.985094
H -3.130057 -2.292521 -1.133974
C -2.385152 -4.270090 -0.962407
H -1.819907 -4.103495 -0.032567
H -2.756424 -5.306925 -0.906001
C -1.433575 -4.138125 -2.142846
H -0.575243 -4.816991 -2.024551
H -1.034916 -3.116329 -2.218071
H -1.915375 -4.387442 -3.100277
C -4.490825 -3.519765 -2.203061
H -5.161823 -2.655118 -2.291602
H -3.873514 -3.504853 -3.115464
C -5.305790 -4.803447 -2.149363
H -4.665241 -5.698899 -2.121734
H -5.955276 -4.893437 -3.033521
H -5.947963 -4.830257 -1.255525
C -6.903245 -1.020639 2.129363
H -7.298377 -0.635027 1.178407
C -8.114137 -1.381689 2.994963
H -7.774227 -1.750436 3.978308
H -8.668352 -0.454292 3.212232
C -9.059650 -2.389013 2.355624
H -8.547984 -3.337239 2.130390
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H -6.884551 1.771963 1.583424
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C -4.547764 5.488559 -0.489209
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H -2.375149 -1.532025 -3.538846
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H 3.546105 -1.602578 -3.204006
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H 1.950996 -2.798039 -1.728427
C 0.922953 -1.025561 -1.030650
C 0.061552 -1.668075 -0.109363
H 0.067852 -2.756410 -0.068814
C -0.778965 -0.965101 0.784069
C -1.682591 -1.595514 1.674288
H -1.754029 -2.683649 1.670824
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H -3.152896 -1.393434 3.258792
C -2.395028 0.530469 2.608510
H -2.986646 1.111376 3.319417
C -1.544388 1.197259 1.689944
H -1.480817 2.282778 1.688577
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H 6.634255 0.268862 3.335539
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C 7.106332 -1.912281 2.038605
H 6.894045 -2.934571 1.699660
H 7.344314 -1.927852 3.110911
H 8.009901 -1.572894 1.506644
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C 2.047229 2.475070 2.414251
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H 0.357335 5.127893 1.084239
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C 6.453044 0.091753 -2.149658
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(^{DIPeP}BDI*)Mg(C_6H_6)Mg(^{DIPeP}BDI*)

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H 0.819077 -4.240467 0.710137
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H 7.634660 0.380901 1.607168
H 7.564127 3.422783 0.556480
H 7.445679 1.933331 -0.407746
H 6.160713 3.146882 -0.502988
H 6.520117 3.632065 2.696159
H 5.037120 3.862003 1.762636
H 5.046082 2.748399 3.133479

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anthracene
C -1.222776 0.721555 -0.000043
C -1.222699 -0.721517 0.000041
C 0.000043 -1.402963 0.000238
C 1.222900 -0.721561 0.000310
C 0.000010 1.402975 0.000128
C 1.222831 0.721483 0.000349
H 0.000063 -2.496569 0.000228
H 0.000142 2.496566 0.000111
C -2.476176 -1.406182 -0.000142
C -3.657857 -0.712231 -0.000148
C -2.476480 1.406223 -0.000002
C -3.658009 0.712088 -0.000142
H -2.473806 -2.499308 -0.000238
H -4.609193 -1.249643 0.000117

H -2.474364 2.499353 0.000230
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H 2.474261 -2.499329 0.000683
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H 4.609158 1.249658 -0.000415

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naphthalene

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C 1.243264 -1.401790 0.000197
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(^{DIPeP}BDI*)Mg(naphthalene)Mg(^{DIPeP}BDI*) same ring

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(^{DIPeP}BDI*)Mg(naphthalene)Mg(^{DIPeP}BDI*) different ring

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H 8.231246 0.882362 0.516521
H 3.773143 1.306066 4.823333
H 5.148547 2.341558 5.226688
H 4.062233 2.779298 3.896599
H 7.473019 1.668847 2.574855
H 6.300308 2.996055 2.517822
H 7.067079 2.552758 4.055910
H 6.926311 -0.494615 3.736239
H 6.522765 0.398750 5.219248
H 5.362691 -0.753293 4.526125

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(^{DIPeP}BDI*)Mg(anthracene)Mg(^{DIPeP}BDI*) same ring

