- Supporting Information -

On the reaction of $GeCl_2$·Dioxane with $KFeCp(CO)_2$: Isolation and characterization of novel bimetallic clusters

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Content:

1. Experimental section

General Considerations

All manipulations were carried out under nitrogen or in vacuo in Schlenk-type glassware on a Schlenk line. Solvents were pre-dried over sodium benzophenone (thf, toluene) or calcium hydride (pentane) and distilled. $GeCl_2$·Dioxane was prepared according to Thorne et al..[1] $KFeCp(CO)_2$ was prepared by reductive cleavage of $[FeCp(CO)_2]_2$ with potassium. ^1H- and ^{13}C- NMR measurements were done at a Bruker DRX250 and Bruker Avance II+ 400 spectrometer. All values are given in ppm against the external standard $SiMe_4$. IR spectra were recorded at 298 K on a Bruker Vertex 70 spectrometer. All compounds were measured in a KBr-pellet under nitrogen atmosphere. The pellets were prepared under argon atmosphere. UV-Vis spectra were recorded in thf solutions at a PG Instruments T60 UV/VIS Spectrophotometer in quartz cuvettes with thf as a blank sample (light source of the spectrometer changes at 360 nm causing absorption jumps in the recorded spectra).

Preparation

$Ge_6[FeCp(CO_2)]_6$. To a solution of $GeCl_2$·Dioxane (2 mmol, 463 mg, 1 eq) in thf (25 mL) cooled to -78°C a solution of $KFeCp(CO)_2$ (4 mmol, 864 mg, 2eq) in thf (25 mL) was added. The resulting reaction mixture was slowly warmed to room temperature under stirring over night. The black solution was then stirred at room temperature for 2 days. Removal of the solvent under vacuum yielded a dark red residue. Washing with pentane and extraction with toluene gave a black toluene solution. Concentration of the extract under vacuum and storage at -28 °C gave dark red crystals of **1** (60 mg, 10 %).

^1H NMR (250 MHz, thf-d8): δ in ppm 4.94 (s, 30H).

^{13}C NMR (62.9 MHz, thf-d8): δ in ppm 85.4 (s), 216.0 (s).

IR (KBr): ν = 1971.24(s, br.), 1917.30(s, br.), 1059.10(w), 1003.97(w, br.), 824.88(m, sh.), 636.10(m, sh.), 572.83(s, sh.), 514.55(m, sh.) cm^{-1}.

[(CO)$_3$Cp$_2$Fe$_2$]-μ-GeCl[FeCp(CO)$_2$]. To a solution of $GeCl_2$·Dioxane (2 mmol, 463 mg, 1 eq) in thf (25 mL) cooled to -78°C a solution of $KFeCp(CO)_2$ (4 mmol, 864 mg, 2eq) in thf (25 mL) was added. The resulting reaction mixture was slowly warmed to room temperature under stirring over night leading to a black reaction solution. Removal of the solvent in vacuum yielded a dark red residue. Washing with pentane and extraction with toluene gave a black toluene solution. The solvent was then removed in vacuum again and the residue was solved in thf. Precipitation with pentane gave a black solid. The protruding solution was filtrated and stored at room temperature forming a black precipitate. Recrystallisation of this precipitate from thf-pentane (3:2) at room temperature gave dark red crystals of **2** (70 mg, 6%).

^{1}H NMR (250 MHz, thf-d8): δ in ppm 4.83 (s, 10H, [(CO)$_3$Cp$_2$Fe$_2$]), 5.18 (s, 5H).

^{13}C NMR (62.9 MHz, thf-d8): δ in ppm 86.5 (s), 87.1 (s), 212.5 (s), 213.8 (s).

IR (KBr): ν= 2008.52(s, sh.), 1958.12(s, sh.), 1937.69(s), 1757.43(s, sh.), 830.71(w), 634.24(w, sh.), 608.54(m, sh.), 583.26(m, sh.), 566.64 (m, sh.), 547.35 (m, sh.), 492.83 (m, sh.) cm^{-1}.

Ge$_6$[FeCp(CO$_2$)]$_6$Cl$_2$. To a solution of $GeCl_2$·Dioxane (2 mmol, 463 mg, 1 eq) in thf (25 mL) cooled to -78°C a solution of $KFeCp(CO)_2$ (4 mmol, 864 mg, 2eq) in thf (25 mL) was added. The resulting reaction mixture was slowly warmed to room temperature under stirring over night. The black solution was then stirred at room temperature for 2 days. Removal of the solvent under vacuum yielded a dark red residue. Washing with pentane and extraction with toluene gave a black toluene solution. The extract was overlayed with pentane what yielded a black precipitate. After filtration and removal of the solvent in vacuo, the resulting dark red residue was solved in a mixture of pentane-thf (2:1). After storage at +6°C, the resulting dark red solution gave black hexagonal crystals of **3** (65 mg, 12%).

^{1}H NMR (400 MHz, thf-d8): δ in ppm 5.09 (t, J= 0.56 Hz, 20H), 4.92 (d, J= 0.56 Hz, 10H).

^{13}C NMR (100.6 MHz, thf-d8): δ in ppm 85.4 (s), 85.5 (s), 85.7 (s).

IR (KBr): ν = 1987.06(s, br.), 1961.54(s, sh.), 1059.09(w), 831.72(m), 632.16(m, sh.), 572.88(s, sh.), 506.63(m) cm^{-1}.

$Ge_6[FeCp(CO_2)]_4[Fe_2Cp_2(CO)_3]_2$. To a solution of $GeCl_2$·Dioxane (0.5 mmol, 116 mg, 1 eq) in thf (15 mL) cooled to -78°C a solution of $KFeCp(CO)_2$ (1 mmol, 216 mg, 2eq) in thf (15 mL) was added. The resulting reaction mixture was slowly warmed to room temperature under stirring overnight. The black solution was then stirred at room temperature for 2 days. The reaction mixture was cooled to -78°C again and a solution of K-benzophenone (1M, 0.33 ml, 0.66 eq) in thf was added. The resulting mixture was warmed to room temperature and then stirred overnight. Removal of the solvent in vacuum yielded a dark red residue. Washing with pentane and extraction with toluene gave a black toluene solution. Concentration of the extract under vacuum and storage at -28 °C gave dark red crystals of **5**.

^{1}H NMR (400 MHz, thf-d8): δ in ppm 4.85 (s, 20H, $[Fe_2Cp_2(CO)_3]$), 5.13 (s, 20H).

^{13}C NMR and IR spectra could not be measured because there were only a few crystals formed of **5** which could not be completely separated from side products (see figure S9).

2. Crystallographic details

Crystals were mounted on the diffractometer at 150 K. The data were collected on a Bruker APEX II DUO diffractometer equipped with an IμS microfocus sealed tube and QUAZAR optics for monochromated MoKα radiation (λ = 0.71073 Å) and equipped with an Oxford Cryosystems cryostat. A semiempirical absorption correction was applied using the program SADABS. The structure was solved by direct methods and refined against F^2 for all observed reflections. Programs used: SHELXS and SHELXL[2] within the Olex2 program package.[3] The prismane **2** contains only half of the molecule in the asymmetrical unit, all Cp rings have to be refined with a disorder model. Compound **3** is refined as inversion twin due to an ambiguous flack parameter in the non-centrosymmetric space group *C*c. A refinement in the centrosymmetric space group *C*2/c with half a molecule in the asymmetrical unit leads to a complicated situation at the atom Ge1, where a Cl and a $FeCp(CO)_2$ group is bound. Due to the torsion angle of the two Cl atoms in **3** (92°), both Cl atoms cannot be symmetrical equivalent. Therefore, a disorder model would be needed, which will not give more information than the refinement in the lower symmetric space group *C*c. The H atom positions in all compounds were refined using a riding model. The supplementary crystallographic data (for CCDC numbers, see Table S1) can be obtained online free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html or from Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ; Fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk.

Table S1: Crystallographic details of the presented structures

	$Ge_6[FeCp(CO)_2]_6$ **1** • 3 toluene	$[(CO)_3Cp_2Fe_2]$-μ-$GeCl[FeCp(CO)_2]$ **2**	$Ge_6[FeCp(CO)_2]_6Cl_2$ **3** • 2 THF	$Ge_6[FeCp(CO)_2]_4[\mu\text{-}Fe_2Cp_2(CO)_3]_2$ **5** • 4 toluene
Empirical formula	$C_{63}H_{54}Fe_6Ge_6O_{12}$	$C_{20}H_{15}ClFe_3GeO_5$	$C_{50}H_{46}Cl_2Fe_6Ge_6O_{14}$	$C_{82}H_{72}Fe_8Ge_6O_{14}$
Formula weight	1773.70	610.91	1712.41	2163.73
Temperature/K	150.1	150.0	150.01	150.0
Crystal system	monoclinic	monoclinic	monoclinic	tetragonal
Space group	*C*2/c	$P2_1/c$	*C*c	$I4_1/a$
a/Å	31.133(2)	13.6340(12)	11.6575(9)	20.9394(10)
b/Å	11.6457(8)	9.1694(8)	21.880(2)	20.9394(10)
c/Å	19.5361(15)	17.4443(15)	22.8176(18)	17.7553(19)
α/°	90	90	90	90
β/°	111.2250(10)	111.6570(10)	95.141(2)	90
γ/°	90	90	90	90
Volume/$Å^3$	6602.7(8)	2026.9(3)	5796.6(9)	7785.0(11)
Z	4	4	4	4
$\rho_{calc}g/cm^3$	1.784	2.002	1.962	1.846
μ/mm^{-1}	4.021	3.736	4.667	3.784
F(000)	3504.0	1208.0	3360.0	4304.0
Crystal size/mm^3	0.39 × 0.151 × 0.148	0.296 × 0.24 × 0.239	0.365 × 0.239 × 0.056	0.226 × 0.21 × 0.117
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.768 to 61.034	4.864 to 61.154	3.584 to 66.42	4.918 to 56.994
Index ranges	$-44 \le h \le 44$, $-16 \le k \le 16$, $-27 \le l \le 27$	$-19 \le h \le 19$, $-13 \le k \le 11$, $-24 \le l \le 24$	$-17 \le h \le 17$, $-33 \le k \le 33$, $-35 \le l \le 35$	$-28 \le h \le 28$, $-28 \le k \le 27$, $-23 \le l \le 23$
Reflections collected	29701	19341	147873	33705
Independent reflections	10079 R_{int} = 0.0416, R_{sigma} = 0.0565	6230 R_{int} = 0.0269, R_{sigma} = 0.0300	22110 R_{int} = 0.0480, R_{sigma} = 0.0320	4915 R_{int} = 0.0545, R_{sigma} = 0.0378
Data/restraints/parameters	10079/430/544	6230/0/271	22110/134/704	4915/68/251
Goodness-of-fit on F^2	1.047	1.050	1.076	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0420, wR_2 = 0.0976	R_1 = 0.0269, wR_2 = 0.0642	R_1 = 0.0322, wR_2 = 0.0755	R_1 = 0.0497, wR_2 = 0.1301
Final R indexes [all data]	R_1 = 0.0769, wR_2 = 0.1094	R_1 = 0.0331, wR_2 = 0.0667	R_1 = 0.0387, wR_2 = 0.0783	R_1 = 0.0776, wR_2 = 0.1540
Largest diff. peak/hole / e $Å^{-3}$	0.99/-0.46	0.70/-0.58	1.17/-0.60	1.28/-0.85
Flack parameter	-	-	0.491(8)	-
CCDC	1878047	1878049	1878046	1878048

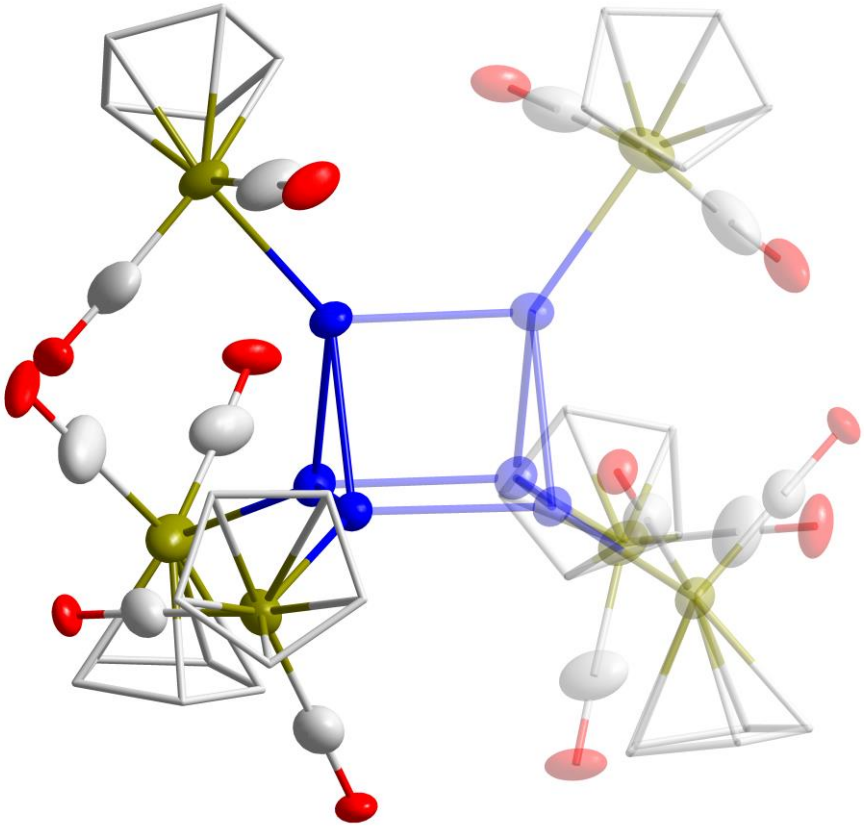

Figure S2: Molecular structure of **1**. The atoms generated by a symmetry operation are showed with 60% transparency. Symmetry operation: -X, Y, 1/2-Z

