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From MgBr via single-electron transfer (SET) to a paramagnetic Mg(II) compound and back to Mg(I): $[MgBr(L^1)^{\bullet}]_2$ and $[K(thf)_3]_2[Mg_2(L^1)_2]$, L^1 = RN=C(Me)C(Me)=NR, R = 2,6-Diisopropylphenyl.

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T. Kruczyński[a], P. Henke[a], T. Augenstein[a], N. Arleth[a], F. Breher[a] and H. Schnöckel[a]

[a] Karlsruhe Institute of Technology (KIT), Institute of Inorganic Chemistry, D-76131 Karlsruhe, Engesserstr. 15, Germany, Fax: +49 721 608 44854, Email: breher@kit.edu (FB), hansgeorg.schnoeckel@kit.edu (HS).

Electronic Supplementary Information (ESI)

1. General information

The experiments were carried out in an atmosphere of dry argon using typical Schlenk technique or in vacuum ampoules and a glove-box. Raman spectra were obtained using a Bruker MultiRaman spectrometer (excitation wavelength 1064 nm). MS spectra were recorded on a Thermo Scientific DFS High Resolution GC/MS. The NMR spectra were recorded on Bruker AV300 MHz, spectrometers at ambient temperature. Solvents for NMR were directly vacuum transported to the NMR tubes. Literature method was used to prepare $(dipNCCH_3)_2$.[1] Solvents (pentane, hexane, toluene, THF, DME, diethyleter) were dried over Na/benzophenone and distilled priori to use under argon.

For the synthesis of **3**, **5** and **6** sealed ampule technique was applied. The solvents were directly condensed from Na/K alloy/bezophenone to the reaction ampules.

2. Metastable magnesium(I) bromide/chloride solution

Metastable magnesium(I) bromide/chloride solution was obtained according to the literature method (Figure S1 A).[2]

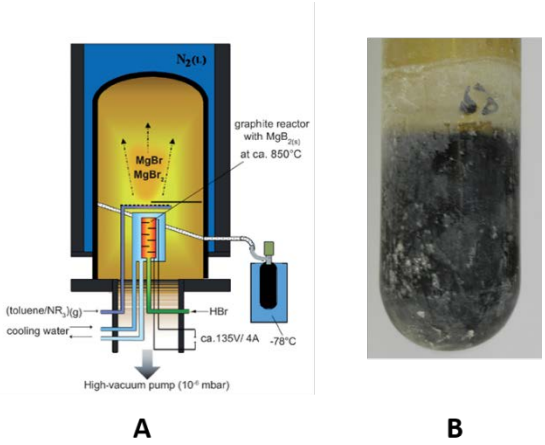


Figure S1 - A - Cocondensation apparatus used in the presented experiments, **B** – MgBr solution.

High temperature molecules of MgBr were cocondensed with the mixture of 100 cm^3 of toluene and 5 cm^3 tributylamine (Figure S2) giving deep brown clear homogenous solution (c_{Br} = 0.207 mol/dm^3, c_{Mg} = 0.212 mol/dm^3) (Figure S2 C). Solution was stored at 190K to prevent thermal disproportionation.

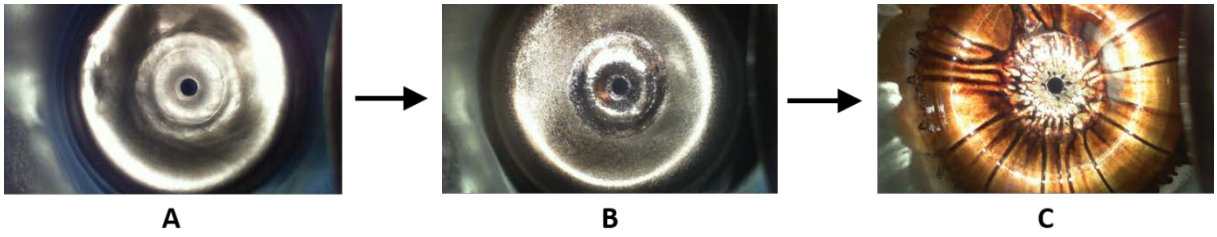
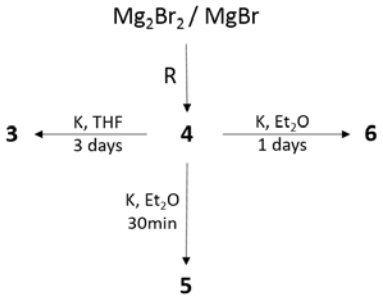


Figure S2 – The result of the MgBr cocondensation process: **A-** solid MgBr/NBu_3/toluene matrix, **B** – melting of the matrix, **C** – MgBr solution.

3. Synthesis

All the compounds presented in the text were obtained according to the Scheme S1.



Scheme S1

Synthetic details:

4 $[(L^1MgBr)_2]$

At the temperature of 195 K 30 cm^3 of freshly obtained MgBr solution was added to the solid R and stirred for about half an hour. Changing of the colour from brown to red was observed. After that time reaction the mixture was slowly heated to room temperature and stirred overnight. Next day all volatile substances were removed at a reduced pressure and the solid residue was extracted with pentane giving red crystals after two days. (1.526g, 1.5mmol, 24% [first fraction]); Anal. Calc. for $C_{56}H_{80}Br_2Mg_2N_4$: C 66.09, H 7.92, N 5.50; Found : C65.73, H 8.11, N 5.23; Raman spectra (crystals in glass capillary): υ = 3059(w), 3024 (m), 2931(s), 2867(m), 1590(s), 1494(w), 1443(s), 1378(m), 1351(s), 1240(s), 1159(w), 1104(w), 1042(w), 889(m), 739(w), 703(w), 627(w), 594(m), 450(m), 364(w), 280(w), 165(m), 115(m) cm^{-1}; MS (70eV) m/z (%): 405 (29) $[DipDAB^+]$, 509 (37) $[½M^+]$, 1017 (0.37) $[M^+]$

4' $[(L^1MgCl)_2]$

$[(L^1MgCl)_2 \cdot THF \cdot C_6H_{14}]$ was obtained like **4** but after removing of all volatile substances solid residue was dissolved in a mixture of hexane and THF from which crystals were obtained after a few days.

3 $[K(thf)_3]_2[L^1MgMgL^1]$

25 mg of potassium was placed together with 70 mg of **4** in a two-vessel ampoule. Directly over this solid THF was condensed giving light red solution. Sealed ampoule was placed in ultrasonic bath and the reaction was continued for 3 days. After this time the solution was decanted from the white powder and the solvent was slowly evaporated in one day giving orange crystals suitable for X-ray diffraction.

