Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

$(thf)_2Ln(Ge_9\{Si(SiMe_3)\}_3)_2$ (Ln = Eu, Sm): the first coordination of germanium metalloid cluster to lanthanides

Svetlana Klementyeva,* Claudio Schrenk, Minghui Zhang, Marat M. Khusniyarov and Andreas Schnepf*

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Experimental Procedures

General Considerations

All manipulations of air-sensitive materials were performed with the rigorous exclusion of oxygen and moisture in flame-dried Schlenk-type glassware either on a dual manifold Schlenk line, interfaced to a high vacuum (10^{-3} torr) line, or in an argon-filled glove box. Elemental analyses were carried out with an Elementar vario MICRO Cube. Tetrahydrofuran was distilled under nitrogen from sodium benzophenoneketyl and degassed before storage over Na/K alloy. *n*-Hexane was distilled under nitrogen from sodium, degassed and stored in vacuo over Na/K alloy. $(thf)_2SmI_2$[1,2], $(thf)_2EuI_2$[2] and KGe_9Hyp_3[3,4] were prepared according to literature procedures.
NMR spectroscopic measurements were performed by using a Bruker AVIIIHD-300 spectrometer. The chemical shifts are given in ppm against the external standard $SiMe_4$. C_6D_6 was dried with Na/K alloy and stored in a glove box under an argon atmosphere. The INEPT pulse program was used for the ^{29}Si NMR spectroscopic experiments.

UV/Vis measurements were performed using a PG Instruments T60 UV/visible spectrophotometer.

X-ray diffraction analysis

Crystals of all compounds were mounted on the diffractometer at 150 K. The data were collected using a Bruker APEX II DUO diffractometer equipped with an IμS microfocus sealed tube and QUAZAR optics for monochromated $Mo_{K\alpha}$ radiation (λ=0.71073 Å) with an Oxford Cryosystems cryostat. A semiempirical absorption correction was applied by using the program SADABS. The structure was solved by direct methods and refined against F2 for all observed reflections; the SHELXS and SHELXL[5] programs were used within the Olex2 program package.[6] The positions of the hydrogen atoms in all compounds were refined using a riding model. In case of $[(thf)_2Eu(Ge_9Hyp_3)_2]$ (**2**), the co crystallized solvent molecules could not be refined properly due to a heavy disorder, so the SQUEEZE program routine implemented in the PLATON program package[7] was used to identify 3 hexane molecules per cluster in a large void of 2560 A³. CCDC 2049433(**2**) and 2049432(**3**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

Magnetic measurements

Magnetic data on microcrystalline samples were collected with a Quantum Design MPMS 3. DC susceptibility data were collected on samples restrained within a polycarbonate gel capsule. Variable-temperature measurements were performed at the applied magnetic field of 0.1 T with 1 K min^{-1} heating rate and 5 K intervals. Magnetic susceptibility data were corrected for sample holder and underlying diamagnetism by using an estimation $\chi_{m,diamag} = 1/2\ M_w \bullet 10^{-6}\ cm^3\ mol^{-1}$, with M_w being the molar mass of the complex.[8] The fits were performed using the program PHI version 3.1.5.[9]

Computational studies

Quantum-chemical calculations were carried out with the RI-DFT version[10] of the Turbomole[11] program package by employing the BP86-functional.[12] The basis sets were of TZVPP quality.[13] The TmoleX client[14] was used as graphical user interface.

Synthesis of $[(thf)_2Eu(Ge_9Hyp_3)_2]$ (2) and $[(thf)_2Sm(Ge_9Hyp_3)_2]$ (3)

$(thf)_2LnI_2$ (1 equiv.) and KGe_9Hyp_3 (2 equiv.) were stirred in THF (20 mL) for 48 h at 85°C. Then THF was removed by evaporation in vacuum and the residue was extracted with *n*-hexane (80 mL) under solvothermal conditions at +85°C for 48 h. The *n*-hexane extract was filtered into a two-section ampule, concentrated to 10 mL under vacuum and flame sealed to grow crystals by slow evaporation. The block-shaped crystals were washed with *n*-hexane and dried in vacuum. The residue after filtration was extracted with *n*-hexane one more time and the second crop of crystals was isolated by the same manner. The isolation of compounds **2** and **3** succeed by the solvothermal extraction with a non-polar solvent like *n*-hexane, which seems to be vital to shift the reaction to the product side as within the primary reaction solution in thf a precipitation of a salt is not observed.
2 (from 42 mg (0.075 mmol) of $(thf)_2EuI_2$ and 215 mg (0.15 mmol) of KGe_9Hyp_3): Orange-brown crystals, first crop 104 mg, second crop 31 mg; yield 135 mg (0.046 mmol; 58%).The reaction mixture was red-orange and the residue was orange-brown in color. Anal. calcd (%) for $C_{62}H_{178}EuGe_{18}O_2Si_{24}$ (3089.46): C 24.10, H 5.81. Found C 23.84, H 5.71.
3 (from 41 mg (0.075 mmol) of $(thf)_2SmI_2$ and 215 mg (0.15 mmol) of KGe_9Hyp_3): Dark-green crystals, first crop 125 mg, second crop 17 mg; yield 142 mg (0.046 mmol; 61%).The reaction mixture was dark brown-green and the residue was brown-greenish in color. Anal. calcd (%) for $C_{62}H_{178}Ge_{18}O_2Si_{24}Sm$ (3087.86): C 24.12, H 5.81.

Found C 24.21, H 5.55. ^{1}H NMR (C_6D_6, 300 MHz): δ=0.42 ppm; $^{13}C\{^{1}H\}$ NMR (C_6D_6, 75 MHz): δ=5.6 ppm; $^{29}Si\{^{1}H\}$ NMR (C_6D_6, 60 MHz): δ=-13.7 (-*Si*Me_3), -94.1 ppm (-*Si*$(SiMe_3)_3$).

Results and Discussion

UV-Vis spectroscopy

Figure S1. The UV-Vis spectrum of **2** recorded at room temperature in *n*-hexane solution. The absorption in visible range is shown as insertion.

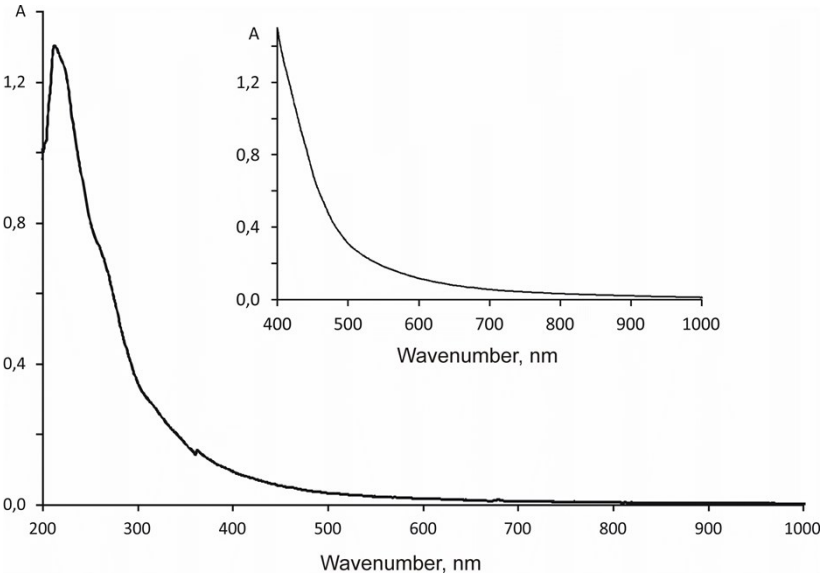


Figure S2. The crystals (a) and solution in *n*-hexane (b) of **2**.

Figure S3. The UV-Vis spectrum of **3** recorded at room temperature in *n*-hexane solution. The absorption in visible range is shown as insertion.

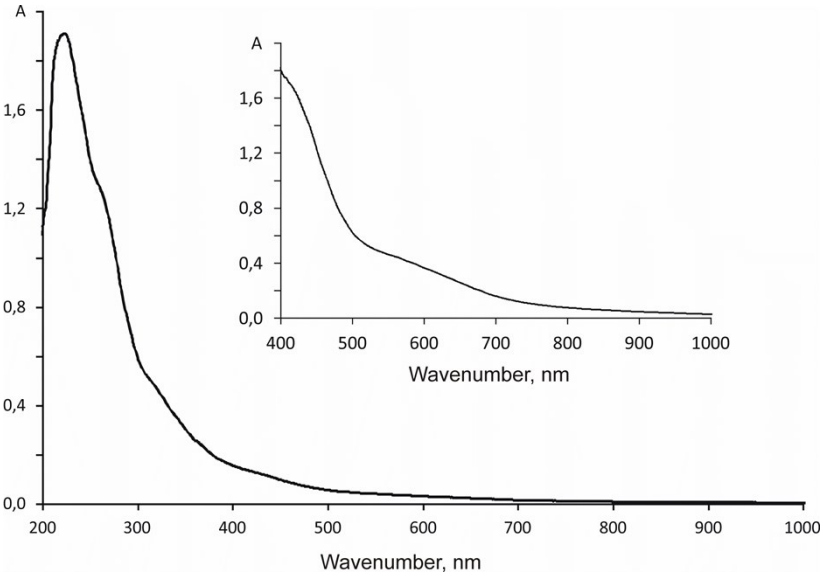


Figure S4. The crystals (a) and solution in *n*-hexane (b) of **3**.