3. Spectroscopical investigations

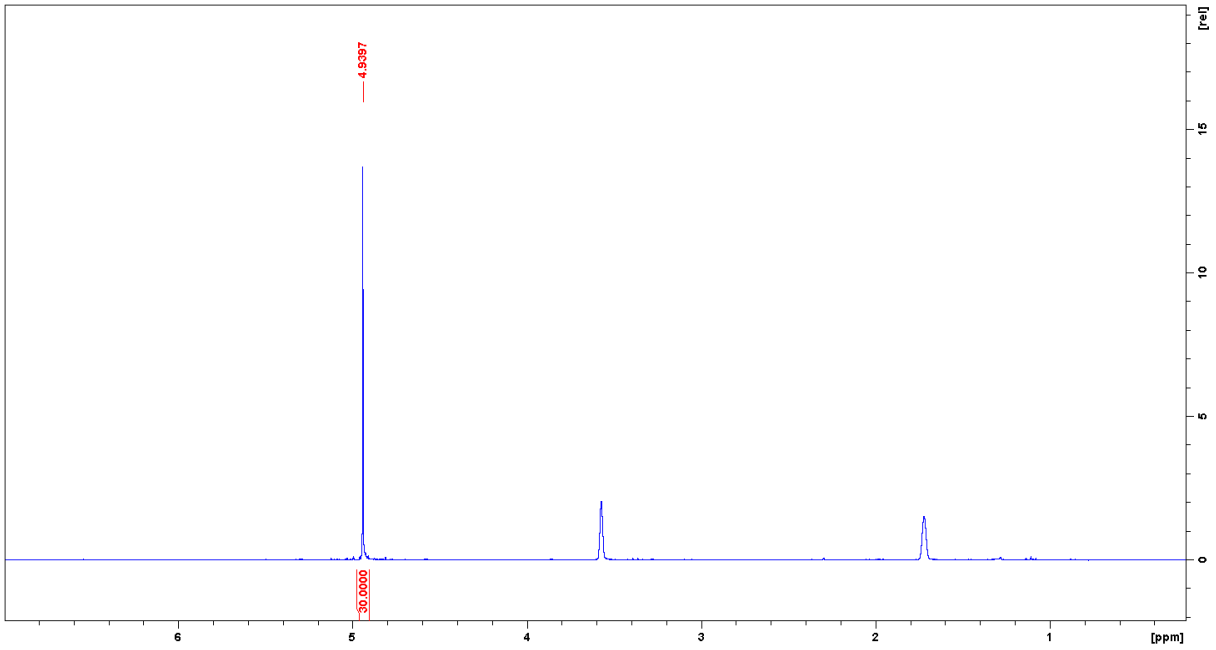

Figure S3: ^{1}H NMR spectrum of **1**.

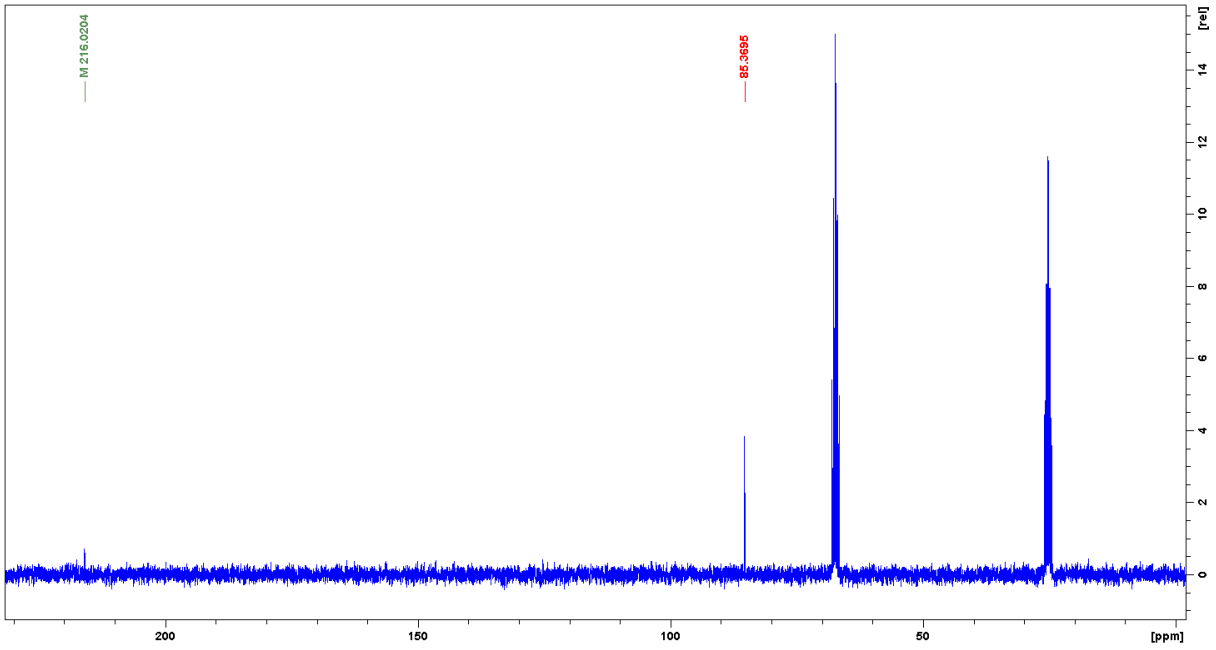

Figure S4: ^{13}C NMR spectrum of **1**.

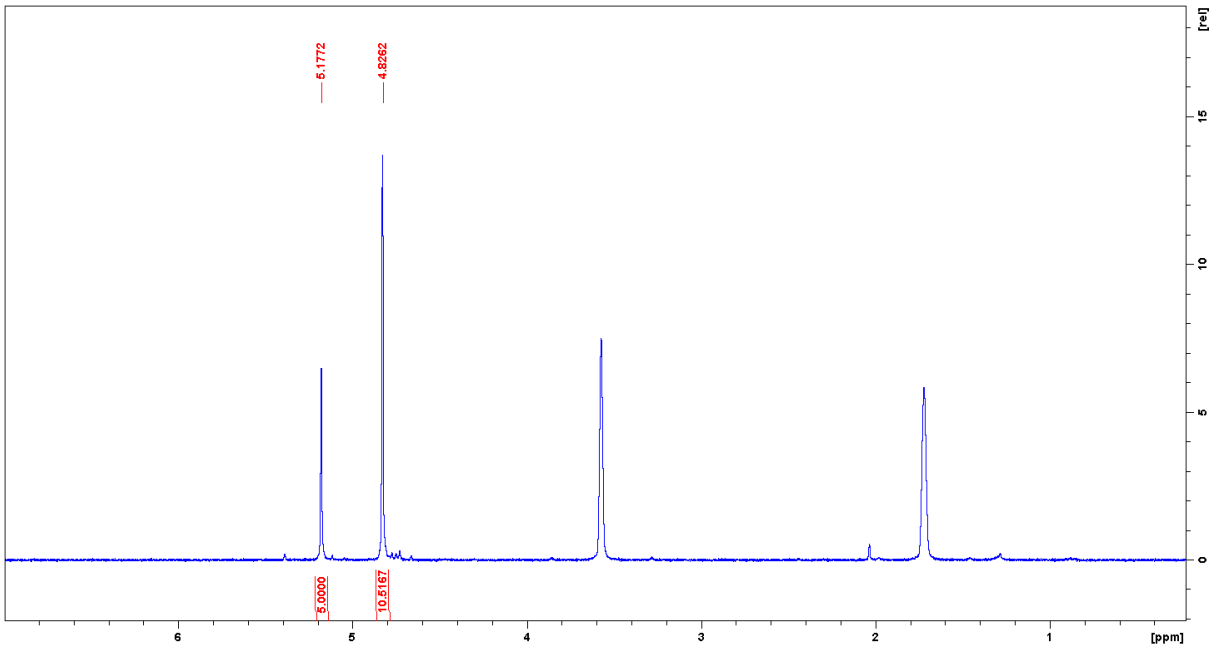

Figure S5: ^{1}H NMR spectrum of **2**.

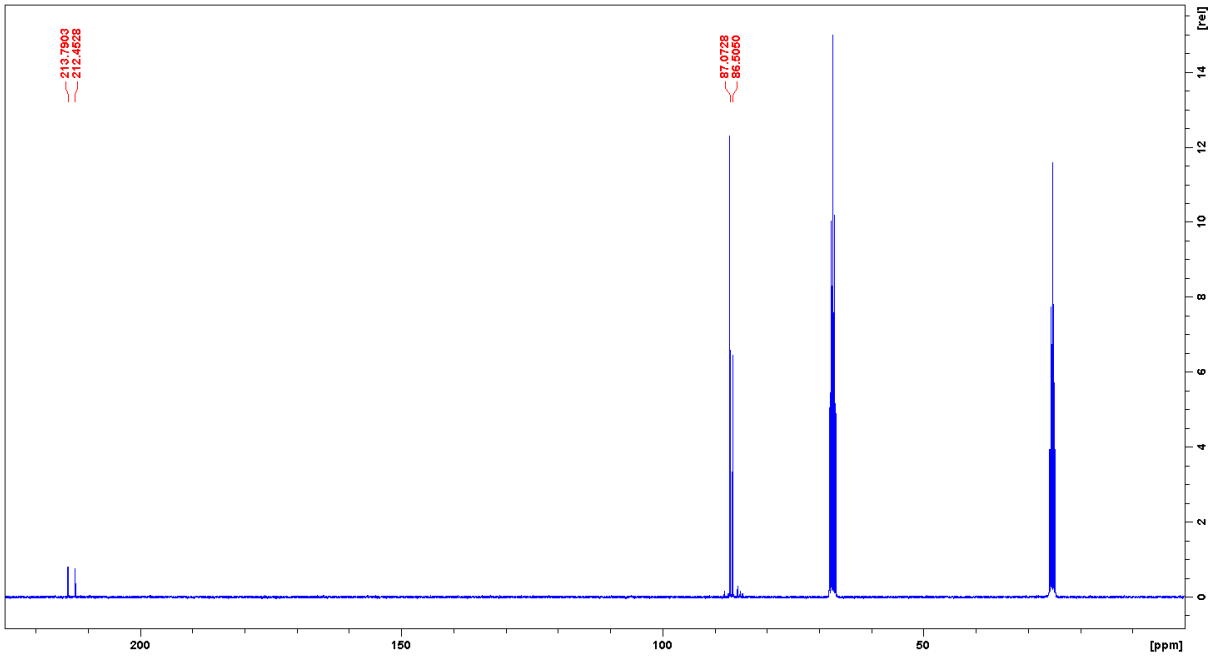

Figure S6: ^{13}C NMR spectrum of **2**.