Mg -2.544661 0.226631 -0.018075
Mg 2.532088 0.089734 -0.197921
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N 4.066943 -0.394660 1.144238
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C -7.615324 -0.289878 -1.880199
C -7.491639 -1.957672 -0.037180
C -6.401110 -2.404492 -2.222553
C -5.442655 -0.563949 -0.586338
C -5.827941 0.465944 0.299484
H -6.900486 0.544142 0.415544
C -5.126536 1.464551 1.002035
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C -5.449058 3.735453 2.321577
C -6.877653 1.765571 2.776125
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C -3.651633 -1.837906 -1.694628
C -3.114813 -1.519543 -2.967559
C -2.563703 -2.557255 -3.728582
H -2.169228 -2.344650 -4.722084
C -2.508034 -3.860938 -3.245397
H -2.086198 -4.657546 -3.862607
C -2.975845 -4.144850 -1.967067
H -2.895547 -5.160438 -1.580852
C -3.541749 -3.150311 -1.169212
C -3.158242 -0.093415 -3.498009
H -2.859944 0.555246 -2.656592
C -2.156999 0.158820 -4.628518
H -1.163356 -0.161583 -4.287529
H -2.399643 -0.481945 -5.491973
C -2.078798 1.602455 -5.100838
H -1.341268 1.706667 -5.910948
H -1.769739 2.273871 -4.287805
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C -4.581007 0.340221 -3.882209
H -5.227426 0.159542 -3.017011
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C -5.146202 -0.352195 -5.113519
H -4.629840 -0.041847 -6.034998
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H -5.081191 -2.972149 0.243003
C -4.313489 -4.936632 0.506739
H -3.355930 -5.474488 0.398836
H -4.567501 -5.023716 1.576458
C -5.410132 -5.607611 -0.309755
H -5.213873 -5.553743 -1.391224
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H -5.510447 -6.671251 -0.043527
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H -2.576150 -3.560900 1.748024
H -2.626638 -2.013968 0.977154
C -4.177618 -2.286007 2.462085
H -3.595049 -1.973502 3.336886
H -4.888485 -3.058412 2.797994
H -4.766665 -1.421918 2.114806
C -3.001458 2.503946 1.661870
C -2.556614 2.383092 3.000535
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H -4.033361 0.931770 3.400144
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H -1.932214 -0.287220 3.301081
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H -0.468594 -0.497350 5.268923
H -1.376691 0.741648 6.158386
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H -2.884057 2.461013 5.790958
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H -4.159898 3.217920 -0.510574
C -3.573962 5.236808 -0.809490
H -4.139449 5.628154 0.052490
H -2.664265 5.855899 -0.869258
C -4.393080 5.419226 -2.079959
H -3.824741 5.140131 -2.980524
H -4.709726 6.466119 -2.203302
H -5.302075 4.796134 -2.060477
C -2.379420 3.139277 -1.650843