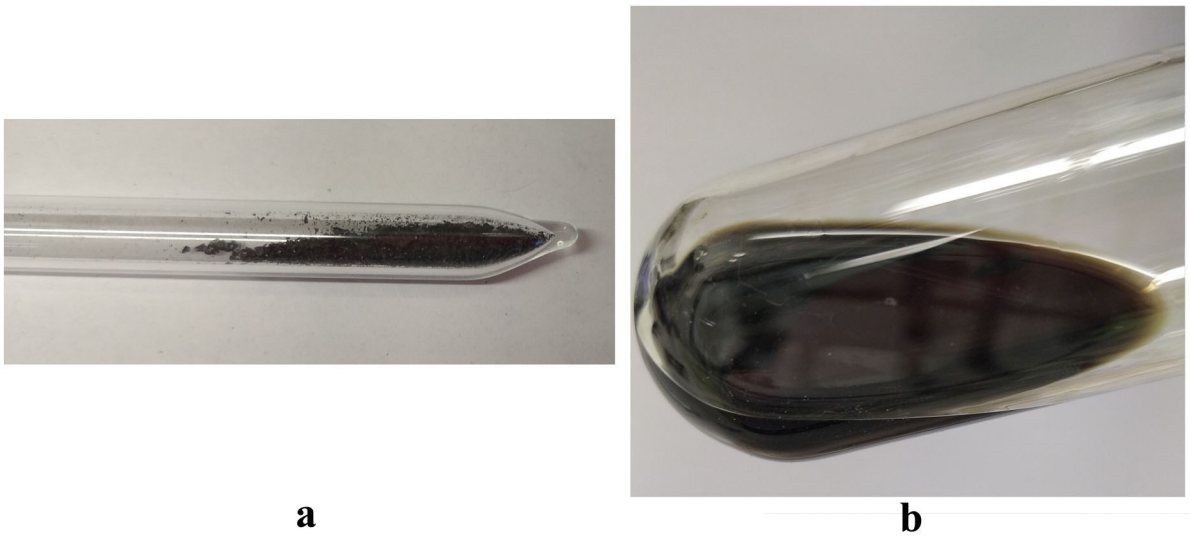


Table S1. Selected Ln-Ge and Ge-Ge distances (pm) for compounds **2**, **3** and the corresponding model compounds together with the calculated 2c-SENs for the two-center Sm-Ge bonds of $[(thf)_2Sm(Ge_9Hyp_3)_2]$.

	Ln-Ge and Ge-Ge distances (pm)				2c-SEN Sm-Ge
	2	**3**	$[(thf)_2Eu(Ge_9Hyp_3)_2]$	$[(thf)_2Sm(Ge_9Hyp_3)_2]$	$[(thf)_2Sm(Ge_9Hyp_3)_2]$
Ln-Ge1	378.97(15)	379.27(11)	379.3	385.7	0.1508
Ln-Ge2	342.48(13)	342.97(9)	342.5	338.8	0.4460
Ln-Ge3	341.20(13)	342.37(10)	341.5	334.9	0.3744
Ln-Ge10	335.15(14)	336.49(9)	343.2	333.8	0.4610
Ln-Ge11	407.83(14)	405.06(11)	362.9	365.6	0.2280
Ln-Ge12	345.71(13)	346.10(9)	339.0	339.7	0.3898
Ge1-Ge2	269.86(17)	269.58(10)	279.7	280.0	
Ge1-Ge3	269.36(18)	269.10(10)	275.1	275.0	
Ge2-Ge3	271.30(16)	271.62(10)	270.1	269.6	
Ge10-Ge11	271.01(17)	271.04(11)	274.9	275.1	
Ge11-Ge12	274.07(16)	273.40(10)	278.7	278.7	
Ge10-Ge12	267.08(17)	267.64(10)	270.4	270.3	

Table S2. Crystal data and structure refinement for **2** and **3**

Identification code	**2**	**3**
Empirical formula	$C_{62}H_{178}EuGe_{18}O_2Si_{24}$	$C_{74}H_{206}Ge_{18}O_2Si_{24}Sm$
Formula weight	3088.77	3259.51
Temperature/K	150	150
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	22.778(3)	22.788(5)
b/Å	24.085(3)	24.181(5)
c/Å	29.746(4)	29.737(6)
α/°	90	90
β/°	112.419(2)	112.337(2)
γ/°	90	90
Volume/Å^3	15085(3)	15157(5)
Z	4	4
ρ_{calc}g/cm^3	1.360	1.428
μ/mm^{-1}	4.152	4.110
F(000)	6164.0	6560.0
Crystal size/mm^3	0.388 × 0.175 × 0.077	0.252 × 0.224 × 0.038
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.318 to 49	2.566 to 52.982
Index ranges	$-26 \le h \le 23$, $-28 \le k \le 28$, $-34 \le l \le 34$	$-28 \le h \le 28$, $-30 \le k \le 30$, $-37 \le l \le 37$
Reflections collected	84484	250840
Independent reflections	25095 [R_{int} = 0.1267, R_{sigma} = 0.1341]	31226 [R_{int} = 0.1136, R_{sigma} = 0.0693]
Data/restraints/parameters	25095/0/1018	31226/363/1183
Goodness-of-fit on F^2	1.017	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0602, wR_2 = 0.1345	R_1 = 0.0488, wR_2 = 0.1037
Final R indexes [all data]	R_1 = 0.1435, wR_2 = 0.1789	R_1 = 0.1029, wR_2 = 0.1262
Largest diff. peak/hole / e Å^{-3}	1.13/-0.90	1.13/-0.67
CCDC number	2049433	2049432

Magnetic measurements

Figure S5. Field-dependent reduced magnetization of **2** measured on a crystalline sample at 2 K. Red curve is the best fit obtained for an S = 7/2 system.

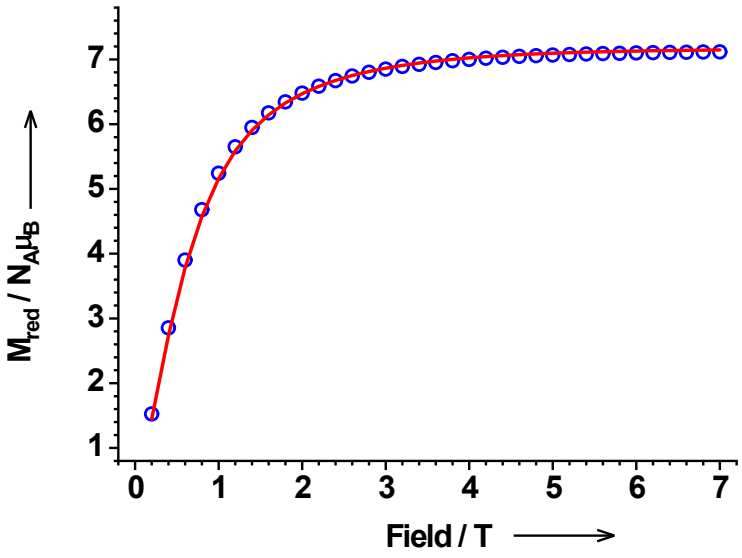


Figure S6. Field-dependent reduced magnetization of **3** measured on a microcrystalline sample at 2 K.

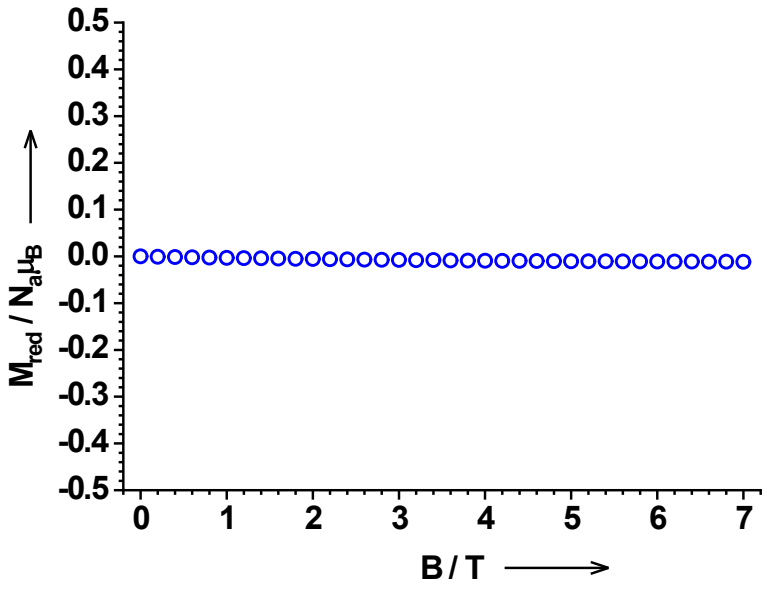


Figure S7. Variable-temperature effective magnetic moment of **2** measured on a microcrystalline sample at external magnetic field of 0.1 T. Red curve is the best fit obtained for an S = 7/2 system.