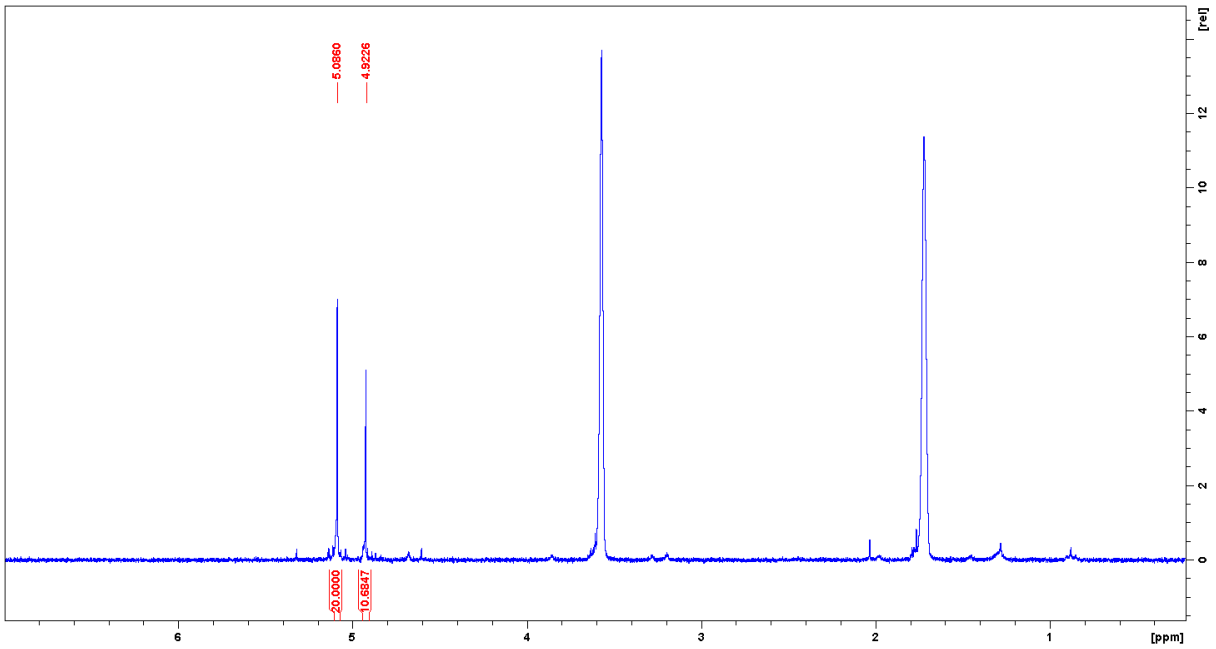

Figure S7: ^{1}H NMR spectrum of **3**.

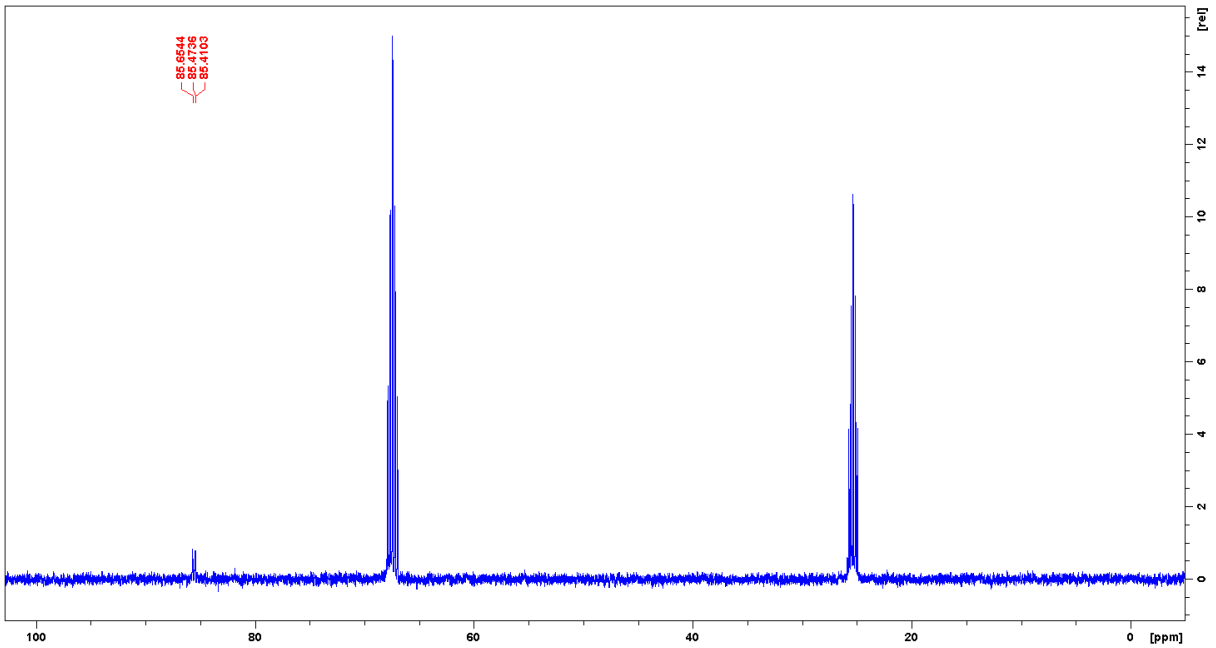

Figure S8: ^{13}C NMR spectrum of **3**.

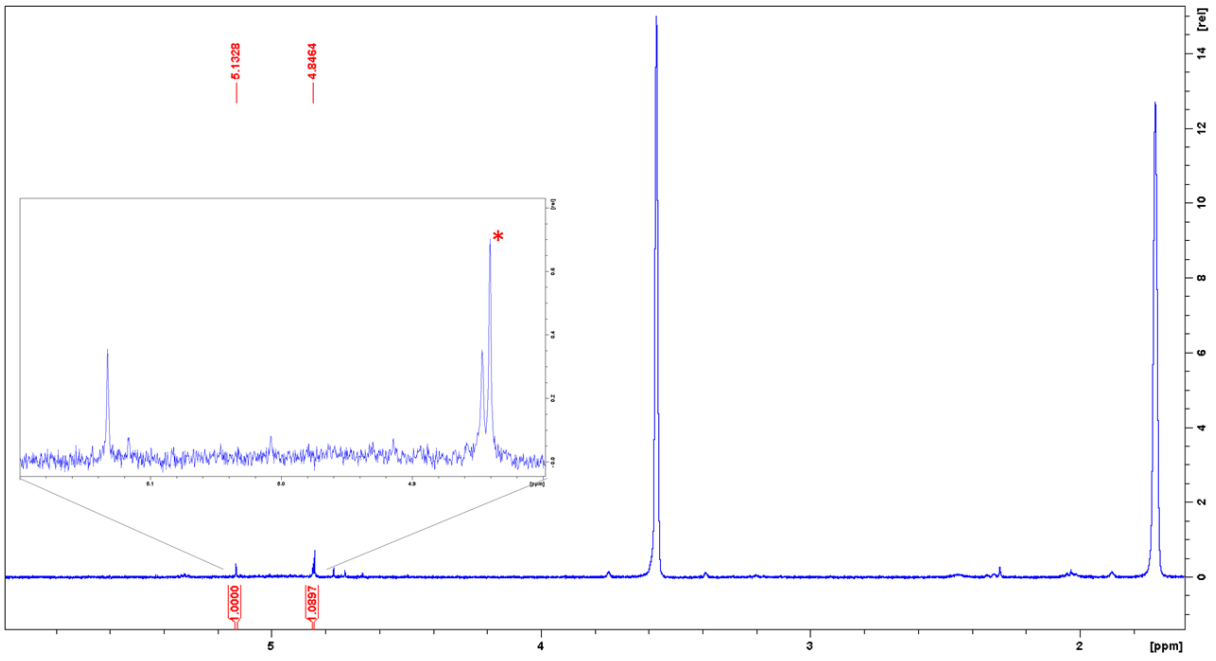

Figure S9: ^{1}H NMR spectrum of **5**. The crystals were washed with cold toluene but it was not possible to remove all the dimer $(CO)_2CpFe\text{-}FeCp(CO)_2$ (*, singulet, 4.84 ppm).

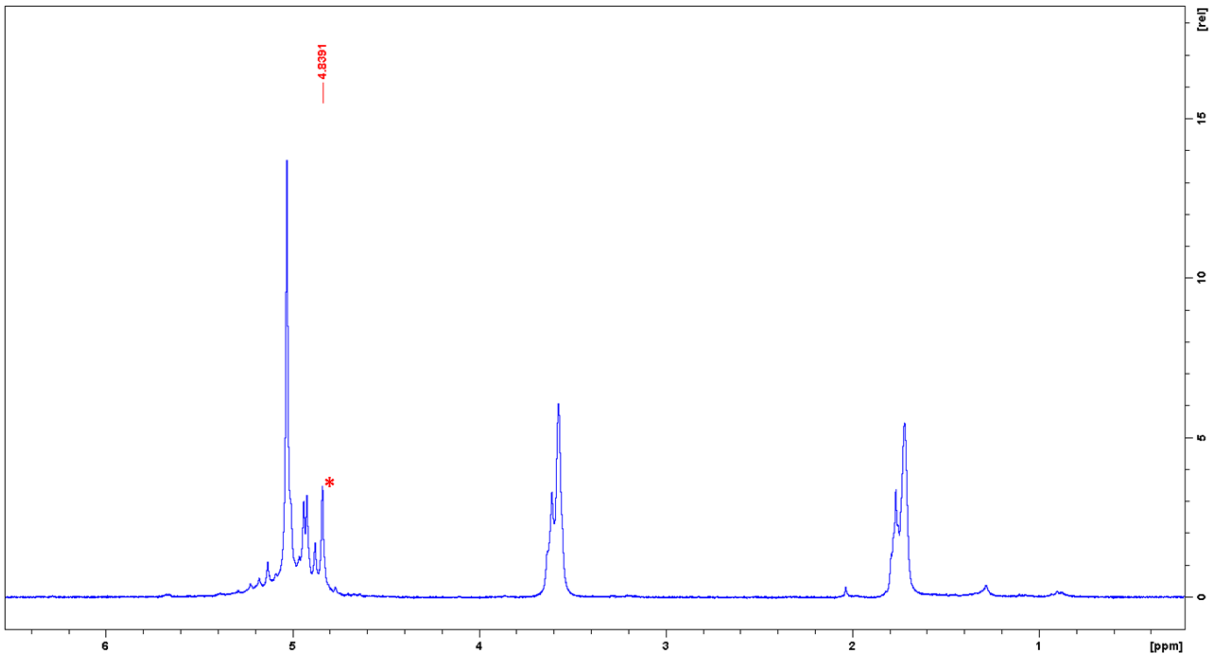

Figure S10: ^{1}H NMR spectrum of a reaction mixture showing the presence of the side product $(CO)_2CpFe\text{-}FeCp(CO)_2$ (*, singulet, 4.84 ppm).

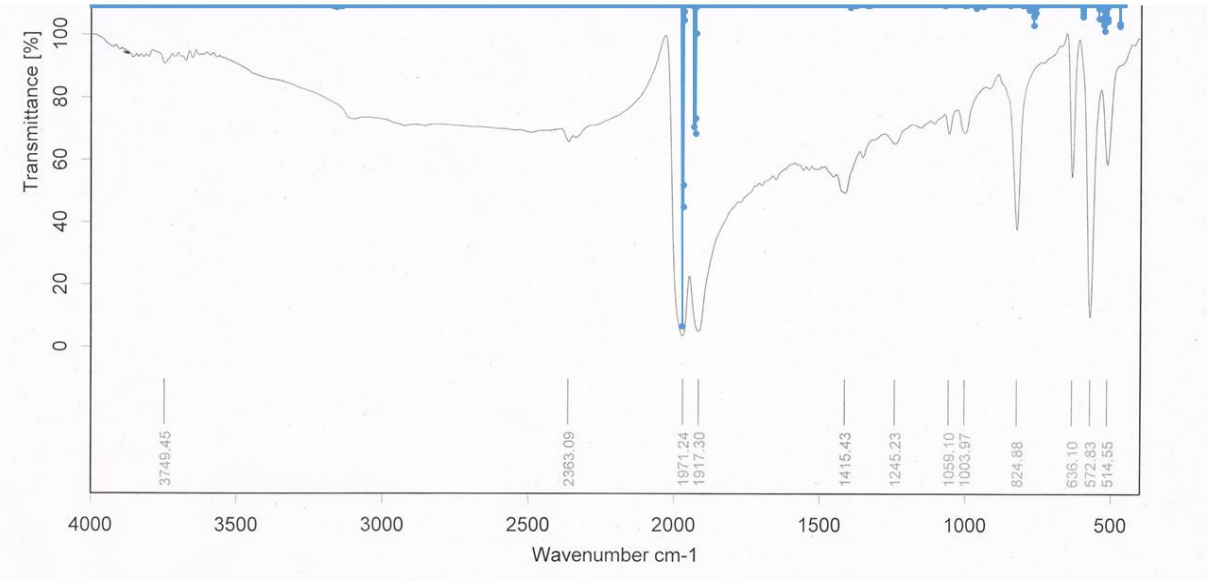

Figure S11: Measured (black) and calculated (blue) IR spectra of **1**.