^{1}H NMR (THF-D_8, 296K, 300 MHz,) δ = 6.89 – 6.59 (12 H, m), 3.93 – 3.79 (8 H, m), 3.58 (28 H, brm), 1.77 (12 H, s), 1.41 (28 H, brm), 1.14(24 H, m), 1.05 (24 H, m) ppm

5 $[KMg(Et_2O)_2L^1]$

Was obtained under the same conditions as **3** in Et_2O as a solvent. After 30 minutes in ultrasonic bath solution changed its colour and white precipitation was observed. Solid was separated by decantation and the clear solution was used for crystallisation. The next day yellow crystals were obtained.

^{1}H NMR (THF-D_8, 296K, 300 MHz,) δ = 7.14 – 6.87 (6 H, m, Ar**H**), 3.53 – 3.44 (4 H, m, C**H**Me_2), 3.39 (8 H, q, OC**H**$_2$Me), 1.77 (6 H, s, C**CH**$_3$), 1.21 (24 H, d, CH**Me**$_2$), 0.90 (12 H, t, OCH_2C**H**$_3$) ppm

MS (70eV) m/z (%):405 (7) $[DipDAB^+]$, 578 (0.02)$[KMg(Et_2O)_2L^1]$

6 $[K_2Mg(Et_2O)L^1(OEt)_2]$

Was obtained like **5** but the reaction time was elongated to one day. Crystallisation conditions were the same.

^{1}H NMR (THF-D_8, 296K, 300 MHz,) δ = 7.20 – 6.91 (6 H, m, Ar**H**), 3.85 (4 H, brs, MgOC**H**$_2$), 3.53 – 3.44 (4 H, m, C**H**Me_2), 3.38 (4 H, q, OC**H**$_2$Me), 1.78 (6 H, s, CC**H**$_3$), 1.20 (24 H, brm, CH**Me**$_2$), 1.12 (6 H, t, $MgOCH_2$C**H**$_3$), 0.91 (6 H, t, OCH_2C**H**$_3$) ppm

MS (70eV) m/z (%):405 (1) [$DipDAB^+$], 428 (0.5) [$MgDipDAB^+$],

Reduction of **4** in dimethoxyethane was performed as well but no crystals were obtained.

4. Crystal structures

Experimental diffraction data were collected on IPDS II 2-circle goniometer diffractometer, equipped with an imaging plate detector. Enhanced X-ray MoK_α radiation source with a graphite monochromator was used. Data collection was carried out at 150 K. Numerical absorption correction (selected measurements) was performed using STOE IPDS software. Structures were solved by direct methods and non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least squares procedure based on F^2. All hydrogen atoms were refined using isotropic model. Solutions and refinements were carried out using the SHELX–97 program package.[3]

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication: CCDC1025302 (**6**); CCDC1025303 (**4'**); CCDC1025304 (**4**); CCDC1025305 (**5**). Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: (+44) 1223-336-033; E-mail: deposit@ccdc.cam.ac.uk)

Each unit cell of **4'** contains one molecule of heptane and one of THF. Solvents are highly disordered and the acceptable disorder model was not found. To solve this problem, a Squeeze procedure was applied.[4]

Table S1- Crystallographic parameters of the obtained structures.

	3	**4**	**4'**	**5**	**6**
empirical formula	$C_{88}H_{144}K_2Mg_2N_4O_8$	$C_{56}H_{80}Mg_2N_4Br_2$	$C_{66}H_{102}Mg_2O_1N_4Cl_2$	$C_{36}H_{60}MgN_2O_2$	$C_{36}H_{60}K_2MgN_2O_3$
M_r	1512.88	1017.68	1087.078	577.17	671.37
T [K]	150(2)	150(2)	150(2)	150(2)	150(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
crystal system	triclinic	monoclinic	monoclinic	orthorhombic	monoclinic
space group	P -1	$P\,2_1/n$	C 2/m	P bca	$P\,2_1/n$
a [Å]	13.009(3)	14.183(3)	18.096(4)	16.250(3)	12.690(3)
b [Å]	13.266(3)	14.692(3)	18.733(4)	16.383(3)	20.959(4)
c [Å]	15.467(3)	14.201(3)	11.813(2)	26.392(5)	14.541(3)
α [deg]	104.90(3)	90.00	90.00	90	90.00
β [deg]	100.42(3)	108.37(3)	123.10(3)	90	97.25(3)
γ [deg]	115.55(3)	90.00	90.00	90	90.00
V [Å^3]	2193.0(10)	2808.3(10)	3354.7(16)	7026(2)	3836.6(13)
Z	1	2	2	8	4
crystal description	block	block	block	block	plate
crystal colour	orange	red	red	orange	orange
crystal dimensions max/mid/min [mm]	0.334/0.3/0.102	0.135/0.135/0.099	0.110/0.101/0.086	0.419/0.397/0.139	0.34/0.298/0.174
ρ_{calcd} [Mg m^{-3}]	1.146	1.203	0.919	1.091	1.162
μ [mm^{-1}]	0.176	1.503	0.147	0.082	0.297
Absorption corrections	numerical	numerical	none	none	numerical
F(000)	826	1076	1004	2544	1456
Θ (range) [deg]	1.834-26.068	2.05-28.278	1.728-26.703	1.543- 26.215	1.714-27.255
Index ranges	-16<h<16	-18<h<15	-22<h<22	-18<h<19	-16<h<16
	13<k<-16	-19<k<19	-23<k<23	-20<k<19	-26<k<26
	-17<l<18	-17<l<18	-14<14	-32<l<32	-18<l<18
Reflections collected / unique	28693/4093	23155/3743	14206/3230	107312/4389	50076/4805
R_{int}	0.1121	0.0776	0.0553	0.1001	0.1222
R_1 $(F_0>4\sigma(F_0))$	0.0727	0.0622	0.0458	0.0483	0.0597
wR_2 *(all data)*	0.1999	0.1265	0.1491	0.1080	0.1558
ρ(min/max) [e Å^{-3}]	-0.589/0.790	-0.581/0.060	-0.260/0.045	-0.192/0.347	-0.480-0.058

CCDC	see ref.[2]	1025304	1025303	1025305	1025302

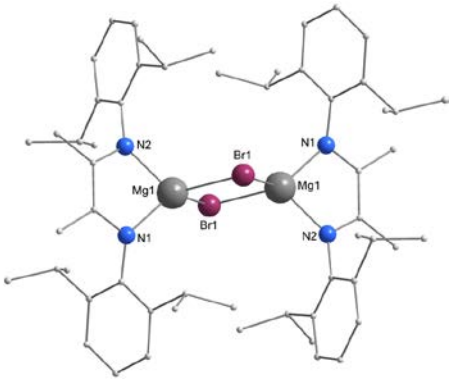


Figure S3 - Molecular structures of **4** in the crystal (H atoms omitted for clarity). Selected bond lengths, distances and angles ([Å]/[°]): Mg1–N1 1.97(1), Mg1–N2 2.015(9), Mg1–Br1 2.527(1), Mg1···Mg1 3.359(2); Mg1–Br1–Mg1 83.35(4), Br1–Mg1–Br1 96.65(4).