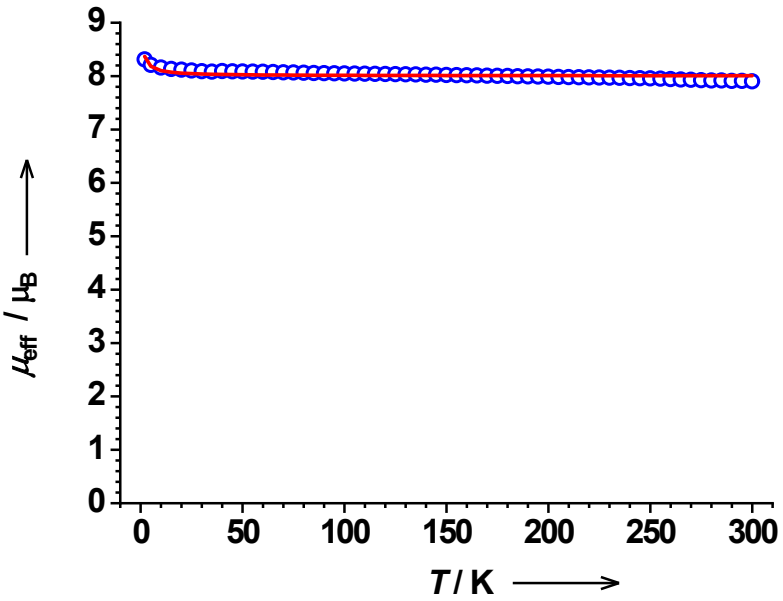
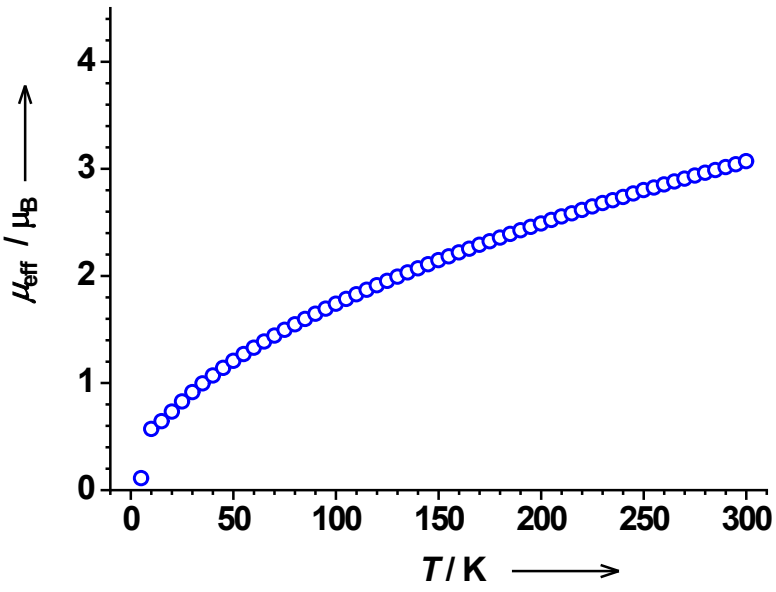


Figure S8. Variable-temperature effective magnetic moment of **3** measured on a microcrystalline sample at external magnetic field of 0.1 T.



NMR Spectroscopy

Figure S9. ^{1}H NMR spectrum of **3** in C_6D_6.

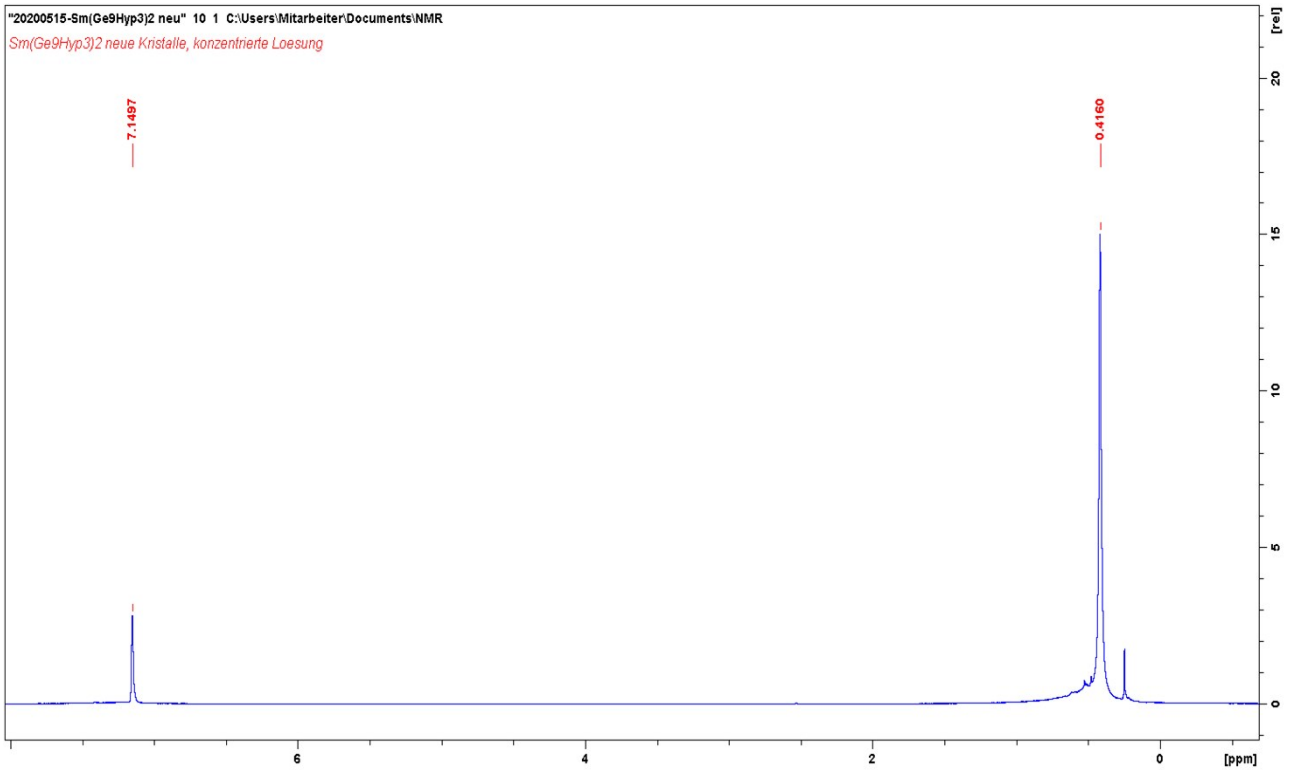


Figure S10. ^{13}C NMR spectrum of **3** in C_6D_6.