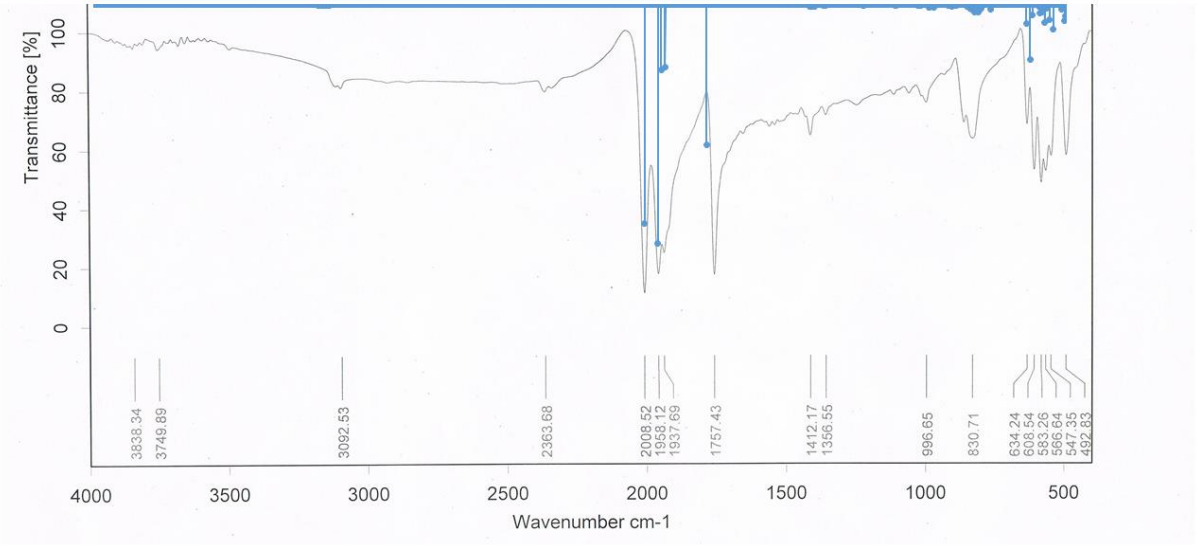

Figure S12: Measured (black) and calculated (blue) IR spectra of **2**.

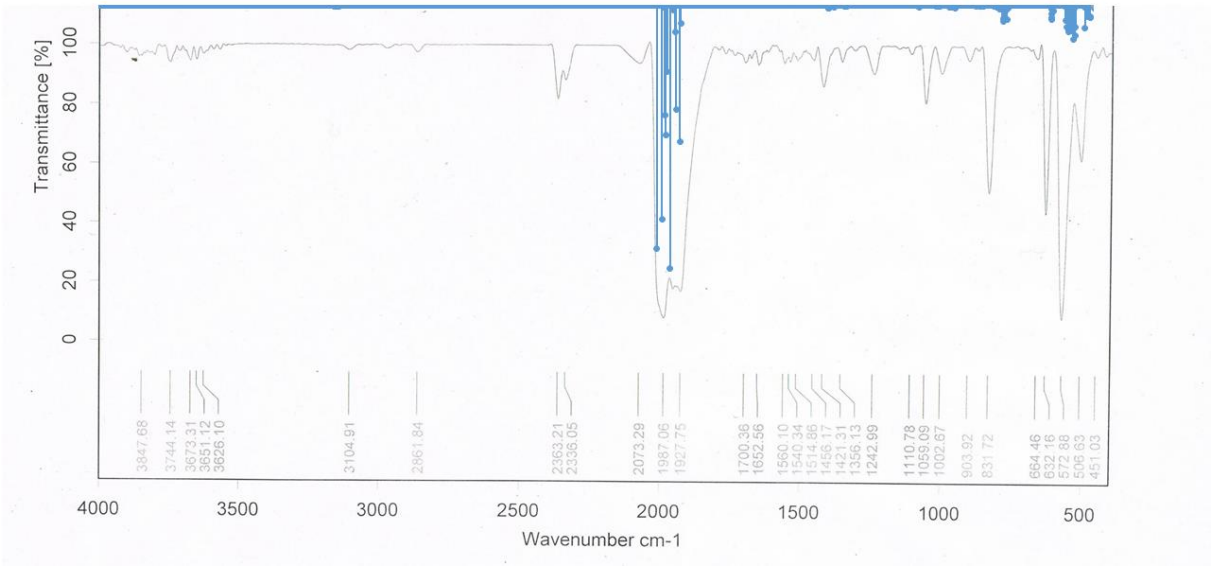

Figure S13: Measured (black) and calculated(blue) IR spectra of **3**.

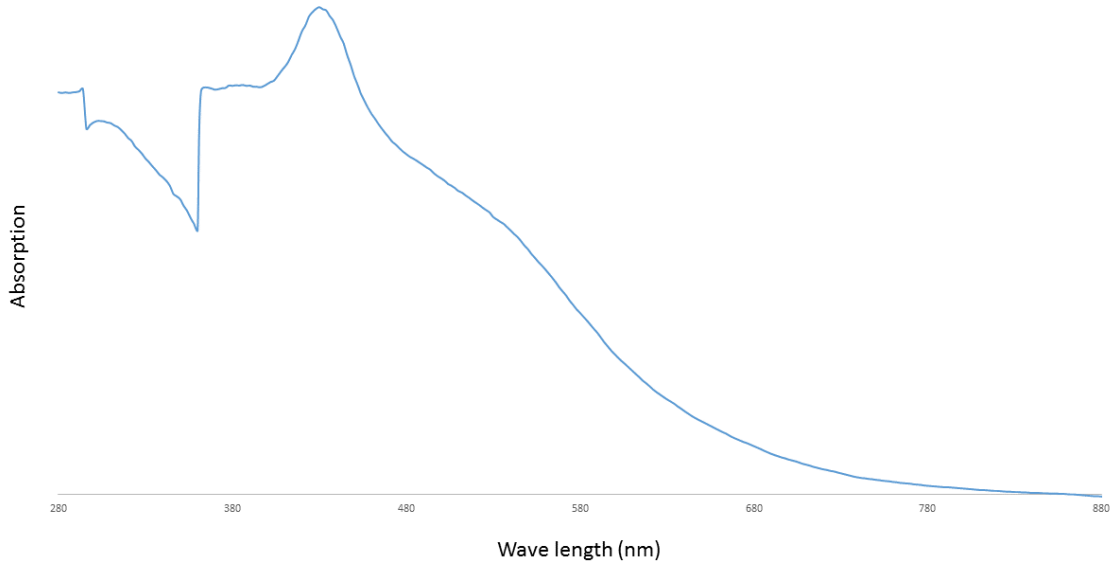

Figure S14: UV-Vis spectrum of **1** in thf solution.

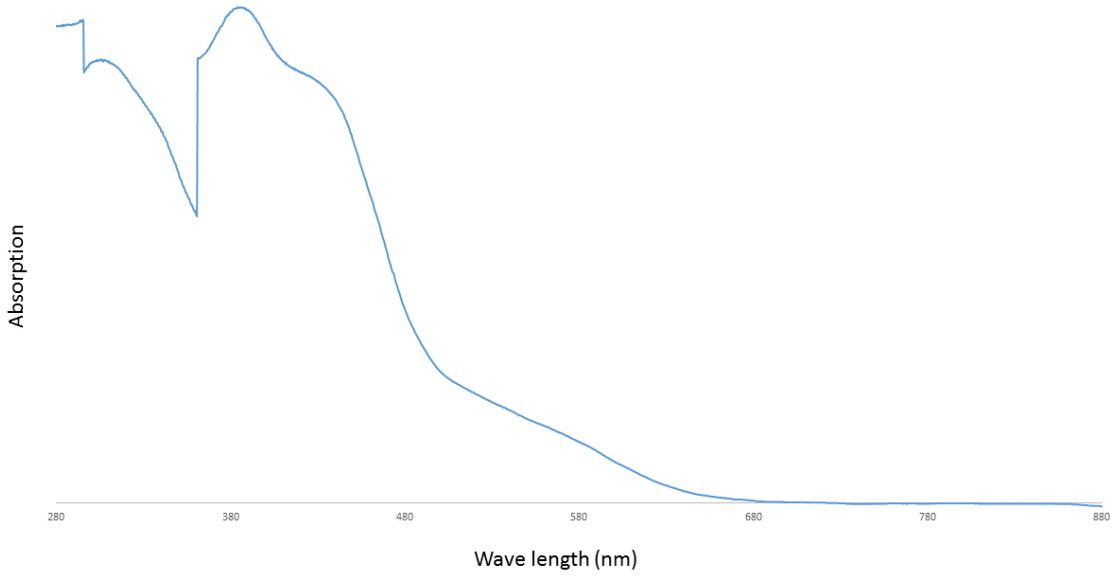

Figure S15: UV-Vis spectrum of **2**.

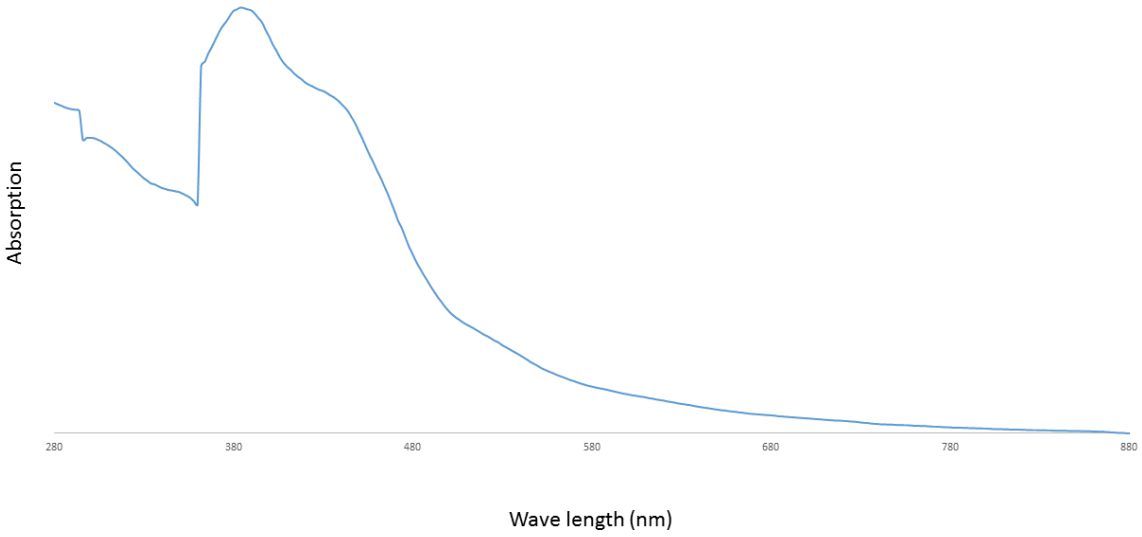

Figure S15: UV-Vis spectrum of **3**.

4. Quantum chemical calculations

All quantum-chemical calculations were carried out with the RI-DFT version of the Turbomole program package and the TmoleX graphical user interface by employing the BP86-functional. The basis sets were of SVP quality.[4] Dispersion forces were modelled with the DFT-D3 correction implemented in TURBOMOLE. [5] Solvent effects were modelled with the COSMO program.[6] To get a reliable value for thermodynamical calculations fort the Gibbs‘ Free Enthalpy the FREEH routine was used. All model compounds are calculated as structural optimized.

4.1 Calculated Enthalpies for the Dimerization and Tetramerization of $GeCl_2$•dioxane

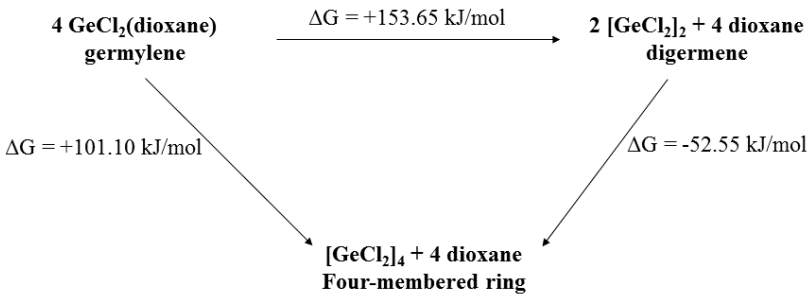

Figure S16: Monomer – Dimer and Monomer – Tetramer equilibrium of $GeCl_2$ to give the digermene or the four membered ring system and dioxane, respectively.