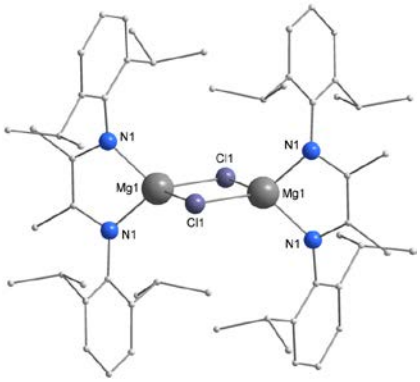


Figure S4 - Molecular structures of **4'** in the crystal (H atoms omitted for clarity). Selected bond lengths, distances and angles ([Å]/[°]): Mg1–N1 2.013(1), Mg1–Cl1 2.373(1), Mg1···Mg1 3.200(2); Mg1–Cl1–Mg1 85.21(3), Cl1–Mg1–Cl1 94.79(3).

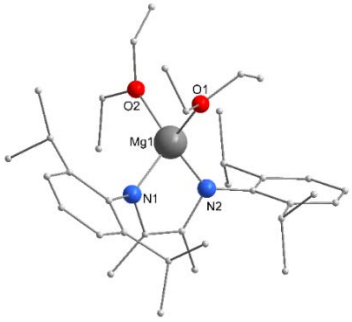


Figure S5 - Molecular structures of **5** in the crystal (H atoms omitted for clarity). Selected bond lengths, distances and angles ([Å]/[°]): Mg1–N1 1.9864(15), Mg1–N2 1.9665(16), Mg1–O1 2.0426(15), Mg1–O2 2.0562(13); N2–Mg1–N1 88.68(7), O1–Mg1–O2 98.98(6), N1–Mg1–O2 117.53(6), N2–Mg1–O1 121.13(6).

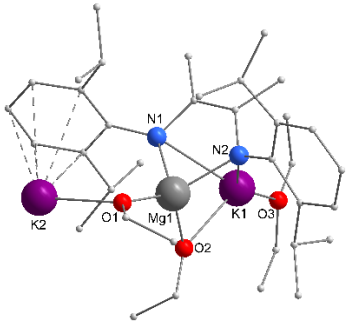


Figure S6 - Molecular structures of **6** in the crystal (H atoms omitted for clarity). Selected bond lengths, distances and angles ([Å]/[°]): K2–O1 2.5758(19), K1–N2 2.873(2), K1–O2 2.5834(19), K1–N1 2.879(2), K1–O3 2.618(2), Mg1–N1 2.065(2), N2–Mg1 2.086(2), O1–Mg1 1.904(2), O2–Mg1 1.907(2); K2–O1–Mg1 107.87(8), N1–Mg1–N2 82.27(8), O1–Mg1–O2 115.38(9), Mg1–O2–K1 85.75(7), N1–K1–N2 56.69(6), O2–K1–O3 129.92(6).

5. Quantum chemical calculations

Theoretical investigations based on DFT methods were performed using the Turbomole[5, 6] software package. The geometries of all molecules were optimized using the B3-LYP functional (also BP86, see below, section 6). Established basis sets for all atoms excluding Mg were of DZP quality from the standard Turbomole basis-set library. For magnesium the basis set contains a McLean–Chandler contraction (12s9p/6s5p) as well as a d-type polarization function (η_d(Mg)=0.175).[7]

Table S2- Calculated energies of compounds mentioned in text (R = L^1).

compound	symetry	E[H]	homo-lumo gap [eV]	most important distances
$(MgL^2)_2$	C_1	-2878.78	3.57	Mg-Mg 2.93
$MgL^2{}_2$	C_1	-2678.64	4.24	Mg-N 2.17
BrMgR	C_1	-3974.86	2.25	Mg-N 2.05 Mg-Br 2.39
MgBr	C_{6v}	-2774.27	2.30	Mg-Br 2.66
R	C_1	-1200.51	4.11	
thf	C_1	-232.43	8.05	
Mg_2Br_2	C_{2v}	-5548.62	4.75	Mg-Br 2.36 Mg-Mg 2.78
$(BrMgR)_2$	C_1	-7949.81	2.18	Mg-Br 2.59 N-Mg 2.06
KBr	C_{6v}	-3174.13	2.99	
$[K(thf)_3]_2[Mg_2R_2]$	C_i	-5395.91	2.07	Mg-Mg 2.99
MgR	C_1	-1400.62	1.41	Mg-N 2.06
MgKR	C_1	-2000.59	1.91	Mg-N 2.06 KN 2.94
BrMg(KR)	C_1	-4574.84	2.29	Br-Mg 2.40 Mg-N 2.01
R^{2-}	C_1	-12.3926	3.83	
$Mg_2Cp^*{}_2$	D_{5h}	-1180.41	4.74	Mg-Mg 2.78
Br^-	C_1	-2574.18	19.45	
Cp^{*-}	C_{5v}	-390.07	4.71	
Na	*Oh*	-162.28	1.69	
NaR	C^1	-1362.81	2.29	Na-N 2.25
$MgRR^2$	C^1	-2639.85	2.22	Mg-N 2.25-2.26

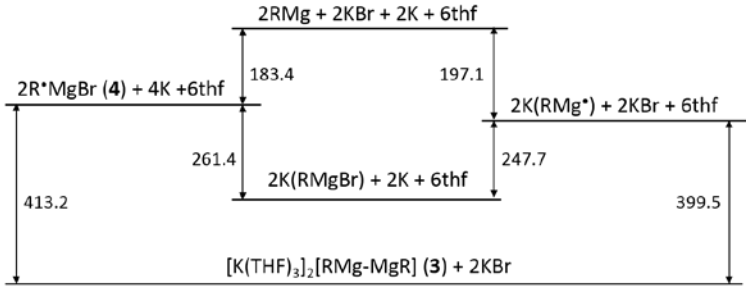


Figure S7 - Calculated energy diagram (kJmol^{-1}) of the gaseous compounds during the formation of **3** (R = L^1).