H -2.073294 2.121914 -1.348448
H -3.022429 2.999810 -2.533399
C -1.121967 3.896382 -2.028389
H -0.503703 4.075731 -1.140469
H -1.345497 4.871262 -2.488918
H -0.510331 3.325017 -2.740735
C -0.083689 -1.088682 1.305461
C -0.050482 0.290773 1.762007
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C 0.366718 1.282667 0.882116
H 0.641391 2.269215 1.269750
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H 0.535666 1.854649 -1.195587
C -0.500229 -0.105392 -0.923147
H -0.513955 -0.305437 -2.000444
C -0.251438 -1.315738 -0.120223
C -0.287295 -2.613593 -0.600752
H -0.459601 -2.784410 -1.663516
C -0.177122 -3.732174 0.264186
C -0.010077 -3.508780 1.670577
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C 6.565296 -0.779050 1.755998
C 6.232438 -1.136817 3.209891
C 7.544529 0.415724 1.816981
C 7.338529 -1.972664 1.155821
C 5.359793 -0.412434 0.810454
C 5.814641 -0.063315 -0.478719
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C 5.183931 0.410261 -1.643820
C 6.206050 0.750165 -2.783601
C 5.621375 1.298247 -4.091184
C 6.987382 -0.534848 -3.134803
C 7.217534 1.798319 -2.279910
C 3.521445 -0.827818 2.383675
C 3.370321 -2.215623 2.629058
C 2.794023 -2.620518 3.833034
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C 2.357343 -1.688747 4.769767
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C 2.460102 -0.329329 4.493468
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C 3.880731 -3.212221 1.607502
H 4.872219 -2.848215 1.306131
C 3.034035 -3.250686 0.320976
H 2.342361 -4.101869 0.379742
H 2.360518 -2.377548 0.267402
C 3.880279 -3.350037 -0.936578
H 4.582688 -4.197010 -0.874386
H 4.477668 -2.437795 -1.094765
H 3.257185 -3.510156 -1.826740
C 4.074279 -4.638096 2.132471
H 3.108486 -5.019552 2.505141
H 4.312024 -5.275603 1.264204
C 5.167271 -4.811050 3.178680
H 5.243374 -5.860594 3.502520
H 4.983386 -4.200707 4.075684
H 6.150569 -4.516819 2.779913
C 3.141748 1.618899 3.004884
H 2.902836 1.750253 1.934294
C 2.150727 2.482262 3.790381
H 1.130445 2.121634 3.591562
H 2.312197 2.349759 4.872142
C 2.230698 3.966304 3.468406
H 3.213321 4.393716 3.717741
H 1.479051 4.528618 4.040231
H 2.046883 4.156652 2.400618
C 4.587608 2.114045 3.166789
H 5.225472 1.472351 2.550676
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H 6.174792 2.354830 4.634689
H 4.935630 1.168195 5.098939
H 4.587839 2.903607 5.205659
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H 0.805716 3.003286 -5.254832
C 2.248179 3.228882 -3.666009
H 2.226832 4.318939 -3.715894
C 3.079298 2.596048 -2.739016
C 2.301259 -1.103384 -3.502113
H 2.383999 -1.376621 -2.432523
C 1.040265 -1.794941 -4.023903
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H 1.832868 -3.753558 -4.604017
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C 3.572480 -1.651339 -4.170455
H 4.433100 -1.176281 -3.687919
H 3.669064 -2.723158 -3.940136
C 3.634705 -1.441563 -5.675866
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C 3.144216 3.614063 -0.430396
C 4.501789 4.675189 -2.328478
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C 2.088318 4.704339 -0.490448
H 2.661099 2.663277 -0.150912
H 1.427443 4.671916 0.388363
H 2.536916 5.708695 -0.529043
H 1.454608 4.588119 -1.379088
C 5.462577 5.387498 -1.385332
H 3.696067 5.370533 -2.614512
H 5.023363 4.426214 -3.268051
H 5.925627 6.258697 -1.873077
H 4.955409 5.750428 -0.478438
H 6.275189 4.719228 -1.057961
C 0.111281 -4.629212 2.529107
C -0.202093 -5.063325 -0.216709
H 7.928560 2.035953 -3.086359
H 6.718039 2.732880 -1.991844
H 7.797555 1.448258 -1.415984
H 7.712555 -0.313734 -3.933373
H 7.545604 -0.933768 -2.277735
H 6.322974 -1.331620 -3.495835
H 6.439906 1.380356 -4.823039
H 4.853535 0.652627 -4.526505

H 5.183922 2.294833 -3.972465
H 7.941021 0.692800 0.832090
H 7.076291 1.309625 2.249375
H 8.399257 0.145602 2.456104
H 7.788009 -1.736149 0.182258
H 8.153399 -2.256910 1.839569
H 6.697735 -2.853796 1.017750
H 5.679507 -2.074572 3.304560
H 7.181612 -1.258593 3.754385
H 5.656686 -0.359127 3.720327
H -7.695701 3.828830 1.065529
H -6.512298 3.504183 -0.222456
H -7.728949 2.283298 0.197936
H -6.258677 4.352409 2.741783
H -4.761665 3.495830 3.135638
H -4.904347 4.353437 1.599629
H -7.582086 2.460502 3.259990
H -7.453468 0.917469 2.381315
H -6.200965 1.378939 3.551432
H -7.110500 0.222108 -2.710121
H -8.486841 -0.819175 -2.295507
H -7.991393 0.480184 -1.195115
H -6.891296 -2.681675 0.530404
H -7.871827 -1.213783 0.675907
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H -5.877002 -3.267570 -1.804407
H -7.364755 -2.763872 -2.615663
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H -0.080129 -7.157250 0.252837
H -0.317587 -5.225289 -1.290783