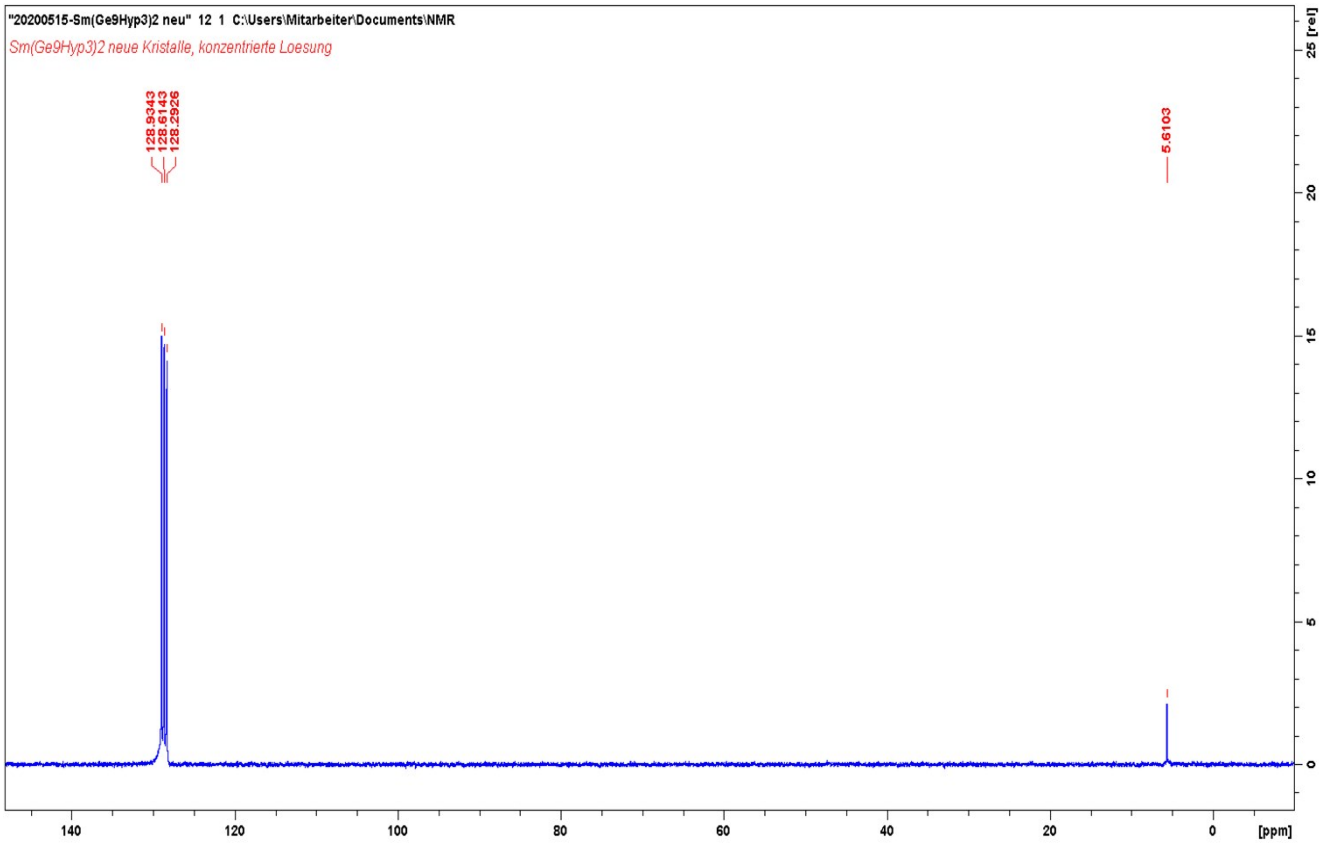
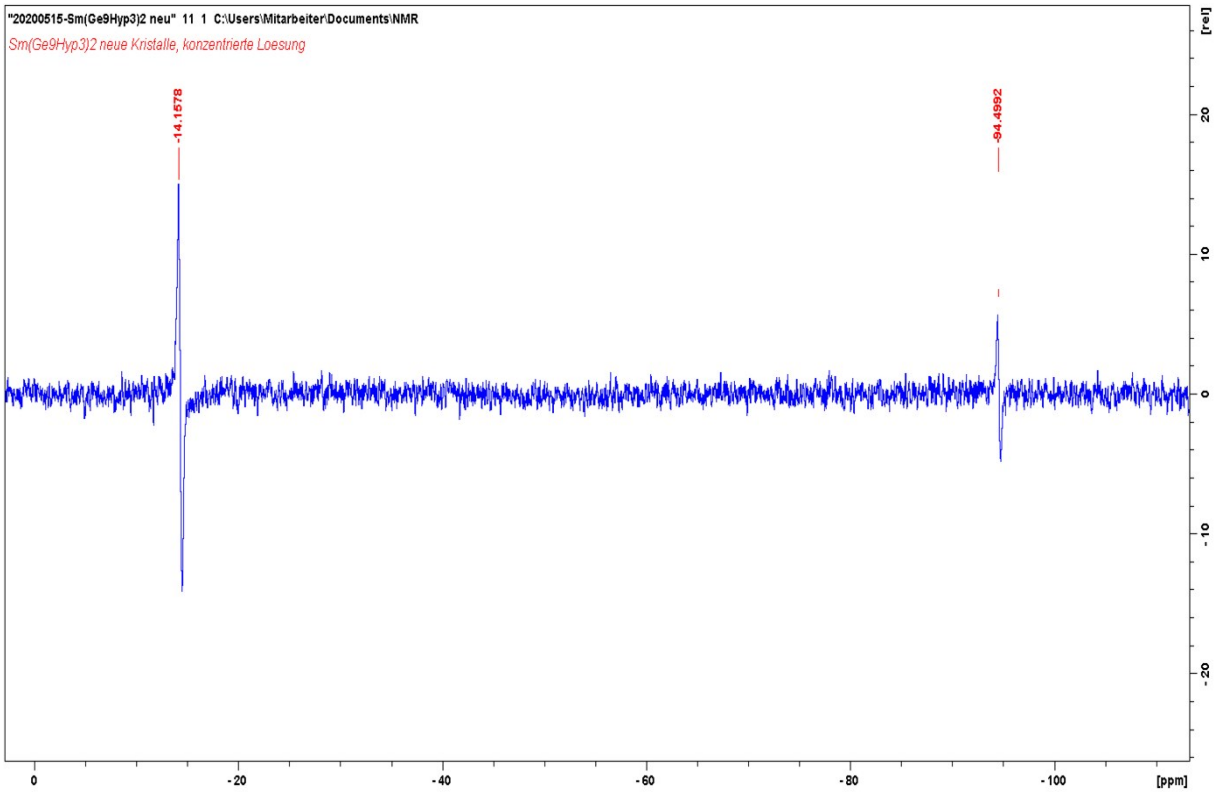
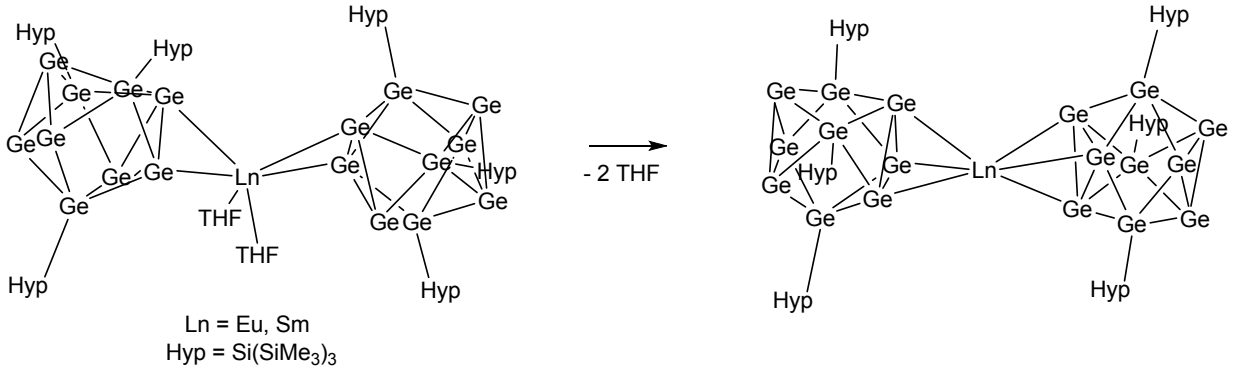


Figure S11. ^{29}Si NMR spectrum of **3** in C_6D_6.



Quantum chemical calculations

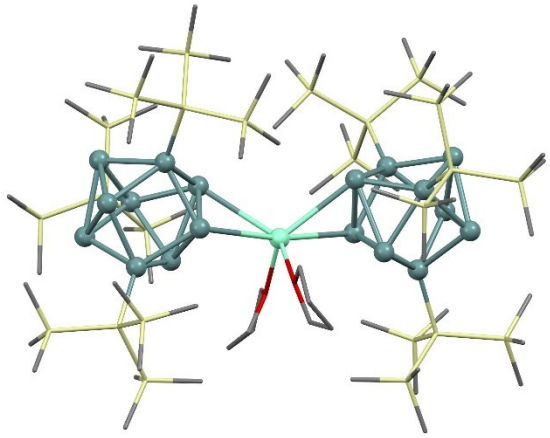
In order to see how the coordinated thf molecules influence the structures we performed additional theoretical studies on model compounds with no coordinating thf molecules $[Ln(Ge_9Hyp_3)_2]$ (Ln = Eu, Sm). Thereby, in case of the model compounds without thf molecules, within the minimum structure the bonding mode of the $Ge_9(Hyp)_3$ units changes to an η^3-coordination mode of both Ge_9 units similar to the transition metal clusters $[Hyp_3Ge_9\text{-}M\text{-}Ge_9Hyp_3]$. The central lanthanide atoms are now bound trigonal antiprismatic to six germanium atoms and the six Hyp-substituents are arranged in a staggered conformation. Hence, removing the thf molecules from **2** or **3** leads to a structural reorganization and a linear arrangement of the two $Ge_9(Hyp)_3$ units around the central lanthanide atom. This is in contrast to most of the base-free lanthanocenes, which still exhibit a bent structure,[15] and only some of them with bulky Cp-ligands adopt centrosymmetric sandwich-type structure with strictly parallel Cp-rings.[15a, 16] Additionally, the presence of coordinating thf molecules within **2** and **3** indicates that the bonding of the thf molecules is more favorable than the coordination of the third germanium atom of the Ge_3-ring of the $Ge_9(Hyp)_3$ unit. This aspect is also supported by quantum chemical calculations showing that the elimination of two thf molecules according to Scheme 1 is endotherm by 54.9 and 55.0 kJ/mol for europium and samarium, respectively.



Scheme S1

1. $[(thf)_2Sm(Ge_9Hyp_3)_2]$

Figure S12. Geometry optimized structure



Point group: C1

Energy: -47620.90874005162 Hartree

HOMO-LUMO-gap: 0.472 eV

Atomic coordinates:

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Ge 15.318751 14.051069 6.967218
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O 12.181894 13.794736 11.121924
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C 11.037450 14.408654 11.804124
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C 10.612662 15.610772 6.782319
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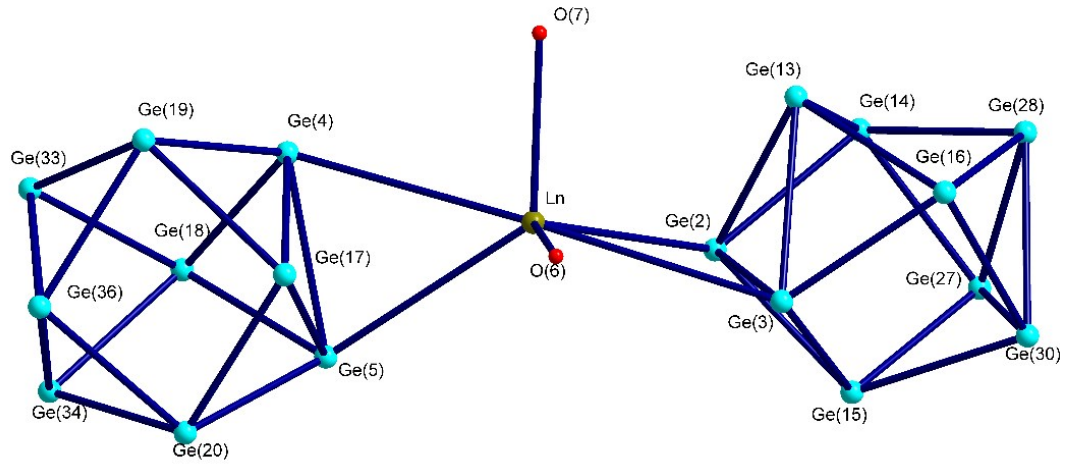
H 19.260038 14.733276 1.586636
H 3.330274 11.975427 6.182793
H 4.956020 11.534640 5.617766
H 4.069665 12.862057 4.833915
H 11.332335 5.008296 8.596863
H 12.721929 3.932480 8.866779
H 11.276186 3.788835 9.888356
H 4.176213 15.806007 7.959221
H 2.864367 14.615419 7.839685
H 3.440304 15.452387 6.383096
H 7.529577 7.714251 12.630682
H 8.332283 7.201143 14.133901
H 7.011267 6.227204 13.455586
H 7.224970 14.041363 13.016497
H 6.251271 12.581449 12.736141
H 7.842285 12.730055 11.972377
H 2.317837 12.868376 10.401852
H 1.501600 11.314869 10.127282
H 2.010006 12.305255 8.746218
H 11.493243 18.158272 7.501195
H 9.994569 18.482018 8.405862
H 13.800151 7.272114 3.866026
H 13.639550 8.062968 5.450077
H 15.004776 8.469852 4.387786
H 12.765550 11.967530 11.951861
H 14.036067 13.243266 11.877419
H 14.456010 22.026242 12.156283
H 12.799819 21.569962 12.600129
H 14.171824 20.989218 13.568912
H 21.767464 13.666594 11.623856
H 20.256243 14.383070 11.018861

H 20.204116 12.917030 12.021832
H 15.031978 20.638313 3.871845
H 15.967250 20.233684 5.330193
H 16.586617 21.440092 4.180719
H 17.973942 8.218836 9.370181
H 19.162451 8.669990 10.609247
H 17.524773 8.175536 11.086786
H 10.016951 14.732950 6.501654
H 11.481899 15.702081 6.114061
H 10.133412 14.167563 11.229060
H 11.200474 15.496040 11.813954
H 15.845787 15.399001 12.724974
H 14.594614 16.280087 13.627490
H 15.951553 15.525632 14.500325
H 7.583096 7.334014 2.750358
H 7.910502 5.655080 3.229525
H 7.780060 6.926037 4.467047
H 15.201521 18.990593 14.978921
H 16.813302 19.726505 14.874419
H 16.567533 18.260044 15.845741
H 13.153626 14.859528 2.282322
H 11.676521 15.555617 2.975815
H 12.967843 14.946710 4.041843
H 18.815080 16.634284 12.586115
H 18.749536 16.631396 14.364110
H 19.152873 18.124752 13.491417
H 6.908262 16.054902 9.312253
H 7.704101 16.109479 10.900130
H 8.256167 14.949247 9.656452
H 13.111981 8.833091 1.213806
H 12.932326 10.597731 1.281421
H 14.495187 9.850610 1.669013
H 11.952705 16.797994 9.415472
H 10.204098 16.448350 9.683407
H 7.242109 10.753468 4.038286
H 7.060004 9.670233 2.648035
H 6.894630 11.425649 2.424508
H 10.387012 3.697231 12.683402
H 10.288865 4.717701 14.133559
H 8.873603 3.782675 13.604403
H 15.068666 9.952663 10.405687
H 15.539840 10.139802 8.701308
H 15.303011 11.581640 9.713604
H 12.669676 12.762452 14.236407
H 13.059663 14.429345 13.754195
H 4.270698 11.226346 12.247603
H 5.269023 9.916327 11.571911
H 3.521138 9.681685 11.793031
H 12.380661 7.765645 15.783005
H 10.970515 6.822923 15.260995
H 12.599282 6.344414 14.740308
H 10.603809 4.720559 4.158807
H 11.989516 5.816654 4.363758
H 10.622141 5.893746 5.495358
H 3.867743 14.346190 11.801086
H 4.069003 15.548921 10.511597
H 4.840075 15.801020 12.092996
H 10.255200 5.608945 1.248905
H 11.631089 6.721888 1.390642
H 10.064677 7.318750 0.807321
H 14.256793 8.285703 12.907500
H 13.502170 9.714414 12.179489
H 13.855561 9.683379 13.925388
H 16.937953 12.878199 2.078450
H 16.775588 13.455499 3.754711
H 15.366816 13.459647 2.677270
H 7.318603 13.671513 5.953890
H 7.003006 15.189482 6.820281
H 6.258178 14.906802 5.229166
H 20.135820 20.640248 10.313515
H 19.831058 19.174344 11.273703
H 19.405729 19.209492 9.552260
H 11.677483 18.717956 12.003313
H 12.899624 18.186744 13.177742
H 12.823736 17.417727 11.579026
H 12.172347 18.010363 1.181635
H 13.745708 17.443751 0.581925
H 13.610522 19.034123 1.358181
H 14.000309 20.964756 9.267493
H 13.413076 19.316532 8.993269
H 12.330447 20.543775 9.708041
H 17.882136 22.350489 9.229338
H 16.974582 20.982955 8.546783
H 16.184283 22.098872 9.685868
H 20.833619 12.122093 5.609017
H 19.212688 12.691591 5.179762
H 19.894126 11.258659 4.371221

Results of the Ahlrichs-Heinzmann population analysis:
calculated shared electron numbers (SEN)

Figure S13. Atom numbers for calculated structure



TWO center shared electron numbers ge 0.1000E-01 :

shared electron number for the pair	1 sm -	2 ge =	0.4460
shared electron number for the pair	1 sm -	3 ge =	0.3744
shared electron number for the pair	1 sm -	4 ge =	0.3898
shared electron number for the pair	1 sm -	5 ge =	0.4610
shared electron number for the pair	1 sm -	13 ge =	0.1508
shared electron number for the pair	1 sm -	17 ge =	0.2280
shared electron number for the pair	2 ge -	3 ge =	1.0144
shared electron number for the pair	2 ge -	13 ge =	0.9105
shared electron number for the pair	2 ge -	14 ge =	1.0069
shared electron number for the pair	2 ge -	15 ge =	0.9920
shared electron number for the pair	2 ge -	16 ge =	-0.0104
shared electron number for the pair	2 ge -	27 ge =	0.1320
shared electron number for the pair	2 ge -	28 ge =	-0.0249
shared electron number for the pair	2 ge -	30 ge =	-0.0306
shared electron number for the pair	3 ge -	13 ge =	0.8422
shared electron number for the pair	3 ge -	15 ge =	1.0251
shared electron number for the pair	3 ge -	16 ge =	1.0124
shared electron number for the pair	3 ge -	27 ge =	-0.0290
shared electron number for the pair	3 ge -	28 ge =	-0.0229
shared electron number for the pair	3 ge -	30 ge =	0.2492
shared electron number for the pair	4 ge -	5 ge =	1.0007
shared electron number for the pair	4 ge -	17 ge =	0.8775
shared electron number for the pair	4 ge -	18 ge =	1.0079
shared electron number for the pair	4 ge -	19 ge =	1.0262

shared electron number for the pair 4 ge - 33 ge = 0.2641
shared electron number for the pair 4 ge - 34 ge = -0.0290
shared electron number for the pair 4 ge - 36 ge = -0.0222
shared electron number for the pair 5 ge - 17 ge = 0.9310
shared electron number for the pair 5 ge - 18 ge = 1.0119
shared electron number for the pair 5 ge - 20 ge = 1.0049
shared electron number for the pair 5 ge - 33 ge = -0.0278
shared electron number for the pair 5 ge - 34 ge = 0.1366
shared electron number for the pair 5 ge - 36 ge = -0.0272
shared electron number for the pair 13 ge - 14 ge = 1.0226
shared electron number for the pair 13 ge - 16 ge = 1.0303
shared electron number for the pair 13 ge - 27 ge = -0.0267
shared electron number for the pair 13 ge - 28 ge = 0.4284
shared electron number for the pair 13 ge - 30 ge = -0.0234
shared electron number for the pair 14 ge - 15 ge = 0.0446
shared electron number for the pair 14 ge - 27 ge = 1.0087
shared electron number for the pair 14 ge - 28 ge = 1.0310
shared electron number for the pair 15 ge - 16 ge = 0.0201
shared electron number for the pair 15 ge - 27 ge = 1.0182
shared electron number for the pair 15 ge - 30 ge = 1.0212
shared electron number for the pair 16 ge - 27 ge = -0.0109
shared electron number for the pair 16 ge - 28 ge = 1.0418
shared electron number for the pair 16 ge - 30 ge = 1.0296
shared electron number for the pair 17 ge - 19 ge = 1.0416
shared electron number for the pair 17 ge - 20 ge = 1.0204
shared electron number for the pair 17 ge - 33 ge = -0.0235
shared electron number for the pair 17 ge - 34 ge = -0.0279
shared electron number for the pair 17 ge - 36 ge = 0.3891
shared electron number for the pair 18 ge - 19 ge = 0.0167
shared electron number for the pair 18 ge - 20 ge = 0.0429
shared electron number for the pair 18 ge - 33 ge = 1.0117
shared electron number for the pair 18 ge - 34 ge = 1.0325
shared electron number for the pair 19 ge - 33 ge = 1.0229
shared electron number for the pair 19 ge - 34 ge = -0.0107
shared electron number for the pair 19 ge - 36 ge = 1.0510
shared electron number for the pair 20 ge - 34 ge = 1.0234
shared electron number for the pair 20 ge - 36 ge = 1.0262
shared electron number for the pair 27 ge - 28 ge = 0.9703
shared electron number for the pair 27 ge - 30 ge = 1.0982
shared electron number for the pair 28 ge - 30 ge = 0.9009
shared electron number for the pair 33 ge - 34 ge = 1.0799
shared electron number for the pair 33 ge - 36 ge = 0.9291
shared electron number for the pair 34 ge - 36 ge = 0.9787