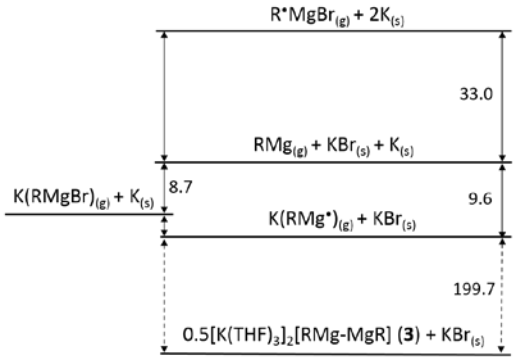


Figure S8 - Calculated energy diagram (kJmol^{-1}) of the possible intermediates on the way to **3** (THF omitted for clarity) (R=L^1)

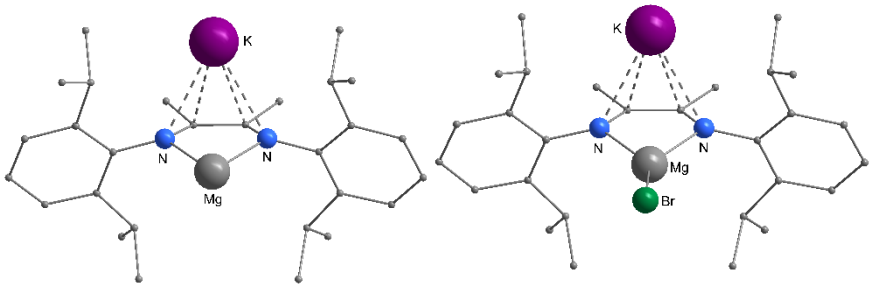


Figure S9 – Optimized structures of the proposed intermediates in a formation of a Mg-Mg bond in **4.**

6. EPR spectroscopic investigations

All spectra were recorded on a Bruker EMXplus cw-X-band spectrometer (microwave frequency: 9.43 GHz) with a liquid nitrogen cooling system for measurements at 100 K attached. The samples were weighted into sealable EPR tubes, the solvent was vacuum transferred onto the solid samples and the tubes were sealed under vacuum subsequently. Simulations were performed using the MATLAB/easyspin program package.[9] The parameters for the simulation of the spectra are given in Table S3. The model used for the simulation of **4** in 2-Methyltetrahydrofurane (MeTHF) consists of an isotropic *g*-tensor along with two equivalent nitrogen and six hydrogen nuclei belonging to the N=C entities and methyl groups in the backbone of the ligand system, respectively. Couplings to bromine (I = 3/2, n.a.(^{79}Br) = 50.69%, n.a.(^{81}Br) = 49.31%) and magnesium (I = 5/2, n.a.(^{25}Mg) = 10%) were added in order to properly fit the simulated spectrum to the experimental one (*cf.* Fig. S10/11). We are aware that the hyperfine coupling to the magnesium clearly falls below the natural line width of the spectrum, but the change of the spectral shape becomes evident, when comparing the two different simulation models (see Fig. S11). In order to compare the spectra obtained for **4** in MeTHF with the singly reduced ligand (L^1), we also freshly prepared [Na(L^1)$^\bullet$] from sodium metal and the neutral ligand in THF (Fig. S12). It immediately becomes apparent that the spectrum considerably changes upon coordination of the MgBr entity. In particular, the dominant central line for [Na(L^1)$^\bullet$] is missing in the EPR spectrum of **4**. An inclusion of bromine isotopes to the simulation (I = 3/2), though with a very small coupling constant of ca. 5 MHz (i.e. below 1% spin density), was inevitably necessary for the successful simulation. Further inclusion of magnesium (also below 1 % spin density) provided further improvements.

Table S3 - Parameters obtained from the simulations of the spectra. Hyperfine couplings A are given in MHz.

	4 (MeTHF)[a]	[Na(L^1)] (THF)
g_{iso}	2.00203	2.0023
A_{iso}(^{14}N)	19.4	15.2
A_{iso}(^{1}H)	13.3	15.3
A_{iso}($^{79/81}$Br)	5.5	-
A_{iso}(^{25}Mg)	2.3	-

Line widths: 0.12 mT for **4** and 0.142 mT for [Na(L^1)]
[a] We used 4MeTHF instead of THF because we have strong spectral evidences that samples of **4** in THF do not form a proper glass.

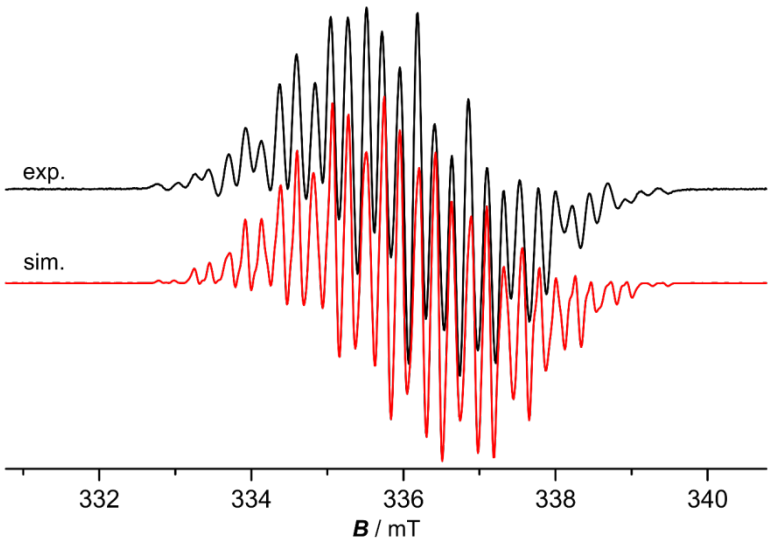


Figure S10 - Experimental (black) and simulated (red) spectrum of **4** in MeTHF at room temperature. The parameters for the simulation are given in Table S3.