4.2 $GeClFeCp(CO)_2$

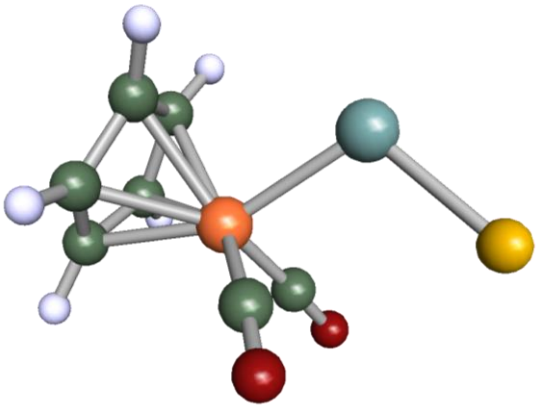

Figure S17: Optimized calculated structure of $GeClFeCp(CO)_2$

Total energy:	-4221.00597854002 H
symmetry used:	C_1
HOMO-LUMO gap:	1.942 eV
lowest vibrational eigenvalue:	18.95 cm^{-1}

Atomic coordinates:

Ge	-2.271607	0.244007	-1.140037
Cl	-2.634185	-1.146760	-2.920529
H	1.900181	1.809249	-0.397353
C	-0.609286	0.656937	1.548297
Fe	-0.129622	-0.230929	-0.339373
H	2.498613	-0.535715	0.861810
C	-0.544944	-1.927305	-0.415567
C	0.440950	-0.183835	-1.991222
H	0.307600	-1.269068	2.309996
O	-0.762953	-3.074052	-0.436653
H	-1.594618	0.657728	2.033609
H	-0.601066	2.576574	0.349801
C	1.561699	0.028106	0.951786
O	0.884805	-0.158919	-3.070756
C	1.239954	1.255191	0.283521
C	0.405837	-0.358698	1.703560
C	-0.091359	1.657490	0.669111

4.3 $[GeClFeCp(CO)_2]_2$

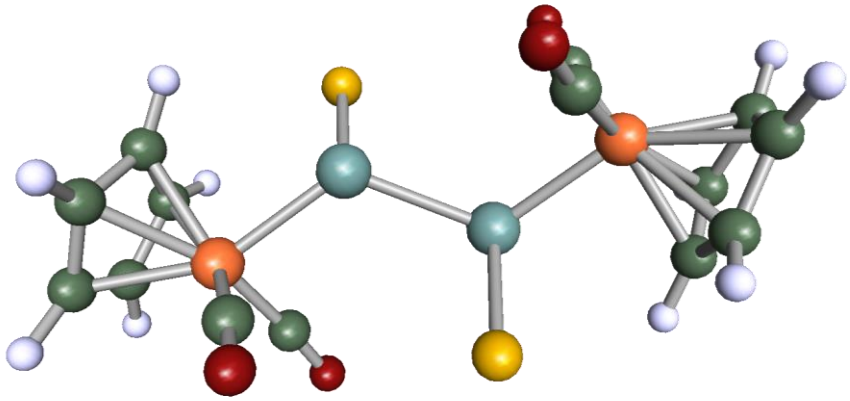

Figure S18: Optimized calculated structure of $[GeClFeCp(CO)_2]_2$

Total energy:	-8442.05762351493 H
symmetry used:	C_1
HOMO-LUMO gap:	1.455 eV
lowest vibrational eigenvalue:	6.73 cm^{-1}

Atomic coordinates:

Ge	-0.822970	0.780787	0.414425	C	-2.790269	0.898274	4.083965
Ge	0.461893	-1.082845	-0.577680	C	-2.710050	2.390050	2.299376
Cl	-2.823068	0.623278	-0.678988	H	3.991653	-1.214841	-1.885744
Cl	2.288941	-0.951474	0.814364	C	1.544410	-2.857249	-3.535016
H	-1.267885	3.810124	3.302085	Fe	1.281500	-0.885933	-2.775745
C	-3.272708	1.147488	2.747193	H	3.565513	-0.290092	-4.427495
Fe	-1.162752	0.983905	2.721594	C	-0.337771	-0.597864	-3.377490
H	-1.374981	2.063929	5.401243	C	1.592875	0.788712	-2.391329
C	-0.911642	-0.745480	2.818537	H	1.542053	-1.750617	-5.517676
C	0.531085	1.384601	2.941195	O	-1.390874	-0.413543	-3.844871
H	-3.033816	0.021933	4.699205	H	0.740207	-3.592735	-3.666532
O	-0.770623	-1.893482	2.973200	H	2.306448	-3.296759	-1.450233
H	-3.945491	0.503805	2.166933	C	3.031541	-1.119211	-3.945111
H	-2.906000	2.871737	1.333025	O	1.850784	1.912843	-2.204598
C	-1.919370	1.966010	4.453293	C	3.261591	-1.607162	-2.605032
O	1.636021	1.686861	3.155920	C	1.970862	-1.883228	-4.515779
C	-1.860597	2.886631	3.340732	C	2.355043	-2.693241	-2.366209

4.4 $[GeClFeCp(CO)_2]_4$

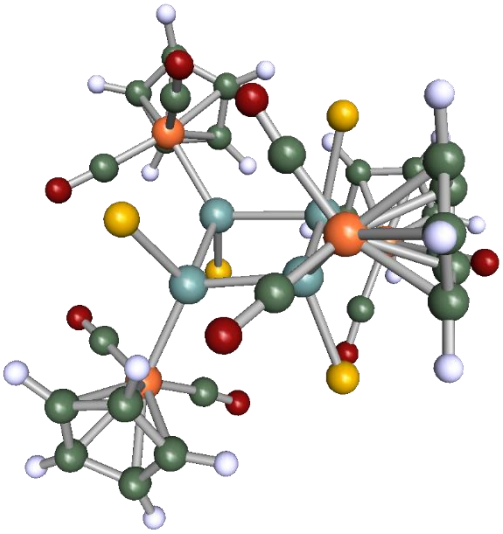

Figure S19: Optimized calculated structure of $[GeClFeCp(CO)_2]_4$

Total energy:	-16884.23680625217 H
symmetry used:	C_1
HOMO-LUMO gap:	1.963 eV
lowest vibrational eigenvalue:	15.74 cm^{-1}

Atomic coordinates:

```
Ge 1.071110 -1.627813 -0.108344
Ge 1.324961 0.855078 -0.357300
Ge -1.158162 1.121492 -0.146633
Ge -1.414679 -1.359863 -0.173489
Cl -2.063921 -1.837961 1.952688
Cl -1.790346 1.757291 -2.245749
Cl 1.542483 -2.461896 -2.179634
Cl 2.109643 1.523026 1.685247
H  0.173707 4.112012 1.927499
C  -2.872923 4.145234 0.450740
Fe -2.142365 2.464518 1.494362
H  -1.899120 4.313933 3.688153
C  -3.551736 1.436514 1.380696
C  -1.388140 1.521734 2.767102
H  -4.221644 4.300431 2.268950
O  -4.517499 0.784706 1.335323
H  -3.579847 4.092872 -0.386925
H  -0.888361 4.049870 -0.602545
C  -1.989544 4.261265 2.595232
O  -0.918060 0.989844 3.689156
C  -0.890145 4.164762 1.660853
C  -3.207563 4.254188 1.850982
C  -1.443206 4.104449 0.341091
H  3.720855 -4.687613 0.049623
C  4.084636 -1.673819 1.537860
Fe 2.250954 -2.745003 1.576557
H  3.846659 -4.820662 2.782741
C  1.388807 -1.851631 2.816858
C  1.065133 -4.015497 1.469423
H  4.108578 -2.279872 3.722944
O  0.898874 -1.308177 3.721369
H  4.148375 -0.578933 1.584742
H  3.972730 -2.089283 -0.681858
C  3.911906 -3.908810 2.175219
O  0.295111 -4.894080 1.416488
C  3.844806 -3.838852 0.734607
```

C	4.051397	-2.574652	2.666613
C	3.965438	-2.463309	0.348271
H	0.358198	3.713462	-2.666049
C	3.408225	3.606993	-1.200843
Fe	2.513731	1.910504	-2.076856
H	2.425476	3.558534	-4.438127
C	3.799059	0.775775	-1.775141
C	1.711410	0.916149	-3.281563
H	4.750196	3.462994	-3.025709
O	4.690791	0.042236	-1.589769
H	4.114760	3.568281	-0.362032
H	1.433784	3.793721	-0.141628
C	2.520886	3.602284	-3.345187
O	1.222533	0.330777	-4.160053
C	1.425143	3.699150	-2.406984
C	3.740101	3.551448	-2.605102
C	1.982295	3.711508	-1.087228
H	-0.679019	-4.475176	-2.207538
C	-3.693703	-4.014810	-0.745435
Fe	-2.694710	-2.471001	-1.777222
H	-2.755734	-4.317501	-3.982858
C	-3.897016	-1.216225	-1.594938
C	-1.846548	-1.649557	-3.074205
H	-5.047534	-3.929948	-2.565966
O	-4.726094	-0.400613	-1.503032
H	-4.385144	-3.852558	0.091263
H	-1.712165	-4.267061	0.304625
C	-2.837942	-4.259459	-2.889429
O	-1.337215	-1.177982	-4.008690
C	-1.740389	-4.356521	-1.953519
C	-4.040627	-4.055216	-2.146812
C	-2.277509	-4.215193	-0.633440

4.5 $GeCl_2$•dioxane

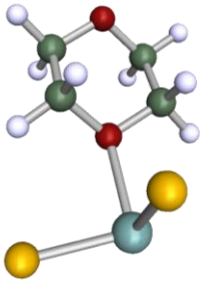

Figure S20: Optimized calculated structure of $GeCl_2$•dioxane

Total energy: -3304.81221156187 H

symmetry used: C_1

HOMO-LUMO gap: 4.326 eV

lowest vibrational eigenvalue: 46.18 cm^{-1}

Atomic coordinates:

C	1.427872	-0.953644	0.389564
O	2.021375	0.312641	0.110402
C	1.190839	1.363837	0.592421
C	-0.191775	1.308337	-0.046972
O	-0.795627	0.008455	0.234317
C	0.054827	-1.075836	-0.256879
H	1.335930	-1.107731	1.493849
H	1.088029	1.305682	1.704893
H	-0.134553	1.439894	-1.150783
H	0.113078	-0.997374	-1.364708
H	2.100780	-1.733115	-0.025428
H	1.681684	2.323795	0.327310
H	-0.869218	2.072392	0.388182
Ge	-2.949045	0.009266	-0.193337
H	-0.454453	-2.017483	0.026151
Cl	-3.124312	-2.226098	0.205978
Cl	-2.495431	-0.033019	-2.434960

4.6 Ge_2Cl_4

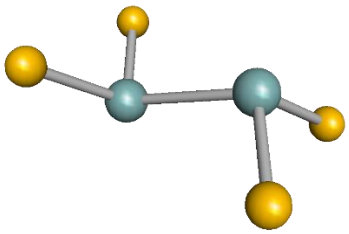

Figure S21: Optimized calculated structure of Ge_2Cl_4

Total energy:	-5994.67425072436 H
symmetry used:	C_1
HOMO-LUMO gap:	2.031 eV
lowest vibrational eigenvalue:	21.33 cm^{-1}

Atomic coordinates:

```
Ge -1.267386 -0.409825 -0.213260
Ge 1.265442 0.405340 0.202209
Cl -2.481591 0.572919 1.354674
Cl -1.928811 0.577194 -2.080450
Cl 1.925473 -0.550868 2.085209
Cl 2.486872 -0.594759 -1.348382
```

4.7 Ge_4Cl_8

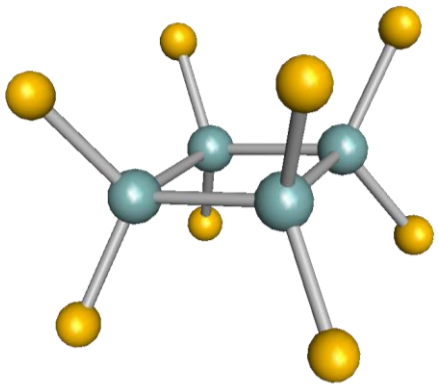

Figure S22: Optimized calculated structure of Ge_4Cl_8

Total energy:	-11989.39727989250 H
symmetry used:	C_1
HOMO-LUMO gap:	2.165 eV
lowest vibrational eigenvalue:	6.13 cm^{-1}

Atomic coordinates:

```
Ge 1.241713 -1.249818 0.001663
Ge 1.245808 1.249548 -0.001711
Ge -1.253654 1.253411 0.004033
Ge -1.257745 -1.246140 -0.003567
Cl -2.126372 -2.114247 1.787772
Cl -2.111337 -2.096523 -1.810724
Cl -2.104744 2.105442 1.811612
Cl -2.120887 2.123744 -1.786916
Cl 2.094963 -2.105942 1.806268
Cl 2.106800 -2.115905 -1.792397
Cl 2.100609 2.103515 -1.806584
Cl 2.113266 2.113895 1.792024
```

4.8 $Ge_6[FeCp(CO)_2]_6$ **1**

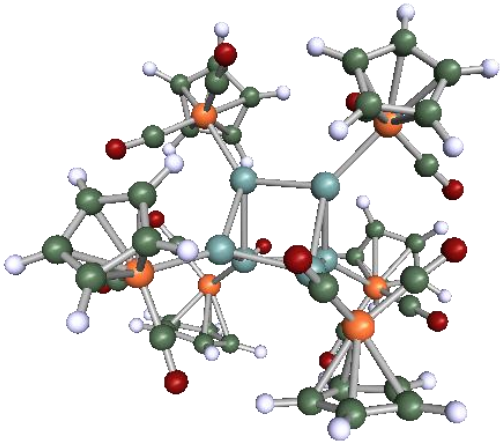

Figure S23: Optimized calculated structure of $Ge_6[FeCp(CO)_2]_6$ **1**

Total energy:	23485.44271627712 H
symmetry used:	C_1
HOMO-LUMO gap:	1.463 eV
lowest vibrational eigenvalue:	23.16 cm^{-1}