THREE and FOUR center SEN greater than 0.010:

n(1 2 3) = 0.1678
n(1 2 3 4) = -0.0268
n(1 2 3 5) = -0.0202
n(1 2 3 13) = 0.0701
n(1 2 3 14) = -0.0192
n(1 2 3 15) = -0.0122
n(1 2 3 16) = -0.0184
n(1 2 3 17) = -0.0231
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n(1 2 4 5) = -0.0164
n(1 2 4 13) = -0.0141
n(1 2 4 17) = -0.0228
n(1 2 5) = -0.0401
n(1 2 5 13) = -0.0197
n(1 2 5 17) = -0.0213
n(1 2 6) = -0.0436
n(1 2 13) = 0.0982
n(1 2 13 14) = -0.0138
n(1 2 13 17) = -0.0180
n(1 2 14) = -0.0358
n(1 2 14 27) = -0.0150
n(1 2 15) = -0.0232
n(1 2 15 27) = -0.0120
n(1 2 17) = -0.0701
n(1 2 27) = -0.0256
n(1 3 4) = -0.1215
n(1 3 4 5) = -0.0328
n(1 3 4 13) = -0.0193
n(1 3 4 17) = -0.0296
n(1 3 5) = -0.0628
n(1 3 5 13) = -0.0225
n(1 3 5 17) = -0.0218
n(1 3 13) = 0.0810
n(1 3 13 16) = -0.0112
n(1 3 13 17) = -0.0155
n(1 3 15) = -0.0248
n(1 3 15 30) = -0.0125
n(1 3 16) = -0.0354
n(1 3 16 30) = -0.0157
n(1 3 17) = -0.0492
n(1 3 30) = -0.0320
n(1 4 5) = 0.1712
n(1 4 5 13) = -0.0138
n(1 4 5 17) = 0.0884
n(1 4 5 18) = -0.0120
n(1 4 5 19) = -0.0169
n(1 4 5 20) = -0.0181
n(1 4 5 33) = -0.0103
n(1 4 13) = -0.0267
n(1 4 13 17) = -0.0119
n(1 4 17) = 0.1091
n(1 4 17 19) = -0.0135
n(1 4 17 20) = -0.0104

n(1 4 18) = -0.0241
n(1 4 18 33) = -0.0127
n(1 4 19) = -0.0347
n(1 4 19 33) = -0.0139
n(1 4 33) = -0.0315
n(1 5 7) = -0.0489
n(1 5 13) = -0.0490
n(1 5 13 17) = -0.0148
n(1 5 17) = 0.1389
n(1 5 17 18) = -0.0104
n(1 5 17 19) = -0.0125
n(1 5 17 20) = -0.0121
n(1 5 17 36) = -0.0111
n(1 5 18) = -0.0276
n(1 5 18 34) = -0.0139
n(1 5 20) = -0.0361
n(1 5 20 34) = -0.0159
n(1 5 34) = -0.0280
n(1 6 7) = -0.0230
n(1 6 10) = 0.0150
n(1 7 12) = 0.0137
n(1 9208) = 0.0104
n(1 10193) = 0.0141
n(1 11206) = 0.0119
n(1 12231) = 0.0135
n(1 13 14) = -0.0175
n(1 13 16) = -0.0142
n(1 13 17) = -0.0287
n(1 13 28) = -0.0189
n(1 17 19) = -0.0210
n(1 17 20) = -0.0195
n(1 17 36) = -0.0241
n(2 3 13) = 0.3590
n(2 3 13 14) = 0.0166
n(2 3 13 15) = 0.0157
n(2 3 13 16) = 0.0164
n(2 3 14) = -0.0394
n(2 3 14 16) = 0.0167
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n(2 3 14 29) = -0.0217
n(2 3 14 30) = 0.0108
n(2 3 15) = 0.2574
n(2 3 15 31) = -0.0195
n(2 3 16) = -0.0413
n(2 3 16 28) = 0.0161
n(2 3 16 32) = -0.0223
n(2 3 27 30) = 0.0350
n(2 3 28) = 0.0118
n(2 3 28 30) = 0.0103
n(2 3 30) = -0.0171
n(2 13 14) = 0.2527
n(2 13 14 29) = -0.0198
n(2 13 15) = -0.0290
n(2 13 15 16) = 0.0212
n(2 13 15 28) = 0.0130
n(2 13 15 30) = 0.0164
n(2 13 15 31) = -0.0211
n(2 13 16) = -0.0316
n(2 13 16 30) = 0.0139
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n(2 13 27 28) = 0.0342
n(2 13 27 30) = 0.0102
n(2 13 28) = -0.0180
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n(2 14 15 27) = 0.0926
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n(2 14 16 28) = 0.0130
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n(2 14 28 30) = 0.0131
n(2 14 29) = -0.0596
n(2 14 29 42) = -0.0228
n(2 14 42) = -0.0225
n(2 15 16 30) = 0.0116
n(2 15 27) = 0.1025
n(2 15 28 30) = 0.0137
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n(2 15 31) = -0.0528
n(2 15 31 45) = -0.0203
n(2 15 45) = -0.0201
n(2 16 32) = -0.0237
n(3 8241) = -0.0182
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n(3 13 16 32) = -0.0219
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n(3 13 28 30) = 0.0373
n(3 14 15 29) = -0.0107
n(3 14 16 28) = 0.0145
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n(3 14 29) = -0.0233
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n(3 15 16 28) = 0.0156
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n(3 15 16 32) = -0.0204
n(3 15 27) = -0.0596
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n(3 15 30) = 0.1690
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n(3 15 46) = -0.0149
n(3 16 27 28) = 0.0152
n(3 16 28) = -0.0662
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n(3 16 47) = -0.0227
n(3 16241) = -0.0122
n(3 27 28) = 0.0110
n(3 27 30) = -0.0127
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n(4 5 18 35) = -0.0191
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n(4 5 19 20) = 0.0182
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n(4 17 18 20) = 0.0262
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n(4 17 20) = -0.0230
n(4 17 20 34) = 0.0147
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n(4 17 34 36) = 0.0116
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n(4 18 19 33) = 0.0771
n(4 18 19 34) = 0.0129
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n(4 18 35) = -0.0378
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n(5 18 35 51) = -0.0142
n(5 18 50) = -0.0117
n(5 18 51) = -0.0131
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n(5 19 37) = -0.0242
n(5 20 33 36) = 0.0138
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n(6 9 23) = -0.0248
n(6 10 24) = -0.0183
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n(8 21121) = -0.0165
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n(8 21239241) = 0.0122
n(8 21240) = 0.0347
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n(8 21241) = 0.0379
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n(9 10 24) = 0.0208
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n(9 23152) = 0.0176
n(9 23152209) = -0.0119
n(9 23153) = 0.0274
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n(9 24208) = -0.0105
n(9208209) = 0.0211
n(10 23 24) = 0.0349
n(10 23 24153) = -0.0127
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n(10 24192243) = -0.0122
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n(10192193) = 0.0185
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Calculated partial atomic charges

****
*
* atomic charges with multicenter corrections *
*
****

atom | charge	atom | charge	atom | charge
1 sm | 0.7357	26 c | -0.0857	51 si | 0.2200
2 ge | -0.1587	27 ge | -0.1045	52 si | 0.2202
3 ge | -0.1391	28 ge | -0.0236	53 si | 0.2477
4 ge | -0.1381	29 si | -0.0070	54 si | 0.2325
5 ge | -0.1373	30 ge | -0.0672	55 si | 0.2429
6 o | -0.2076	31 si | 0.0322	56 si | 0.2516
7 o | -0.2147	32 si | 0.0134	57 si | 0.2214
8 c | -0.2596	33 ge | -0.0514	58 c | -0.2939
9 c | 0.0279	34 ge | -0.1113	59 c | -0.2951
10 c | 0.0203	35 si | 0.0018	60 c | -0.2848
11 c | 0.0357	36 ge | -0.0430	61 c | -0.2992
12 c | 0.0281	37 si | -0.0056	62 c | -0.2926
13 ge | -0.1592	38 si | 0.0037	63 c | -0.2886
14 ge | 0.1184	39 c | -0.2958	64 c | -0.2903
15 ge | 0.1481	40 c | -0.2936	65 c | -0.2670
16 ge | 0.0847	41 si | 0.2244	66 c | -0.2736
17 ge | -0.1707	42 si | 0.2526	67 c | -0.2774
18 ge | 0.1542	43 si | 0.2324	68 c | -0.2847
19 ge | 0.1033	44 si | 0.2183	69 c | -0.2831
20 ge | 0.1436	45 si | 0.2501	70 c | -0.2945
21 si | 0.1973	46 si | 0.2255	71 c | -0.2938
22 c | -0.2664	47 si | 0.2449	72 c | -0.2718
23 c | -0.0745	48 si | 0.2221	73 c | -0.2848
24 c | -0.0863	49 si | 0.2172	74 c | -0.2921
25 c | -0.0838	50 si | 0.2400	75 c | -0.2912