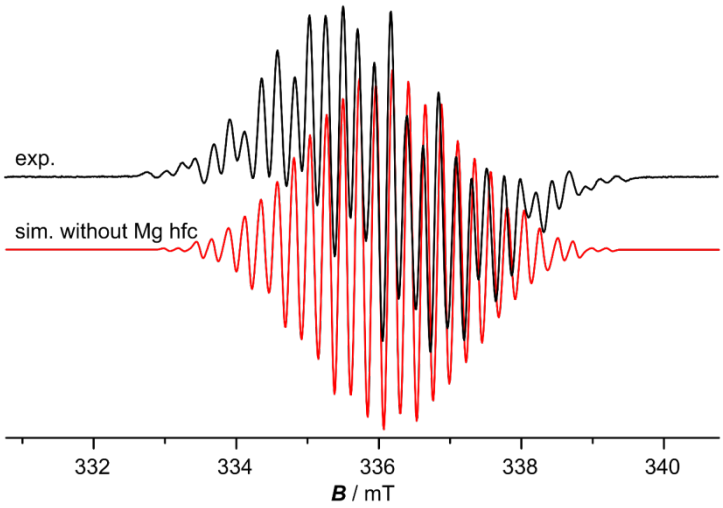


Figure S11 - Comparison of the experimental (black) and simulated spectrum without Magnesium hyperfine interaction (red). The parameters used for the calculation of the spectra are given in Table S3.

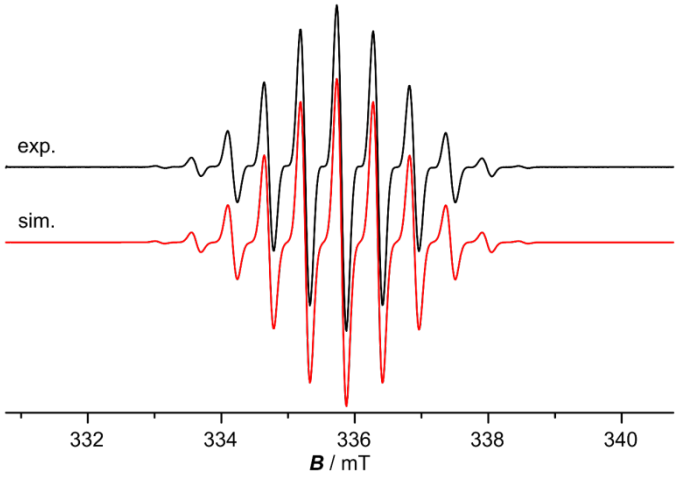


Figure S12 - Experimental (black) and simulated spectrum of [Na(L^1)] in THF at room temperature. The parameters used for the calculation of the spectrum are given in Table S3.

For the simulation of the spectrum of **4** acquired in frozen toluene solution at 100K, we applied the dipole interaction *via* $S^T DS$ with the largest coupling in z-direction, as the criterion for strongly coupled pairs does not apply in this case, see Fig. S13. Due to the large line width of the spectrum, we did not obtain certain values for the nitrogen and hydrogen hyperfine coupling constants, as they fall clearly below the line width. Therefore, we used the values obtained from the simulation of **4** in MeTHF solution.

Table S4 - Parameters for the spectrum of **4** in frozen toluene solution at 100K. Line width: x = 25 MHz, y = 35 MHz, z = 25 MHz. Hyperfine coupling constants A are given in MHz. The dipolar coupling constant D is given in MHz.

	4 (toluene, 100K)
g_1, g_2, g_3	2.0021, 2.0025, 2.0041
A (^{14}N)	<10, 20, <10
D	100±10

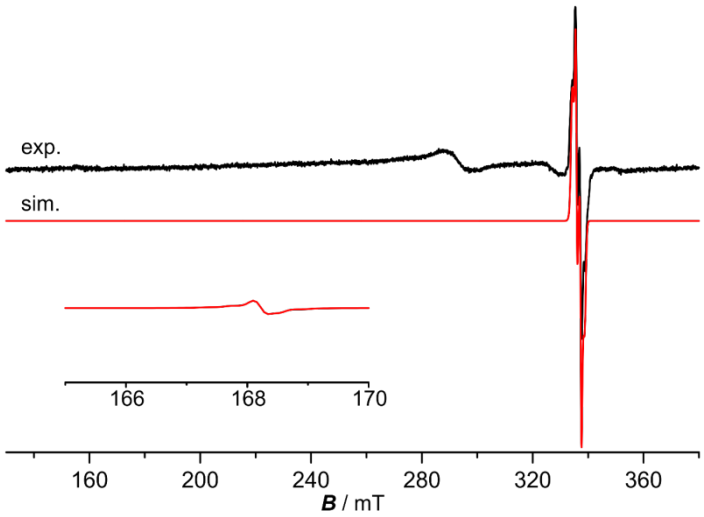


Figure S13 - Experimental (*black*) and simulated (*red*) spectrum of **4** in frozen toluene solution at 100K. The inset shows the region of the expected half-field signal of the simulated spectrum (*red*, magnification: 50x). Note that due to the very small intensity of this $\Delta m_s = \pm 2$ transition, an experimental observation was not possible (covered with background noise). Parameters for the simulation are given in Table S4.

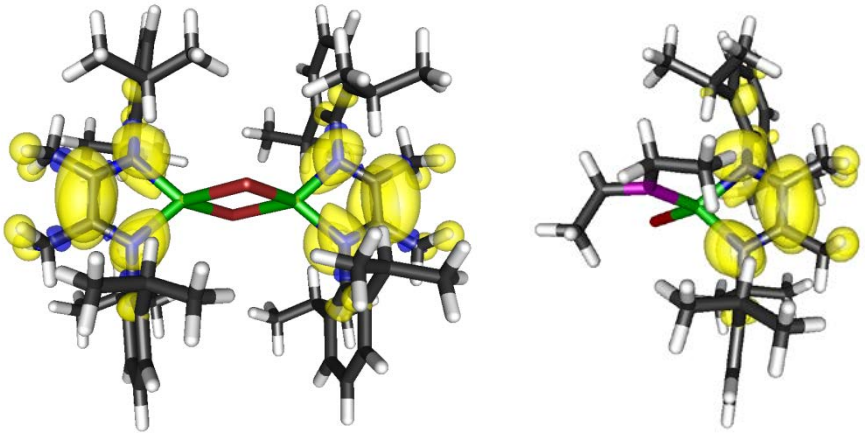


Figure S14 – Calculated spin density of **4** (dimer, left, and monomer, right, Et_2O as solvent) at the BP86/def2-TZVP level. Compilations of the atomic spin density calculations are provided at the end of the ESI.