Atomic coordinates:

```
Ge 0.409807 -2.527528 -0.173999
Ge -0.755894 -0.531786 -
1.194764
Ge 1.474811 -0.623331 1.150005
Fe -0.670385 -4.567536 0.567135
Cl 1.944515 -3.332755 -1.690489
Ge -0.803836 0.533207 1.166088
Ge 1.519557 0.624753 -1.087392
Fe -2.351826 -0.586123 -
3.043267
Fe 3.246173 -0.664803 2.815807
C 1.218704 -4.974707 1.494741
C 0.861138 -6.036008 0.602124
C -0.382232 -6.611537 1.060115
C -0.795320 -5.889234 2.219022
C 0.190349 -4.867555 2.488151
C -2.109853 -3.670867 0.955884
C -1.164589 -4.805292 -1.090925
Ge 0.403251 2.528176 0.193587
Fe -2.473891 0.591552 2.948438
Fe 3.357522 0.668527 -2.679427
C -3.850265 -1.166394 -1.628853
C -4.237866 0.042267 -2.295177
C -4.332204 -0.239682 -3.708573
C -3.992608 -1.610656 -3.907443
C -3.689152 -2.188295 -2.618219
C -1.150475 -1.499032 -3.930363
C -1.722711 0.960269 -3.537151
C 1.783672 -0.592184 4.374844
C 4.145661 0.414401 1.770340
C 2.763152 -1.594160 4.666132
C 4.052730 -0.951645 4.755661
C 3.854115 0.442214 4.510115
C 2.451651 0.671868 4.266823
C 3.841877 -2.131969 2.076981
H 2.133719 -4.372351 1.425697
H 1.436803 -6.342822 -0.280803
H -0.917120 -7.448955 0.592507
H -1.708203 -6.069751 2.802645
H 0.144282 -4.133587 3.303146
O -3.122787 -3.137129 1.207700
O -1.543813 -5.016920 -2.176165
```

Fe -0.651701 4.563427 -0.593592	O -1.487851 -1.979392 3.891454
Cl 1.882039 3.336400 1.762169	C 2.954191 1.594256 -4.550610
C 1.274293 4.977356 -1.439266	C 4.244647 0.948323 -4.585115
C 0.866985 6.045836 -0.576981	C 4.032294 -0.444409 -4.344496
C -0.359190 6.604631 -1.097597	C 2.620488 -0.669788 -4.158814
C -0.712730 5.864484 -2.265004	C 1.960812 0.595617 -4.297604
C 0.293305 4.849340 -2.477080	C 3.919929 2.138027 -1.919195
C -2.075012 3.663804 -1.030817	C 4.216229 -0.407780 -1.597269
C -1.209079 4.806079 1.043654	H 2.767662 2.666264 -4.701166
H 2.190140 4.384028 -1.321487	H 5.211310 1.438418 -4.761586
H 1.399192 6.368935 0.327142	H 4.813465 -1.215202 -4.292649
H -0.922016 7.442630 -0.665063	H 2.144122 -1.630857 -3.924681
H -1.599838 6.028830 -2.891406	H 0.882261 0.774567 -4.229613
H 0.291393 4.106214 -3.285179	O 4.326182 3.149012 -1.498710
O -3.077641 3.128262 -1.317737	O 4.863394 -1.130165 -0.952883
O -1.630968 5.019331 2.112692	H -3.693995 -1.295706 -0.551083
C -4.478884 0.243854 3.535205	H -4.419804 1.018959 -1.829529
C -4.151083 1.617052 3.738811	H -3.380869 -3.225714 -2.436284
C -3.796944 2.187060 2.459170	H -4.610218 0.479506 -4.490563
C -3.914729 1.158241 1.470929	H -3.962320 -2.137891 -4.870542
C -4.325848 -0.047187 2.128776	O -0.408829 -2.112420 -4.589286
C -1.311726 1.512944 3.878315	O -1.334531 1.990147 -3.937026
C -1.861703 -0.951330 3.473520	H 0.708451 -0.768336 4.261909
H -4.786605 -0.471015 4.310017	H 2.567600 -2.665988 4.805998
H -4.161371 2.150506 4.698863	H 1.987649 1.634636 4.015734
H -3.484498 3.224189 2.282809	H 5.010152 -1.444508 4.970875
H -3.714428 1.281130 0.399786	H 4.638846 1.211062 4.493064
H -4.485370 -1.027582 1.662640	O 4.816254 1.138436 1.152284
O -0.598187 2.132336 4.562132	O 4.266264 -3.141595 1.671291

Vibrational analysis:

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.16	0.10805	YES	YES
8	a	24.71	0.24406	YES	YES
9	a	25.65	0.07956	YES	YES
10	a	27.36	0.13672	YES	YES
11	a	29.71	0.06393	YES	YES
12	a	33.13	0.41939	YES	YES
13	a	35.67	0.21347	YES	YES
14	a	36.37	0.34878	YES	YES
15	a	40.85	0.07446	YES	YES
16	a	41.83	0.40656	YES	YES
17	a	43.08	0.02860	YES	YES
18	a	43.95	0.06342	YES	YES
19	a	45.74	0.12886	YES	YES
20	a	46.91	0.17875	YES	YES
21	a	47.14	0.44345	YES	YES

22	a	47.87	0.16617	YES	YES
23	a	48.15	0.27173	YES	YES
24	a	51.24	0.11156	YES	YES
25	a	52.79	0.06525	YES	YES
26	a	53.90	0.13372	YES	YES
27	a	56.01	0.14826	YES	YES
28	a	57.30	0.36995	YES	YES
29	a	58.08	0.64795	YES	YES
30	a	60.80	0.28465	YES	YES
31	a	65.61	0.02950	YES	YES
32	a	65.83	0.10053	YES	YES
33	a	69.28	0.01542	YES	YES
34	a	69.38	0.14903	YES	YES
35	a	72.78	0.74770	YES	YES
36	a	72.92	0.69789	YES	YES
37	a	74.36	0.01208	YES	YES
38	a	76.63	0.10018	YES	YES
39	a	77.87	0.47847	YES	YES
40	a	79.08	0.34901	YES	YES
41	a	80.45	0.08339	YES	YES
42	a	82.53	0.18963	YES	YES
43	a	84.07	0.59617	YES	YES
44	a	86.14	0.06007	YES	YES
45	a	92.15	2.10913	YES	YES
46	a	99.77	0.48892	YES	YES
47	a	99.99	0.81022	YES	YES
48	a	103.33	0.99247	YES	YES
49	a	104.62	0.58847	YES	YES
50	a	105.62	1.02501	YES	YES
51	a	109.39	0.48654	YES	YES
52	a	110.23	4.93924	YES	YES
53	a	111.48	0.38593	YES	YES
54	a	115.71	0.21183	YES	YES
55	a	117.93	0.00321	YES	YES
56	a	121.09	0.62911	YES	YES
57	a	121.73	0.07296	YES	YES
58	a	121.88	1.34100	YES	YES
59	a	128.44	0.16375	YES	YES
60	a	132.89	0.92927	YES	YES
61	a	134.99	0.02705	YES	YES
62	a	136.95	0.20675	YES	YES
63	a	140.02	0.03623	YES	YES
64	a	140.99	0.26179	YES	YES
65	a	145.62	7.14771	YES	YES
66	a	145.78	0.11092	YES	YES
67	a	151.83	0.55821	YES	YES
68	a	152.36	0.64474	YES	YES
69	a	159.96	1.21017	YES	YES
70	a	167.76	7.08542	YES	YES
71	a	169.72	4.57540	YES	YES
72	a	176.74	13.56798	YES	YES
73	a	182.55	3.33455	YES	YES
74	a	187.32	2.04555	YES	YES
75	a	201.26	2.40676	YES	YES
76	a	203.20	1.72646	YES	YES
77	a	214.61	18.47288	YES	YES

78	a	250.91	0.29706	YES	YES
79	a	259.96	10.59343	YES	YES
80	a	262.15	17.25135	YES	YES
81	a	264.31	13.06237	YES	YES
82	a	280.42	2.43824	YES	YES
83	a	306.85	49.42197	YES	YES
84	a	313.00	18.74604	YES	YES
85	a	341.62	2.42106	YES	YES
86	a	341.91	1.71607	YES	YES
87	a	344.88	3.97936	YES	YES
88	a	345.72	3.88062	YES	YES
89	a	346.12	1.10742	YES	YES
90	a	347.20	1.74267	YES	YES
91	a	360.53	6.78923	YES	YES
92	a	361.02	2.42055	YES	YES
93	a	361.93	3.76118	YES	YES
94	a	362.85	0.81058	YES	YES
95	a	363.77	3.57009	YES	YES
96	a	364.89	1.69183	YES	YES
97	a	369.22	2.75978	YES	YES
98	a	370.29	2.35811	YES	YES
99	a	371.44	1.75262	YES	YES
100	a	371.64	3.41751	YES	YES
101	a	376.65	0.76169	YES	YES
102	a	377.50	1.23147	YES	YES
103	a	441.24	1.38619	YES	YES
104	a	441.78	0.43722	YES	YES
105	a	447.00	0.30497	YES	YES
106	a	447.50	0.84522	YES	YES
107	a	452.14	1.14194	YES	YES
108	a	452.42	0.82716	YES	YES
109	a	499.02	10.61370	YES	YES
110	a	500.64	0.66317	YES	YES
111	a	500.73	9.43947	YES	YES
112	a	501.73	0.28476	YES	YES
113	a	502.38	2.26718	YES	YES
114	a	502.86	2.97486	YES	YES
115	a	513.18	43.18778	YES	YES
116	a	514.01	39.01787	YES	YES
117	a	522.65	40.77963	YES	YES
118	a	524.07	27.70503	YES	YES
119	a	531.99	80.62672	YES	YES
120	a	533.19	6.94461	YES	YES
121	a	565.74	77.73036	YES	YES
122	a	567.20	108.97657	YES	YES
123	a	569.25	9.40600	YES	YES
124	a	569.34	8.08215	YES	YES
125	a	569.59	2.37704	YES	YES
126	a	569.62	4.33038	YES	YES
127	a	573.15	123.40513	YES	YES
128	a	574.27	84.58917	YES	YES
129	a	577.45	0.61443	YES	YES
130	a	577.67	1.75469	YES	YES
131	a	578.40	67.35923	YES	YES
132	a	579.19	90.92657	YES	YES
133	a	579.57	28.30308	YES	YES

134	a	580.87	85.54939	YES	YES
135	a	581.90	33.75424	YES	YES
136	a	583.46	3.53934	YES	YES
137	a	587.83	97.00657	YES	YES
138	a	588.35	26.76263	YES	YES
139	a	589.53	88.71046	YES	YES
140	a	591.67	0.83409	YES	YES
141	a	594.02	12.35798	YES	YES
142	a	594.83	78.26460	YES	YES
143	a	600.10	54.94116	YES	YES
144	a	601.32	2.17245	YES	YES
145	a	643.33	21.55225	YES	YES
146	a	649.04	8.05463	YES	YES
147	a	649.62	44.54286	YES	YES
148	a	649.92	30.40508	YES	YES
149	a	650.20	14.72473	YES	YES
150	a	650.85	51.06933	YES	YES
151	a	800.91	8.73629	YES	YES
152	a	806.86	50.25045	YES	YES
153	a	809.31	16.43588	YES	YES
154	a	810.59	12.97339	YES	YES
155	a	812.77	4.66144	YES	YES
156	a	813.17	6.01541	YES	YES
157	a	813.28	4.79342	YES	YES
158	a	813.83	17.81005	YES	YES
159	a	814.34	29.47959	YES	YES
160	a	814.95	20.50523	YES	YES
161	a	815.22	9.45116	YES	YES
162	a	817.00	37.64898	YES	YES
163	a	817.33	2.45973	YES	YES
164	a	818.25	9.77260	YES	YES
165	a	818.66	47.09910	YES	YES
166	a	819.84	58.03854	YES	YES
167	a	820.19	5.04176	YES	YES
168	a	820.71	6.70985	YES	YES
169	a	826.63	2.37576	YES	YES
170	a	828.16	11.94252	YES	YES
171	a	829.07	7.00977	YES	YES
172	a	830.05	9.32341	YES	YES
173	a	831.28	11.85541	YES	YES
174	a	832.10	3.49273	YES	YES
175	a	832.93	5.13775	YES	YES
176	a	833.34	10.19344	YES	YES
177	a	840.33	5.23372	YES	YES
178	a	842.90	5.16553	YES	YES
179	a	849.22	4.31643	YES	YES
180	a	851.92	3.63287	YES	YES
181	a	888.68	1.80309	YES	YES
182	a	890.56	0.85697	YES	YES
183	a	894.54	0.04555	YES	YES
184	a	895.34	0.10263	YES	YES
185	a	896.83	0.78649	YES	YES
186	a	897.43	0.26021	YES	YES
187	a	899.92	1.95962	YES	YES
188	a	903.70	2.47681	YES	YES
189	a	908.95	0.74710	YES	YES