76 c | -0.2809
77 c | -0.2907
78 c | -0.2865
79 c | -0.2916
80 c | -0.2754
81 c | -0.2962
82 c | -0.2925
83 c | -0.2821
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87 c | -0.2809
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95 c | -0.2832
96 c | -0.2858
97 c | -0.2979
98 c | -0.2831
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100 c | -0.2678
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103 c | -0.2879
104 c | -0.2940
105 c | -0.2871
106 c | -0.2823
107 c | -0.2832
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109 h | 0.0718
110 h | 0.0648
111 h | 0.0602
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113 h | 0.0770
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116 h | 0.0664
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139 h | 0.0535
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141 h | 0.0674
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157 h | 0.0649
158 h | 0.0592
159 h | 0.0639
160 h | 0.0645
161 h | 0.0677
162 h | 0.0707
163 h | 0.0672
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165 h | 0.0642
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167 h | 0.0595
168 h | 0.0683
169 h | 0.0628
170 h | 0.0718
171 h | 0.0685
172 h | 0.0737
173 h | 0.0640
174 h | 0.0615
175 h | 0.0633
176 h | 0.0707
177 h | 0.0702
178 h | 0.0797
179 h | 0.0659
180 h | 0.0660
181 h | 0.0686
182 h | 0.0683
183 h | 0.0595
184 h | 0.0667
185 h | 0.0691
186 h | 0.0624
187 h | 0.0758
188 h | 0.0643
189 h | 0.0626
190 h | 0.0777
191 h | 0.0669
192 h | 0.0684
193 h | 0.0618
194 h | 0.0676
195 h | 0.0682
196 h | 0.0684
197 h | 0.0649
198 h | 0.0710
199 h | 0.0602
200 h | 0.0629
201 h | 0.0751
202 h | 0.0682
203 h | 0.0685
204 h | 0.0658
205 h | 0.0695
206 h | 0.0571
207 h | 0.0668
208 h | 0.0541
209 h | 0.0504
210 h | 0.0709
211 h | 0.0550
212 h | 0.0697
213 h | 0.0609
214 h | 0.0702
215 h | 0.0747
216 h | 0.0596
217 h | 0.0725
218 h | 0.0658
219 h | 0.0669
220 h | 0.0726
221 h | 0.0632
222 h | 0.0757
223 h | 0.0690
224 h | 0.0635
225 h | 0.0629
226 h | 0.0710
227 h | 0.0652
228 h | 0.0661

229 h | 0.0636	248 h | 0.0630	267 h | 0.0684
230 h | 0.0702	249 h | 0.0667	268 h | 0.0652
231 h | 0.0530	250 h | 0.0637	269 h | 0.0632
232 h | 0.0457	251 h | 0.0675	270 h | 0.0756
233 h | 0.0699	252 h | 0.0766	271 h | 0.0673
234 h | 0.0618	253 h | 0.0641	272 h | 0.0673
235 h | 0.0660	254 h | 0.0680	273 h | 0.0596
236 h | 0.0625	255 h | 0.0698	274 h | 0.0643
237 h | 0.0650	256 h | 0.0711	275 h | 0.0670
238 h | 0.0693	257 h | 0.0667	276 h | 0.0605
239 h | 0.0625	258 h | 0.0658	277 h | 0.0776
240 h | 0.0774	259 h | 0.0695	278 h | 0.0611
241 h | 0.0336	260 h | 0.0605	279 h | 0.0684
242 h | 0.0672	261 h | 0.0671	280 h | 0.0688
243 h | 0.0696	262 h | 0.0661	281 h | 0.0761
244 h | 0.0581	263 h | 0.0650	282 h | 0.0594
245 h | 0.0806	264 h | 0.0640	283 h | 0.0641
246 h | 0.0677	265 h | 0.0772	284 h | 0.0625
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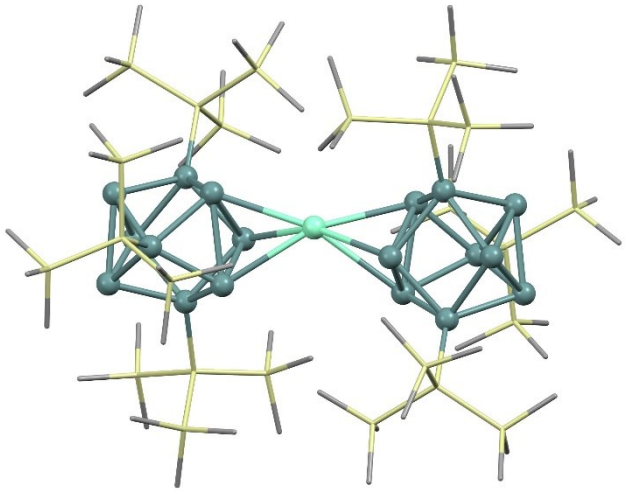
2. [Sm(Ge_9Hyp_3)$_2$]

Figure S13. Geometry optimized structure



Point group: C1

Energy: -47662.87950875043 Hartree

HOMO-LUMO-gap: 0.657eV

Atomic coordinates:

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Ge 0.159251 -2.177603 4.402737
Ge -1.624646 1.281328 4.319929
Ge 1.433373 -0.915144 2.511338
Ge 0.448875 1.619836 2.846814
Si 4.411205 1.739839 4.547103
Ge -1.261938 -0.760556 2.826334
Si -0.463385 -4.535885 4.550030
Si -3.543178 2.762405 4.201465
Sm -0.409452 0.415558 0.054804
Ge -0.405404 -1.513389 -2.563823
Ge 1.297554 0.594868 -2.634781
Ge -1.478280 1.027463 -2.932286
Ge 1.528268 -1.374703 -4.264974
Ge -2.087160 -0.968448 -4.436408
Ge 0.310739 2.164214 -4.389212
Ge -0.245449 -1.522805 -6.172934
Ge 1.378646 0.531608 -6.073034
Si 3.418345 -2.911529 -4.302675
Ge -1.323522 0.969946 -6.017261
Si -4.444092 -1.575776 -4.594582
Si 0.661376 4.567938 -4.426515
Si -4.703006 -2.721161 -6.679306
Si -4.888058 -3.031036 -2.753251
Si 0.237075 -5.561202 2.511863
Si 0.745675 -5.429826 6.410374
Si -2.816994 -4.788252 4.883591
C -4.554160 -1.505266 -8.129863
C -3.394793 -4.076870 -6.891327
C -6.421861 -3.535983 -6.746066
C -4.030722 -4.707428 -2.993786
C -6.759967 -3.327424 -2.583329
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Si -5.816306 0.377827 -4.502685
C -5.254510 1.690394 -5.749290
C -7.623785 -0.073274 -4.892689
C -5.754545 1.143417 -2.763863
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C 2.019887 -5.075412 2.085360
C 0.159327 -7.456158 2.664856
C -3.312013 -6.599626 4.568583
C -3.304241 -4.339833 6.663285
C -3.808627 -3.692422 3.693884
C 0.161580 -7.211243 6.742738
C 2.609494 -5.463718 6.047761
C 0.459772 -4.415670 7.988042
H -4.430351 -5.247592 -3.862699
H -4.185690 -5.338982 -2.106249
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H 2.989452 -4.461708 5.807295
H 3.156346 -5.828755 6.930469
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Si -0.330786 5.456440 -6.410338
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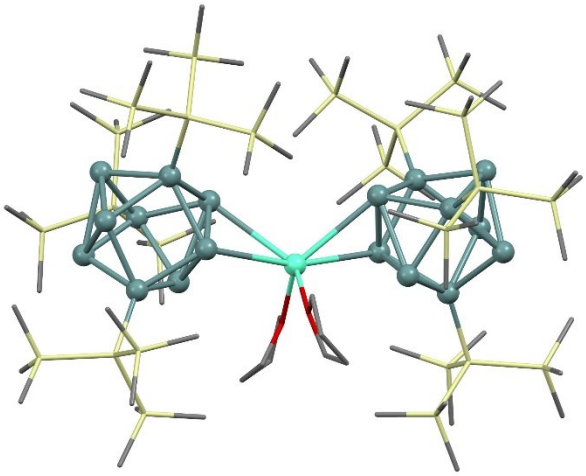
3. $[(thf)_2Eu(Ge_9Hyp_3)_2]$