Notes and references

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atomic populations from spin density for monomeric **4**, solvated by one Et_2O solvent molecule (nitrogen and carbon atoms of the dad entity are highlighted in yellow):

atomic populations from spin density:

atom	sum	n(s)	n(p)	n(d)	n(f)	n(g)
1 h	-0.00019	-0.00019	0.00000	0.00000	0.00000	0.00000
2 h	0.00024	0.00023	0.00000	0.00000	0.00000	0.00000
3 h	0.00004	0.00003	0.00001	0.00000	0.00000	0.00000
4 c	0.01003	0.00028	0.00973	0.00002	0.00000	0.00000
5 h	0.00015	0.00015	0.00000	0.00000	0.00000	0.00000
6 c	-0.00392	-0.00026	-0.00367	0.00001	0.00000	0.00000
7 h	0.00086	0.00086	0.00000	0.00000	0.00000	0.00000
8 c	0.00035	0.00013	0.00021	0.00001	0.00000	0.00000
9 h	-0.00001	-0.00001	-0.00000	0.00000	0.00000	0.00000
10 c	-0.00013	-0.00003	-0.00014	0.00004	0.00000	0.00000
11 c	-0.00175	0.00065	-0.00247	0.00006	0.00000	0.00000
12 h	0.00017	0.00017	0.00000	0.00000	0.00000	0.00000
13 h	-0.00004	-0.00004	-0.00000	0.00000	0.00000	0.00000
14 h	-0.00001	-0.00001	0.00000	0.00000	0.00000	0.00000
15 c	0.01523	0.00210	0.01300	0.00012	0.00001	0.00000
16 c	0.00715	0.00072	0.00608	0.00035	-0.00000	0.00000
17 h	-0.00003	-0.00003	0.00000	0.00000	0.00000	0.00000
18 c	0.01921	0.00337	0.01570	0.00013	0.00001	0.00000
19 c	-0.00218	-0.00065	-0.00200	0.00047	0.00000	0.00000
20 h	0.00057	0.00040	0.00017	0.00000	0.00000	0.00000
21 h	0.00074	0.00074	0.00001	0.00000	0.00000	0.00000
22 h	0.00031	0.00031	-0.00000	0.00000	0.00000	0.00000
23 h	0.00029	0.00029	0.00000	0.00000	0.00000	0.00000
24 c	0.00022	0.00007	0.00016	-0.00001	0.00000	0.00000
25 h	0.01065	0.01064	0.00001	0.00000	0.00000	0.00000
26 c	-0.00048	-0.00019	-0.00038	0.00009	0.00001	0.00000
27 c	-0.00359	-0.00120	-0.00332	0.00093	0.00000	0.00000
28 h	-0.00005	-0.00005	0.00000	0.00000	0.00000	0.00000
29 h	0.00001	-0.00000	0.00001	0.00000	0.00000	0.00000
30 h	0.00003	0.00003	0.00000	0.00000	0.00000	0.00000
31 c	-0.00012	-0.00002	-0.00015	0.00004	0.00000	0.00000
32 n	0.23734	0.00645	0.23091	0.00002	-0.00005	0.00000
33 h	0.01259	0.01254	0.00005	0.00000	0.00000	0.00000
34 h	-0.00004	-0.00006	0.00002	0.00000	0.00000	0.00000
35 h	0.00002	0.00002	-0.00000	0.00000	0.00000	0.00000
36 h	0.00166	0.00154	0.00012	0.00000	0.00000	0.00000
37 h	0.00076	0.00076	-0.00000	0.00000	0.00000	0.00000
38 h	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000
39 c	0.19797	0.00358	0.19078	0.00364	-0.00003	0.00000
40 c	0.00040	0.00019	0.00016	0.00005	0.00000	0.00000
41 h	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
42 c	0.00044	0.00014	0.00028	0.00001	-0.00000	0.00000
43 c	0.00069	0.00045	0.00021	0.00003	0.00000	0.00000
44 o	0.00207	0.00083	0.00124	0.00000	0.00000	0.00000
45 br	0.00436	0.00009	0.00442	-0.00014	-0.00000	0.00000
46 h	0.00006	0.00006	0.00000	0.00000	0.00000	0.00000
47 h	0.00003	0.00003	0.00000	0.00000	0.00000	0.00000
48 mg	0.02161	-0.00075	0.01683	0.00554	0.00000	0.00000
49 h	-0.00000	-0.00000	-0.00000	0.00000	0.00000	0.00000
50 c	-0.00000	-0.00001	0.00000	0.00000	0.00000	0.00000
51 h	0.00031	0.00031	0.00000	0.00000	0.00000	0.00000
52 c	0.17424	0.00331	0.16768	0.00333	-0.00008	0.00000
53 h	0.00904	0.00901	0.00003	0.00000	0.00000	0.00000
54 h	-0.00001	-0.00001	0.00000	0.00000	0.00000	0.00000
55 h	-0.00022	-0.00041	0.00019	0.00000	0.00000	0.00000
56 h	0.00005	0.00005	-0.00000	0.00000	0.00000	0.00000
57 c	-0.00237	-0.00077	-0.00279	0.00119	-0.00000	0.00000
58 n	0.24421	0.00651	0.23770	0.00005	-0.00005	0.00000
59 h	0.00011	0.00011	0.00000	0.00000	0.00000	0.00000
60 h	0.01283	0.01280	0.00002	0.00000	0.00000	0.00000

61 h	0.00009	0.00009	0.00000	0.00000	0.00000	0.00000
62 c	0.00059	0.00018	0.00033	0.00007	0.00000	0.00000
63 h	0.00037	0.00038	-0.00001	0.00000	0.00000	0.00000
64 c	0.00266	0.00027	0.00215	0.00024	-0.00000	0.00000
65 h	0.00043	0.00035	0.00008	0.00000	0.00000	0.00000
66 c	0.00007	0.00003	0.00000	0.00003	0.00000	0.00000
67 h	0.00001	0.00001	-0.00000	0.00000	0.00000	0.00000
68 h	0.00006	0.00005	0.00000	0.00000	0.00000	0.00000
69 h	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000
70 c	-0.00086	-0.00046	-0.00136	0.00095	0.00001	0.00000
71 h	0.00013	0.00013	0.00000	0.00000	0.00000	0.00000
72 h	0.00005	0.00005	-0.00000	0.00000	0.00000	0.00000
73 c	0.01204	0.00295	0.00890	0.00018	0.00001	0.00000
74 c	0.00010	-0.00000	0.00011	0.00000	0.00000	0.00000
75 c	0.00004	0.00003	-0.00030	0.00031	-0.00000	0.00000
76 h	0.00001	0.00001	-0.00000	0.00000	0.00000	0.00000
77 c	0.01018	0.00255	0.00754	0.00009	0.00001	0.00000
78 h	0.00027	0.00026	0.00001	0.00000	0.00000	0.00000
79 c	0.00023	0.00008	0.00006	0.00009	0.00000	0.00000
80 h	-0.00001	-0.00001	0.00000	0.00000	0.00000	0.00000
81 c	0.00020	0.00023	-0.00008	0.00005	0.00000	0.00000
82 h	0.00057	0.00057	0.00000	0.00000	0.00000	0.00000
83 h	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000
84 c	-0.00034	0.00016	-0.00050	0.00000	0.00000	0.00000
85 c	0.00100	0.00002	0.00101	-0.00003	0.00000	0.00000
86 h	0.00021	0.00020	0.00000	0.00000	0.00000	0.00000
87 h	-0.00005	-0.00005	0.00000	0.00000	0.00000	0.00000