190	a	912.16	0.76618	YES	YES
191	a	913.72	1.24295	YES	YES
192	a	916.12	2.01037	YES	YES
193	a	987.51	10.22386	YES	YES
194	a	988.37	5.69962	YES	YES
195	a	989.03	1.52998	YES	YES
196	a	990.27	5.77526	YES	YES
197	a	993.90	4.49296	YES	YES
198	a	994.05	4.29555	YES	YES
199	a	1003.04	5.68347	YES	YES
200	a	1006.08	5.92570	YES	YES
201	a	1006.32	1.26763	YES	YES
202	a	1008.51	4.02701	YES	YES
203	a	1009.39	4.20170	YES	YES
204	a	1009.89	7.16693	YES	YES
205	a	1039.83	0.61134	YES	YES
206	a	1042.64	1.66869	YES	YES
207	a	1044.40	2.37344	YES	YES
208	a	1044.57	0.83513	YES	YES
209	a	1044.67	0.99442	YES	YES
210	a	1044.85	0.53476	YES	YES
211	a	1045.00	0.66524	YES	YES
212	a	1046.81	1.83140	YES	YES
213	a	1051.60	1.97181	YES	YES
214	a	1053.03	0.04167	YES	YES
215	a	1055.15	1.90718	YES	YES
216	a	1056.51	2.00334	YES	YES
217	a	1115.28	1.88119	YES	YES
218	a	1115.45	2.02946	YES	YES
219	a	1116.21	0.32806	YES	YES
220	a	1116.84	4.80329	YES	YES
221	a	1117.95	2.97214	YES	YES
222	a	1118.05	2.26109	YES	YES
223	a	1244.42	0.19642	YES	YES
224	a	1244.74	0.09386	YES	YES
225	a	1246.72	0.46723	YES	YES
226	a	1247.32	0.20543	YES	YES
227	a	1250.51	0.05106	YES	YES
228	a	1251.45	0.05217	YES	YES
229	a	1371.33	3.39432	YES	YES
230	a	1372.24	3.13818	YES	YES
231	a	1373.24	3.00714	YES	YES
232	a	1373.31	0.32680	YES	YES
233	a	1376.31	0.39825	YES	YES
234	a	1376.73	3.60806	YES	YES
235	a	1376.84	4.14754	YES	YES
236	a	1377.16	1.13130	YES	YES
237	a	1377.40	0.46085	YES	YES
238	a	1377.63	0.14912	YES	YES
239	a	1378.32	0.62564	YES	YES
240	a	1378.53	0.42658	YES	YES
241	a	1414.11	2.26639	YES	YES
242	a	1414.67	5.67470	YES	YES
243	a	1414.88	2.66604	YES	YES
244	a	1415.32	3.02066	YES	YES
245	a	1419.96	1.68474	YES	YES

246	a	1420.14	1.67746	YES	YES
247	a	1432.56	6.50289	YES	YES
248	a	1433.45	9.25002	YES	YES
249	a	1433.86	5.38406	YES	YES
250	a	1433.98	8.92813	YES	YES
251	a	1434.79	10.43103	YES	YES
252	a	1435.54	4.11334	YES	YES
253	a	1955.46	63.98136	YES	YES
254	a	1958.51	492.29360	YES	YES
255	a	1971.51	374.65909	YES	YES
256	a	1974.72	96.37346	YES	YES
257	a	1982.10	15.75845	YES	YES
258	a	1992.94	950.98068	YES	YES
259	a	2003.66	240.44450	YES	YES
260	a	2008.73	470.18545	YES	YES
261	a	2012.34	397.02096	YES	YES
262	a	2017.84	4.95426	YES	YES
263	a	2021.60	773.61043	YES	YES
264	a	2039.47	877.73876	YES	YES
265	a	3152.72	0.20722	YES	YES
266	a	3153.00	0.21525	YES	YES
267	a	3154.54	0.22973	YES	YES
268	a	3155.00	0.21997	YES	YES
269	a	3155.77	0.34392	YES	YES
270	a	3155.88	0.20670	YES	YES
271	a	3158.28	1.16319	YES	YES
272	a	3158.36	1.49419	YES	YES
273	a	3161.18	1.58273	YES	YES
274	a	3161.33	1.54906	YES	YES
275	a	3165.26	0.35617	YES	YES
276	a	3165.82	0.14926	YES	YES
277	a	3168.01	1.71469	YES	YES
278	a	3168.17	1.46231	YES	YES
279	a	3169.24	1.51383	YES	YES
280	a	3169.76	1.50102	YES	YES
281	a	3172.51	3.81509	YES	YES
282	a	3172.72	3.50388	YES	YES
283	a	3173.19	0.25995	YES	YES
284	a	3173.24	1.32015	YES	YES
285	a	3173.46	0.23660	YES	YES
286	a	3174.09	0.78278	YES	YES
287	a	3176.44	0.27833	YES	YES
288	a	3176.73	2.99426	YES	YES
289	a	3180.54	1.21781	YES	YES
290	a	3180.75	1.21840	YES	YES
291	a	3185.35	0.33941	YES	YES
292	a	3186.72	0.47419	YES	YES
293	a	3198.56	0.50082	YES	YES
294	a	3198.66	0.55370	YES	YES

4.9 $[(CO)_3Cp_2Fe_2]$-μ-GeCl$[FeCp(CO)_2]$ 2

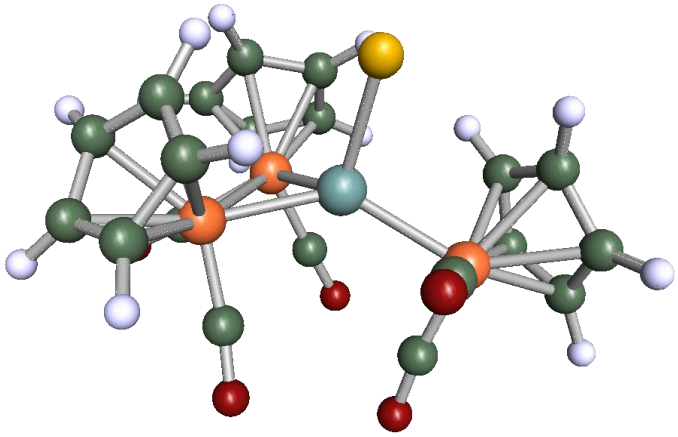

Figure S24: Optimized calculated structure of $[(CO)_3Cp_2Fe_2]$-μ-$GeCl[FeCp(CO)_2]$ **2**

Total energy:	-7475.43530080433 H
symmetry used:	C_1
HOMO-LUMO gap:	2.096 eV
lowest vibrational eigenvalue:	18.48 cm^{-1}

Atomic coordinates:

```
Ge -0.535876 0.232448 0.231367
Fe -0.737701 1.100108 2.411010
Fe -0.401960 -1.921248 -0.66664
Fe 1.407596 -0.047035 -1.043724
Cl -2.160093 1.470941 -0.896556
C 0.772762 2.568318 2.622340
H 1.847725 2.356651 2.558319
C -1.418590 3.066791 2.042380
H -2.307620 3.297836 1.443113
C -1.381302 2.821192 3.463150
H -2.243082 2.844847 4.143001
C -0.034707 2.513055 3.821804
H 0.326871 2.260192 4.827158
C -0.085015 2.920504 1.531927
H 0.227647 3.071469 0.491821
C 0.191997 -0.179749 3.156561
C -2.251146 0.230564 2.428150
C 0.033075 -2.562575 0.883000
C 1.440824 -1.953781 -1.171262
C -2.015241 -3.247069 -0.715440
H -2.358341 -3.828444 0.151448
C -1.016363 -3.667753 -1.669077
H -0.452094 -4.608702 -1.643841
C -0.868377 -2.613993 -2.625475
H -0.162970 -2.602682 -3.466654
C -1.772159 -1.556750 -2.272898
H -1.899788 -0.599918 -2.790392
C -2.490247 -1.947292 -1.094817
H -3.258071 -1.356138 -0.581149
C 0.785094 0.684632 -2.964111
H -0.163330 0.461946 -3.465014
C 1.020150 1.783292 -2.072933
H 0.283210 2.549797 -1.805412
C 2.381844 1.700109 -1.633940
H 2.880104 2.389392 -0.938739
C 2.997539 0.556642 -2.275254
H 4.033153 0.218712 -2.140504
C 2.004695 -0.061055 -3.094347
H 2.142244 -0.970574 -3.692525
C 2.267872 -0.097968 0.457421
O 0.825868 -0.950447 3.758895
O -3.266741 -0.347280 2.452809
O 0.273794 -3.109198 1.890823
O 2.232755 -2.791794 -1.489229
O 2.904018 -0.077936 1.443423
```

Vibrational analysis:

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.48	1.57975	YES	YES
8	a	23.00	0.27486	YES	YES
9	a	42.48	0.56508	YES	YES
10	a	46.74	0.40215	YES	YES
11	a	51.42	0.48548	YES	YES
12	a	60.53	0.20503	YES	YES
13	a	66.83	0.43994	YES	YES
14	a	76.08	0.30279	YES	YES
15	a	85.39	1.19679	YES	YES
16	a	94.73	0.15815	YES	YES
17	a	96.96	1.04428	YES	YES
18	a	99.89	1.01290	YES	YES
19	a	108.77	0.41930	YES	YES
20	a	118.12	0.78155	YES	YES
21	a	127.42	2.55776	YES	YES
22	a	135.72	2.05379	YES	YES
23	a	145.33	1.39194	YES	YES
24	a	147.60	0.65298	YES	YES
25	a	154.15	0.93156	YES	YES
26	a	156.46	3.56730	YES	YES
27	a	166.00	6.76651	YES	YES
28	a	173.05	6.02736	YES	YES
29	a	194.11	2.11145	YES	YES
30	a	203.23	8.71441	YES	YES
31	a	222.15	11.54771	YES	YES
32	a	272.21	15.35573	YES	YES
33	a	276.73	56.65776	YES	YES
34	a	296.27	79.77673	YES	YES
35	a	353.01	17.18688	YES	YES
36	a	353.74	3.16328	YES	YES
37	a	360.47	5.29871	YES	YES
38	a	362.50	14.45824	YES	YES
39	a	377.88	17.62741	YES	YES
40	a	381.80	3.05660	YES	YES
41	a	387.03	8.58571	YES	YES
42	a	398.43	0.47192	YES	YES
43	a	427.11	1.52808	YES	YES
44	a	454.71	3.56465	YES	YES
45	a	459.97	0.30801	YES	YES
46	a	501.24	33.83446	YES	YES
47	a	505.53	82.73190	YES	YES
48	a	508.32	114.26483	YES	YES
49	a	519.10	28.02463	YES	YES
50	a	549.75	176.75641	YES	YES
51	a	563.48	109.39313	YES	YES
52	a	573.15	19.47618	YES	YES
53	a	574.34	21.23569	YES	YES
54	a	575.62	16.78275	YES	YES
55	a	578.74	0.83856	YES	YES