Figure S14. Geometry optimized structure



Point group: C1

Energy: -47662.87950875043 Hartree

HOMO-LUMO-gap: 0.657eV

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Ge 11.690389 10.221612 8.194092
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C 15.687471 10.536309 9.714668
C 10.995289 14.467524 11.887838
C 12.943389 13.101106 12.170007
C 10.491568 15.732808 6.809497
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Ge 17.556184 13.834774 8.220903
Ge 16.289745 17.103560 9.610644
Ge 9.862313 11.248903 9.971999
Ge 10.112679 9.583666 6.230384
Ge 7.686669 11.278238 8.575504
Ge 10.300699 8.699558 9.758357
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C 10.988069 13.873648 13.292102
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Si 15.852924 17.003346 3.569498
Ge 18.588722 16.035325 9.145296
Si 18.798081 11.794764 8.706171
Si 16.168118 18.764690 11.383194
Ge 7.572929 9.421046 6.787457
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Si 10.634447 9.237443 3.871861
Ge 7.735420 8.872749 9.471968
Si 5.662676 12.555059 9.019290
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Si 12.975696 9.616672 3.638383
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Si 16.847725 15.352837 2.152127
Si 13.526152 17.219078 3.117816
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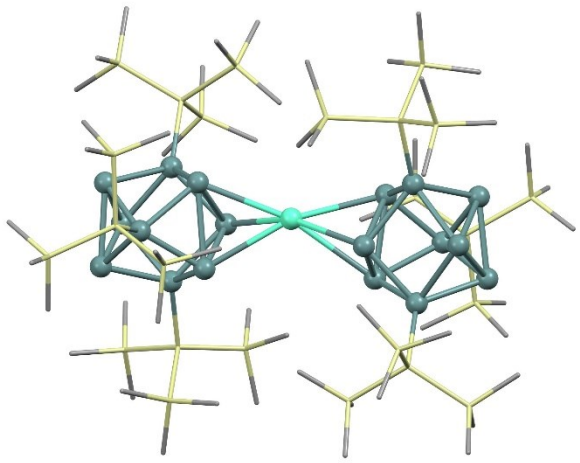
4. [Eu(Ge_9Hyp_3)$_2$]

Figure S14. Geometry optimized structure



Point group: C1

Energy: -47208.24296914469 Hartree

HOMO-LUMO-gap: 0.724 eV

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References

(1) Girard, P.; Namy, J.-L.; Kagan, H. B. *J. Am. Chem. Soc.* **1980**, *102*, 2693-2698.

(2) S*ynthetic Methods of Organometallic and Inorganic Chemistry* (Eds.: W. A. Herrmann, G. Brauer), Georg Thieme Verlag, Thieme Medical Publishers, Stuttgart, **1996**.

(3) Li, F.; Sevov, S. C. *Inorg. Chem.* **2012**, *51*, 2706-2708.

(4) Kysliak, O.; Schnepf, A. *Dalton Trans.* **2016**, *45*, 2404-2408.

(5) (a) Sheldrick, G. M. *Acta Crystallogr. Sect. A* **2008**, *64*, 112-122; (b) Sheldrick, G. M. *Acta Crystallogr. Sect. C* **2015**, *71*, 3-8.

(6) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Crystallogr.* **2009**, *42*, 339-341.

(7) Spek, A. L. Acta Cryst. 2009, D65, 148 - 155.

(8) Kahn, O. *Molecular magnetism*, VCH Publishers, Inc.(USA), **1993**.

(9) Chilton, N. F.; Anderson, R. P.; Turner, L. D.; Soncini, A.; Murray, K. S. *J. Comput. Chem.* **2013**, *34*, 1164-1175.

(10) Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, *240*, 283-290.

(11) Treutler, O.; Ahlrichs, R. *J. Chem. Phys.* **1995**, *102*, 346-354.

(12) (a) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822-88824; (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100.

(13) Schäfer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, *97*, 2571-2577.

(14) Steffen, C.; Thomas, K.; Huniar, U.; Hellweg, A.; Rubner, O.; Schroer, A. *J. Comput. Chem.* **2010**, *31*, 2967-2970.

(15) (a) Xémard, M.; Goudy, V.; Braun, A.; Tricoire, M.; Cordier, M.; Ricard, L.; Castro, L.; Louyriac, E.; Kefalidis, C. E.; Clavaguéra, C.; Maron, L.; Nocton, G. Reductive Disproportionation of CO_2 with Bulky Divalent Samarium Complexes; *Organometallics* **2017**, *36*, 4660-4668. (b) Sitzmann, H.; Dezember, T.; Schmitt, O.; Weber, F.; Wolmershäuser, G.; Ruck, M. Metallocenes of Samarium, Europium, and Ytterbium with the Especially Bulky Cyclopentadienyl Ligands $C_5H(CHMe_2)_4$, $C_5H_2(CMe_3)_3$, and $C_5(CHMe_2)_5$; *Z. Anorg. Allg. Chem.* **2000**, *626*, 2241-2244. (c) Visseaux, M.; Barbier-Baudry, D.; Blacque, O.; Hafid, A.; Richard, P.; Weber, F. New base-free metallocenes of samarium and neodymium, an approach to stereoelectronic control in organolanthanide chemistry; *New J. Chem.* **2000**, *24*, 939-942. (d) Nocton, G.; Ricard, L. N-aromatic heterocycle adducts of bulky $[1,2,4\text{-}(Me_3C)_3C_5H_2]_2Sm$: synthesis, structure and solution analysis; *Dalton Trans.* **2014**, *43*, 4380-4387. (e) Evans, W. J.; Hughes, L. A.; Hanusa, T. P. Synthesis and crystallographic characterization of an unsolvated, monomeric samarium bis(pentamethylcyclopentadienyl) organolanthanide complex, $(C_5Me_5)_2Sm$; *J. Am. Chem. Soc.* **1984**, *106*, 4270-4272. (f) Evans, W. J.; Perotti, J. M.; Brady, J. C.; Ziller, J. W. Tethered Olefin Studies of Alkene versus Tetraphenylborate Coordination and Lanthanide Olefin Interactions in Metallocenes; *J. Am. Chem. Soc.* **2003**, *125*, 5204-5212. (g) Evans, W. J.; Hughes, L. A.; Hanusa, T. P. Synthesis and x-ray crystal structure of bis (pentamethylcyclopentadienyl) complexes of samarium and europium: $(C_5Me_5)_2Sm$ and $(C_5Me_5)_2Eu$; *Organometallics* **1986**, *5*, 1285-1291. (h) Weber, F.; Sitzmann, H.; Schultz, M.; Sofield, C. D.; Andersen, R. A. Synthesis and Solid State Structures of Sterically Crowded d^0-Metallocenes of Magnesium, Calcium, Strontium, Barium, Samarium, and Ytterbium; *Organometallics* **2002**, *21*, 3139-3146. (i) Kuiper, M. H.; Lueken, H. Synthesis, Structure and Magnetism of Bis [1,2,4-tris(trimethylsilyl)cyclopentadienyl] europium; *Z. Anorg. Allg. Chem.* **2007**, *633*, 1407-1409. (j) Schultz, M.; Burns, C. J.; Schwartz, D. J.; Andersen, R. A. Solid-State Structures of Base-Free Ytterbocenes and Inclusion Compounds of Bis(pentamethylcyclopentadienyl)ytterbium with Neutral Carboranes and Toluene: The Role of Intermolecular Contacts; *Organometallics* **2000**, *19*, 781-789. (k) Palumbo, C. T.; Ziller, J. W.; Evans, W. J. Structural characterization of the bent metallocenes, $[C_5H_3(SiMe_3)_2]_2Sm$ and $[C_5H_3(CMe_3)_2]_2Ln$ (Ln = Eu, Sm), and the mono(cyclopentadienyl) tetraphenylborate complex, $[C_5H_3(CMe_3)_2]Eu(\mu\text{-}\eta^6\text{:}\eta^1\text{-}Ph)_2BPh_2$; *J. Organomet. Chem.* **2018**, *867*, 142-148.

(16) (a) Kelly, R. P.; M. Bell, T. D.; Cox, R. P.; Daniels, D. P.; Deacon, G. B.; Jaroschik, F.; Junk, P. C.; Le Goff, X. F.; Lemercier, G.; Martinez, A.; Wang, J.; Werner, D. Divalent Tetra- and Penta-phenylcyclopentadienyl Europium and

Samarium Sandwich and Half-Sandwich Complexes: Synthesis, Characterization, and Remarkable Luminescence Properties; *Organometallics* **2015**, *34*, 5624-5636. (b) van Velzen, N. J. C.; Harder, S. Deca-arylsamarocene: an unusually inert Sm (II) sandwich complex; *Organometallics* **2018**, *37*, 2263-2271. (c) Ruspic, C.; Moss, J. R.; Schürmann, M.; Harder, S. Remarkable Stability of Metallocenes with Superbulky Ligands: Spontaneous Reduction of Sm^{III} to Sm^{II}; *Angew. Chem. Int. Ed.* **2008**, *47*, 2121-2126. (d) Harder, S.; Naglav, D.; Ruspic, C.; Wickleder, C.; Adlung, M.; Hermes, W.; Eul, M.; Pöttgen, R.; Rego, D. B.; Poineau, F. Czerwinski, K. R.; Herber, R. H.; Nowik, I. Physical Properties of Superbulky Lanthanide Metallocenes: Synthesis and Extraordinary Luminescence of $[Eu^{II}(Cp^{BIG})_2]$ (Cp^{BIG}=(4-*n*Bu-$C_6H_4)_5$-Cyclopentadienyl); *Chem. Eur. J.* **2013**, *19*, 12272-12280. (e) Deacon, G. B.; Forsyth, C. M.; Jaroschik, F.; Junk, P. C.; Kay, D. L.; Maschmeyer, T.; Masters, A. F.; Wang, J.; Field, L. D. Accessing Decaphenylmetallocenes of Ytterbium, Calcium, and Barium by Desolvation of Solvent-Separated Ion Pairs: Overcoming Adverse Solubility Properties; *Organometallics* **2008**, *27*, 4772-4778.