atomic populations from spin density for dimeric **4** (nitrogen and carbon atoms of the dad subunits are highlighted in yellow):

atom	sum	n(s)	n(p)	n(d)	n(f)	n(g)
1 h	0.00007	0.00006	0.00000	0.00000	0.00000	0.00000
2 h	0.00031	0.00031	0.00000	0.00000	0.00000	0.00000
3 h	-0.00004	-0.00004	0.00000	0.00000	0.00000	0.00000
4 h	-0.00004	-0.00004	0.00000	0.00000	0.00000	0.00000
5 h	0.00006	0.00006	0.00000	0.00000	0.00000	0.00000
6 c	0.00017	0.00004	0.00011	0.00003	-0.00000	0.00000
7 h	0.00006	0.00006	-0.00000	0.00000	0.00000	0.00000
8 h	-0.00002	-0.00002	-0.00000	0.00000	0.00000	0.00000
9 c	-0.00041	0.00003	-0.00045	0.00001	0.00000	0.00000
10 c	0.00110	0.00002	0.00108	-0.00001	-0.00000	0.00000
11 c	0.00070	0.00001	0.00070	-0.00001	-0.00000	0.00000
12 h	0.00030	0.00029	0.00001	0.00000	0.00000	0.00000
13 h	0.00051	0.00050	0.00000	0.00000	0.00000	0.00000
14 h	0.00009	0.00009	0.00000	0.00000	0.00000	0.00000
15 c	-0.00004	-0.00000	-0.00006	0.00002	0.00000	0.00000
16 c	-0.00019	0.00006	-0.00026	0.00001	0.00000	0.00000
17 c	0.00366	0.00032	0.00303	0.00031	-0.00000	0.00000
18 c	0.01020	0.00261	0.00757	0.00001	0.00001	0.00000
19 c	0.00009	0.00031	-0.00024	0.00002	0.00000	0.00000
20 h	0.00052	0.00051	0.00000	0.00000	0.00000	0.00000
21 c	0.00004	0.00032	-0.00030	0.00002	0.00000	0.00000
22 h	0.00005	0.00005	-0.00000	0.00000	0.00000	0.00000
23 h	-0.00002	-0.00002	0.00000	0.00000	0.00000	0.00000
24 h	-0.00006	-0.00005	-0.00001	0.00000	0.00000	0.00000
25 h	0.00007	0.00006	0.00000	0.00000	0.00000	0.00000
26 h	-0.00005	-0.00028	0.00023	0.00000	0.00000	0.00000
27 h	-0.00009	-0.00009	-0.00000	0.00000	0.00000	0.00000
28 h	0.01180	0.01178	0.00002	0.00000	0.00000	0.00000
29 h	0.00010	0.00010	-0.00000	0.00000	0.00000	0.00000
30 c	-0.00192	-0.00075	-0.00231	0.00113	0.00001	0.00000
31 c	0.01125	0.00264	0.00854	0.00006	0.00001	0.00000
32 c	-0.00412	-0.00088	-0.00427	0.00102	0.00000	0.00000
33 c	-0.00004	0.00000	-0.00006	0.00001	0.00000	0.00000
34 c	0.00991	0.00260	0.00717	0.00012	0.00001	0.00000
35 h	0.00011	0.00011	-0.00000	0.00000	0.00000	0.00000
36 h	-0.00001	-0.00002	0.00000	0.00000	0.00000	0.00000
37 c	0.01112	0.00265	0.00828	0.00018	0.00001	0.00000