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(^{DIPeP}BDI*)Mg(naphthalene)Mg(^{DIPeP}BDI*) different ring

Mg 2.922450 0.116325 -0.264383
Mg -2.850534 -0.121245 -0.034973
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C 6.407536 -3.680715 -0.112746
C 5.568524 -1.221292 0.387240
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H -0.351963 -4.156004 3.112971
H 0.334710 -2.532382 2.962197
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C 3.605204 -3.372267 2.370302
H 4.459889 -2.754020 2.073262
H 3.250633 -2.934273 3.317683
C 4.047902 -4.808912 2.607488
H 3.265291 -5.404217 3.102194
H 4.942144 -4.849644 3.248459
H 4.293767 -5.315252 1.660460
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H 5.925554 -1.556338 -2.092091
C 5.756110 -2.213551 -4.104672
H 4.967629 -2.457661 -4.837286
H 6.296358 -1.357631 -4.543528
C 6.724219 -3.379090 -3.952281
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H 7.151438 -3.671742 -4.923888
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H 4.057721 -0.302029 -4.061169
H 3.536676 -0.253814 -2.433835
C 5.400226 0.806839 -2.765903
H 4.944658 1.767489 -3.039283
H 6.329576 0.703072 -3.348864
H 5.685933 0.850513 -1.701754
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C 2.430035 2.183620 2.588407
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H 3.639299 6.167312 -0.441355
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H 3.568331 0.442909 2.943763
C 3.191843 1.314264 4.842562
H 3.987957 2.070748 4.764910
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H -1.979025 -1.245296 2.480098
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H -0.979190 -2.486613 0.609488
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H 1.431393 2.439257 -3.643281
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C 1.098932 1.256324 -1.144025
H 1.133860 2.347162 -1.105962
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C -5.375708 3.752514 -2.212527
C -7.356816 2.648179 -1.239973
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C -7.373237 -2.302964 -1.820842
C -8.077399 -1.330180 0.368836
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C -2.361079 2.678626 -2.209259
C -1.444123 3.720683 -2.349807
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C -1.270354 4.661940 -1.338643
H -0.577928 5.493978 -1.477021
C -1.968094 4.532746 -0.143537
H -1.792848 5.256807 0.652336
C -2.860779 3.475793 0.066703
C -2.637090 1.686605 -3.321860
H -3.729591 1.565733 -3.341326
C -2.059174 0.283103 -3.056139
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H -1.753184 0.175319 -1.998470
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H -3.321778 -0.693425 -4.520611
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C -2.219210 2.153153 -4.719021
H -1.132291 2.336054 -4.729620
H -2.364265 1.303470 -5.407129
C -2.981292 3.357836 -5.253343
H -2.631079 3.634938 -6.259615
H -2.863210 4.240483 -4.606558
H -4.060006 3.147495 -5.325619
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H -3.244202 2.330294 4.050734
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C -5.139953 5.276974 1.312819
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H -4.630798 5.654888 0.412049
H -4.724620 5.819852 2.176026
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18
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(^{DIPeP}BDI)CaI

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(^{DIPeP}BDI)CaI + Cyclohexane

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(^{DIPeP}BDI)CaI + C_6H_6

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5. References

[S1] (a) Rigaku Oxford Diffraction, **2019**, *CrysAlisPro Software system*, version 1.171.40.67a, Rigaku Corporation, Oxford, UK (compounds (^{DIPeP}BDI)Ca(μ^6,μ^6-anthracene)Ca(^{DIPeP}BDI) (**7**), (^{DIPeP}BDI)Ca(μ^A,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**6**), (^{DIPeP}BDI*)Mg(μ^2,μ^A-naphthalene)Ca(^{DIPeP}BDI) (**4**)).

(b) Rigaku Oxford Diffraction, **2020**, *CrysAlisPro Software system*, version 1.171.40.84a, Rigaku Corporation, Oxford, UK (compound (^{DIPeP}BDI*)Mg(μ^2,μ^A-anthracene)Ca(^{DIPeP}BDI) (**5**)).

(c) Rigaku Oxford Diffraction, **2022**, *CrysAlisPro Software system*, version 1.171.42.72a, Rigaku Corporation, Oxford, UK (compound [(^{DIPeP}BDI)Ca(H)·(THF)]$_2$·2Hexane (**2**)).

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