38 h	0.01319	0.01317	0.00003	0.00000	0.00000	0.00000
39 h	0.00008	0.00008	0.00000	0.00000	0.00000	0.00000
40 c	0.00019	0.00003	0.00013	0.00004	0.00000	0.00000
41 c	0.00034	0.00009	0.00027	-0.00002	-0.00000	0.00000
42 h	0.00053	0.00053	0.00000	0.00000	0.00000	0.00000
43 c	0.00334	0.00030	0.00275	0.00030	-0.00000	0.00000
44 c	0.00013	-0.00000	0.00010	0.00003	0.00000	0.00000
45 h	0.00016	0.00016	0.00000	0.00000	0.00000	0.00000
46 h	0.00006	0.00006	-0.00000	0.00000	0.00000	0.00000
47 h	-0.00001	-0.00001	-0.00000	0.00000	0.00000	0.00000
48 c	0.00012	-0.00000	0.00010	0.00003	0.00000	0.00000
49 c	-0.00186	-0.00075	-0.00218	0.00107	0.00001	0.00000
50 h	-0.00006	-0.00006	-0.00000	0.00000	0.00000	0.00000
51 c	-0.00019	0.00002	-0.00059	0.00038	0.00000	0.00000
52 h	0.00062	0.00062	0.00000	0.00000	0.00000	0.00000
53 h	0.00009	0.00009	-0.00000	0.00000	0.00000	0.00000
54 h	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
55 n	0.23782	0.00585	0.23180	0.00023	-0.00005	0.00000
56 c	-0.00012	0.00012	-0.00056	0.00032	0.00000	0.00000
57 c	0.19351	0.00347	0.18614	0.00397	-0.00008	0.00000
58 h	0.00008	0.00008	0.00000	0.00000	0.00000	0.00000
59 h	-0.00001	-0.00025	0.00024	0.00000	0.00000	0.00000
60 c	0.00030	0.00004	0.00028	-0.00002	-0.00000	0.00000
61 h	0.00015	0.00015	0.00000	0.00000	0.00000	0.00000
62 h	-0.00008	-0.00008	-0.00001	0.00000	0.00000	0.00000
63 h	-0.00003	-0.00005	0.00002	0.00000	0.00000	0.00000
64 h	-0.00029	-0.00030	0.00001	0.00000	0.00000	0.00000
65 h	0.01214	0.01211	0.00002	0.00000	0.00000	0.00000
66 n	0.23678	0.00582	0.23080	0.00021	-0.00005	0.00000
67 br	0.01183	0.00195	0.01010	-0.00022	0.00000	0.00000
68 h	0.01299	0.01296	0.00002	0.00000	0.00000	0.00000
69 h	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
70 c	0.19438	0.00353	0.18703	0.00390	-0.00008	0.00000
71 c	-0.00412	-0.00087	-0.00431	0.00105	0.00000	0.00000
72 c	-0.00412	-0.00086	-0.00431	0.00105	0.00000	0.00000
73 mg	0.03276	-0.00067	0.02718	0.00625	0.00000	0.00000
74 h	0.01296	0.01294	0.00002	0.00000	0.00000	0.00000
75 h	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
76 c	0.19432	0.00353	0.18697	0.00389	-0.00008	0.00000
77 h	0.01214	0.01212	0.00002	0.00000	0.00000	0.00000
78 mg	0.03276	-0.00067	0.02717	0.00626	0.00000	0.00000
79 h	0.00008	0.00008	0.00000	0.00000	0.00000	0.00000
80 h	-0.00008	-0.00008	-0.00001	0.00000	0.00000	0.00000
81 h	-0.00004	-0.00005	0.00002	0.00000	0.00000	0.00000
82 n	0.23674	0.00581	0.23076	0.00021	-0.00005	0.00000
83 h	-0.00029	-0.00029	0.00001	0.00000	0.00000	0.00000
84 br	0.01186	0.00196	0.01013	-0.00022	0.00000	0.00000
85 h	0.00009	0.00009	0.00000	0.00000	0.00000	0.00000
86 c	0.00030	0.00004	0.00028	-0.00002	-0.00000	0.00000
87 h	0.00015	0.00015	0.00000	0.00000	0.00000	0.00000
88 h	0.00061	0.00061	0.00000	0.00000	0.00000	0.00000
89 h	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
90 h	-0.00001	-0.00025	0.00024	0.00000	0.00000	0.00000
91 c	0.00013	-0.00000	0.00010	0.00003	0.00000	0.00000
92 c	-0.00012	0.00012	-0.00056	0.00032	0.00000	0.00000
93 h	-0.00006	-0.00006	-0.00000	0.00000	0.00000	0.00000
94 c	0.00012	-0.00000	0.00009	0.00003	0.00000	0.00000
95 c	-0.00020	0.00002	-0.00059	0.00038	0.00000	0.00000
96 c	0.19357	0.00347	0.18620	0.00397	-0.00008	0.00000
97 h	-0.00001	-0.00001	-0.00000	0.00000	0.00000	0.00000
98 h	0.00006	0.00006	-0.00000	0.00000	0.00000	0.00000
99 h	0.00053	0.00053	0.00000	0.00000	0.00000	0.00000
100 n	0.23782	0.00585	0.23179	0.00023	-0.00005	0.00000
101 c	0.00034	0.00009	0.00027	-0.00002	-0.00000	0.00000
102 c	-0.00186	-0.00075	-0.00218	0.00107	0.00001	0.00000
103 h	0.00016	0.00016	0.00000	0.00000	0.00000	0.00000
104 h	0.00011	0.00011	-0.00000	0.00000	0.00000	0.00000
105 h	0.01319	0.01316	0.00003	0.00000	0.00000	0.00000
106 c	0.00019	0.00003	0.00013	0.00003	0.00000	0.00000

107 c	0.00334	0.00030	0.00274	0.00030	-0.00000	0.00000
108 h	0.00010	0.00010	-0.00000	0.00000	0.00000	0.00000
109 c	0.01111	0.00265	0.00827	0.00018	0.00001	0.00000
110 h	0.00008	0.00008	0.00000	0.00000	0.00000	0.00000
111 c	-0.00412	-0.00088	-0.00426	0.00102	0.00000	0.00000
112 h	-0.00009	-0.00009	-0.00000	0.00000	0.00000	0.00000
113 c	0.00992	0.00260	0.00719	0.00012	0.00001	0.00000
114 c	0.01124	0.00264	0.00853	0.00006	0.00001	0.00000
115 h	-0.00001	-0.00001	0.00000	0.00000	0.00000	0.00000
116 h	0.01183	0.01181	0.00002	0.00000	0.00000	0.00000
117 c	-0.00004	0.00000	-0.00006	0.00001	0.00000	0.00000
118 c	-0.00192	-0.00075	-0.00230	0.00113	0.00001	0.00000
119 h	0.00007	0.00006	0.00000	0.00000	0.00000	0.00000
120 h	-0.00006	-0.00005	-0.00001	0.00000	0.00000	0.00000
121 h	-0.00005	-0.00028	0.00023	0.00000	0.00000	0.00000
122 h	0.00052	0.00051	0.00000	0.00000	0.00000	0.00000
123 c	0.00009	0.00031	-0.00024	0.00002	0.00000	0.00000
124 h	0.00005	0.00005	-0.00000	0.00000	0.00000	0.00000
125 c	0.00004	0.00033	-0.00030	0.00002	0.00000	0.00000
126 h	-0.00002	-0.00002	0.00000	0.00000	0.00000	0.00000
127 h	0.00050	0.00050	0.00000	0.00000	0.00000	0.00000
128 c	-0.00018	0.00006	-0.00025	0.00001	0.00000	0.00000
129 c	0.01018	0.00261	0.00754	0.00001	0.00001	0.00000
130 c	0.00365	0.00033	0.00302	0.00031	-0.00000	0.00000
131 c	-0.00004	-0.00000	-0.00006	0.00002	0.00000	0.00000
132 h	0.00009	0.00009	0.00000	0.00000	0.00000	0.00000
133 c	0.00071	0.00001	0.00071	-0.00001	-0.00000	0.00000
134 h	0.00030	0.00029	0.00001	0.00000	0.00000	0.00000
135 c	0.00107	0.00002	0.00106	-0.00001	-0.00000	0.00000
136 h	-0.00002	-0.00002	-0.00000	0.00000	0.00000	0.00000
137 c	-0.00040	0.00003	-0.00044	0.00001	0.00000	0.00000
138 c	0.00017	0.00004	0.00011	0.00003	-0.00000	0.00000
139 h	0.00006	0.00006	0.00000	0.00000	0.00000	0.00000
140 h	0.00006	0.00006	-0.00000	0.00000	0.00000	0.00000
141 h	-0.00004	-0.00004	0.00000	0.00000	0.00000	0.00000
142 h	-0.00004	-0.00004	0.00000	0.00000	0.00000	0.00000
143 h	0.00031	0.00031	0.00000	0.00000	0.00000	0.00000
144 h	0.00007	0.00006	0.00000	0.00000	0.00000	0.00000