56	a	581.15	124.74371	YES	YES
57	a	583.62	10.62646	YES	YES
58	a	586.41	25.92286	YES	YES
59	a	591.17	51.74420	YES	YES
60	a	599.85	61.94394	YES	YES
61	a	600.88	9.53547	YES	YES
62	a	624.46	73.14595	YES	YES
63	a	633.59	398.25174	YES	YES
64	a	646.60	134.44105	YES	YES
65	a	774.44	31.88737	YES	YES
66	a	806.68	1.25446	YES	YES
67	a	808.59	23.22923	YES	YES
68	a	811.14	16.64464	YES	YES
69	a	811.64	13.89316	YES	YES
70	a	813.60	33.54561	YES	YES
71	a	814.21	1.34343	YES	YES
72	a	816.10	22.86402	YES	YES
73	a	818.61	54.23983	YES	YES
74	a	825.89	43.82567	YES	YES
75	a	833.43	49.94715	YES	YES
76	a	837.97	5.71344	YES	YES
77	a	843.68	29.36876	YES	YES
78	a	851.78	24.33711	YES	YES
79	a	861.04	9.30473	YES	YES
80	a	898.92	0.45825	YES	YES
81	a	902.57	3.58247	YES	YES
82	a	909.89	0.61520	YES	YES
83	a	911.70	0.39735	YES	YES
84	a	916.39	10.74360	YES	YES
85	a	927.22	5.70572	YES	YES
86	a	979.57	14.20477	YES	YES
87	a	984.00	13.93232	YES	YES
88	a	985.71	10.06169	YES	YES
89	a	992.92	8.72968	YES	YES
90	a	996.69	17.76353	YES	YES
91	a	998.33	16.24107	YES	YES
92	a	1028.04	1.61388	YES	YES
93	a	1028.99	1.14759	YES	YES
94	a	1030.46	0.83509	YES	YES
95	a	1030.84	1.11124	YES	YES
96	a	1033.48	0.08432	YES	YES
97	a	1038.69	0.48578	YES	YES
98	a	1114.55	2.54237	YES	YES
99	a	1116.60	5.27873	YES	YES
100	a	1118.50	6.40350	YES	YES
101	a	1232.55	0.30771	YES	YES
102	a	1234.14	0.30555	YES	YES
103	a	1235.35	0.11133	YES	YES
104	a	1369.72	4.82083	YES	YES
105	a	1370.54	2.35010	YES	YES
106	a	1372.80	0.93181	YES	YES
107	a	1373.07	0.69682	YES	YES
108	a	1375.72	3.81581	YES	YES
109	a	1377.40	2.57399	YES	YES
110	a	1408.62	8.47793	YES	YES
111	a	1411.95	12.99755	YES	YES

112	a	1413.98	4.99768	YES	YES
113	a	1423.48	7.23577	YES	YES
114	a	1425.94	12.26250	YES	YES
115	a	1426.47	7.38999	YES	YES
116	a	1798.52	1020.54744	YES	YES
117	a	1947.72	451.40274	YES	YES
118	a	1962.04	472.74322	YES	YES
119	a	1973.58	1738.74434	YES	YES
120	a	2020.92	1595.31599	YES	YES
121	a	3157.73	1.10085	YES	YES
122	a	3158.37	0.49173	YES	YES
123	a	3164.45	0.53699	YES	YES
124	a	3164.75	0.04664	YES	YES
125	a	3168.11	0.06075	YES	YES
126	a	3171.03	0.22824	YES	YES
127	a	3178.44	0.68405	YES	YES
128	a	3178.85	1.20598	YES	YES
129	a	3179.19	0.70138	YES	YES
130	a	3179.75	1.61803	YES	YES
131	a	3181.02	0.49194	YES	YES
132	a	3182.79	1.45356	YES	YES
133	a	3191.48	0.64861	YES	YES
134	a	3194.82	0.32087	YES	YES
135	a	3198.37	1.20953	YES	YES

4.10 $Ge_6[FeCp(CO)_2]_6Cl_2$ 3

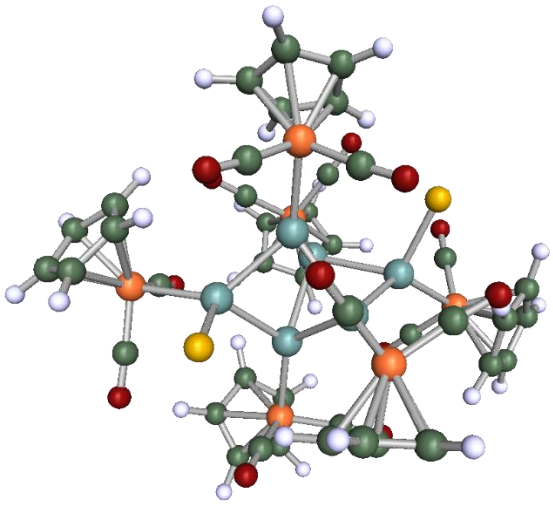

Figure S25: Optimized calculated structure of $Ge_6[FeCp(CO)_2]_6Cl_2$ **3**

Total energy: -22565.12752535429 H

symmetry used: C_1

HOMO-LUMO gap: 1.566 eV

lowest vibrational eigenvalue: 7.23 cm^{-1}

Atomic coordinates:

```
Ge 0.463723 -1.676092 -0.879979
Ge 1.779301 0.547402 -0.583183
Ge -1.779280 -0.547340 -
0.583061
Ge 0.994748 -0.783741 1.507290
Fe 1.013285 -3.770493 -1.999107
Ge -0.463728 1.676177 -0.880018
Fe 3.983597 1.220981 -1.376791
Ge -0.994593 0.783891 1.507285
Fe -3.983522 -1.221014 -
1.376831
Fe 2.225206 -1.736046 3.384688
C -0.314480 -4.476399 -1.125347
C 2.169820 -4.092956 -0.732108
C 1.390715 -2.595932 -3.765704
H 1.471841 -1.501854 -3.809490
C 0.190941 -3.360772 -3.930919
H -0.810481 -2.953281 -4.122218
C 0.541817 -4.757738 -3.819703
H -0.156365 -5.602024 -3.900909
C 1.944836 -4.851558 -3.580071
H 2.522180 -5.776117 -3.447651
C 2.470215 -3.507538 -3.532406
H 3.514866 -3.226799 -3.345838
Fe -1.013308 3.770562 -1.999129
C 3.235183 1.461805 -2.927646
C 4.337178 -0.459315 -1.687453
C 5.245237 2.927116 -1.490224
H 5.491527 3.454464 -2.421997
C 5.969972 1.835946 -0.927925
H 6.873551 1.371771 -1.344776
C 5.297248 1.439389 0.288075
H 5.591937 0.614430 0.949263
C 4.172501 2.304713 0.476917
H 3.471488 2.272249 1.321346
C 4.123784 3.217495 -0.626233
H 3.373634 4.005508 -0.771703
Fe -2.225114 1.736065 3.384720
C -3.234991 -1.461743 -2.927627
C -4.337194 0.459258 -1.687555
C -5.245110 -2.927163 -1.490408
H -5.491364 -3.454533 -2.422175
C -5.969918 -1.836021 -0.928163
H -6.873485 -1.371896 -1.345102
C -5.297320 -1.439397 0.287886
H -5.592051 -0.614375 0.948982
C -4.172591 -2.304771 0.476854
H -3.471631 -2.272258 1.321332
C -4.123740 -3.217508 -0.626310
H -3.373577 -4.005530 -0.771704
C 3.700483 -1.538572 2.473788
C 2.285525 -0.125842 4.039458
C 2.809565 -3.422730 4.544234
H 3.837212 -3.624690 4.873904
C 1.827841 -2.668177 5.251575
H 1.966759 -2.182049 6.226875
C 0.617292 -2.646472 4.463626
H -0.328339 -2.157173 4.732472
C 0.859853 -3.400262 3.269830
H 0.136335 -3.589715 2.466020
C 2.213243 -3.866293 3.305664
H 2.708937 -4.453772 2.522053
O -1.197243 -5.011656 -0.569731
O 2.958161 -4.384704 0.081383
C 0.314543 4.476453 -1.125470
C -2.169685 4.093101 -0.731982
C -1.390952 2.595911 -3.765597
H -1.472190 1.501830 -3.809410
C -0.191126 3.360632 -3.930978
H 0.810239 2.953035 -4.122401
C -0.541920 4.757642 -3.819868
H 0.156327 5.601871 -3.901203
C -1.944892 4.851585 -3.580069
H -2.522161 5.776201 -3.447729
C -2.470374 3.507620 -3.532326
H -3.515040 3.226968 -3.345762
O 2.786349 1.637488 -3.996763
O 4.646505 -1.560845 -1.930402
C -3.700424 1.538367 2.473871
C -2.285245 0.125804 4.039440
C -2.809619 3.422611 4.544339
H -3.837290 3.624403 4.874073
C -1.827758 2.668193 5.251642
H -1.966546 2.182027 6.226946
C -0.617233 2.646678 4.463606
H 0.328493 2.157491 4.732375
C -0.859985 3.400478 3.269813
H -0.136549 3.590048 2.465943
C -2.213436 3.866329 3.305751
H -2.709261 4.453739 2.522175
O -2.786042 -1.637364 -3.996678
O -4.646703 1.560696 -1.930698
O 4.733130 -1.432530 1.934442
O 2.361535 0.934322 4.534337
O 1.197377 5.011553 -0.569837
O -2.957840 4.384975 0.081609
O -4.733093 1.432178 1.934635
O -2.361249 -0.934403 4.534232
```

Vibrational analysis:

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.23	0.11995	YES	YES
8	a	7.29	0.18292	YES	YES
9	a	12.49	0.21029	YES	YES
10	a	17.43	0.14629	YES	YES
11	a	19.96	0.19670	YES	YES
12	a	20.16	0.65265	YES	YES
13	a	22.67	0.01679	YES	YES
14	a	22.85	0.19703	YES	YES
15	a	26.43	0.04709	YES	YES
16	a	29.03	0.11055	YES	YES
17	a	30.46	0.00041	YES	YES
18	a	33.89	0.06287	YES	YES
19	a	35.97	0.01798	YES	YES
20	a	39.00	0.03468	YES	YES
21	a	39.82	0.01298	YES	YES
22	a	45.67	0.00113	YES	YES
23	a	46.60	0.08028	YES	YES
24	a	48.76	0.19510	YES	YES
25	a	50.47	0.06290	YES	YES
26	a	50.57	0.11861	YES	YES
27	a	51.57	0.17765	YES	YES
28	a	52.66	0.20082	YES	YES
29	a	53.00	0.32641	YES	YES
30	a	57.25	0.00143	YES	YES
31	a	58.90	0.00128	YES	YES
32	a	60.00	0.00001	YES	YES
33	a	65.06	1.64216	YES	YES
34	a	71.53	0.73811	YES	YES
35	a	71.62	0.14244	YES	YES
36	a	71.90	0.66540	YES	YES
37	a	74.67	0.58925	YES	YES
38	a	76.17	0.01167	YES	YES
39	a	76.74	0.01406	YES	YES
40	a	82.77	0.10207	YES	YES
41	a	83.09	0.09609	YES	YES
42	a	87.52	0.00178	YES	YES
43	a	97.45	0.28850	YES	YES
44	a	97.71	0.32192	YES	YES
45	a	101.47	3.17539	YES	YES
46	a	103.73	0.09031	YES	YES
47	a	103.82	0.10898	YES	YES
48	a	104.84	0.04053	YES	YES
49	a	112.65	0.29825	YES	YES
50	a	116.97	0.09778	YES	YES
51	a	117.43	0.18513	YES	YES
52	a	119.09	0.19000	YES	YES
53	a	119.24	0.09075	YES	YES
54	a	120.08	0.15607	YES	YES
55	a	121.79	0.00022	YES	YES

56	a	130.45	0.00204	YES	YES
57	a	131.75	0.04788	YES	YES
58	a	134.53	0.03008	YES	YES
59	a	136.43	0.04436	YES	YES
60	a	138.05	0.00086	YES	YES
61	a	138.81	0.01421	YES	YES
62	a	145.63	0.18309	YES	YES
63	a	145.81	0.41134	YES	YES
64	a	159.24	0.64368	YES	YES
65	a	161.41	3.76757	YES	YES
66	a	162.25	4.83383	YES	YES
67	a	166.71	4.68496	YES	YES
68	a	167.14	6.34909	YES	YES
69	a	175.05	21.60778	YES	YES
70	a	184.84	8.53908	YES	YES
71	a	185.23	9.36476	YES	YES
72	a	218.51	0.07366	YES	YES
73	a	219.38	0.05732	YES	YES
74	a	224.17	0.05499	YES	YES
75	a	255.77	32.60298	YES	YES
76	a	256.67	31.90380	YES	YES
77	a	267.96	44.39384	YES	YES
78	a	276.86	0.06617	YES	YES
79	a	333.61	4.15992	YES	YES
80	a	333.82	5.16748	YES	YES
81	a	335.12	4.13881	YES	YES
82	a	335.52	7.05955	YES	YES
83	a	335.76	0.00817	YES	YES
84	a	336.01	3.96389	YES	YES
85	a	350.39	2.19611	YES	YES
86	a	350.41	5.38883	YES	YES
87	a	352.43	4.45355	YES	YES
88	a	352.58	1.93993	YES	YES
89	a	353.89	1.34083	YES	YES
90	a	353.93	7.39743	YES	YES
91	a	363.79	9.44902	YES	YES
92	a	363.92	0.01795	YES	YES
93	a	364.32	8.46635	YES	YES
94	a	365.03	3.42160	YES	YES
95	a	366.15	7.93098	YES	YES
96	a	366.32	0.94011	YES	YES
97	a	446.24	0.09213	YES	YES
98	a	446.50	0.17509	YES	YES
99	a	447.07	0.20491	YES	YES
100	a	447.57	0.27800	YES	YES
101	a	450.17	0.28067	YES	YES
102	a	450.27	0.06430	YES	YES
103	a	495.23	0.86545	YES	YES
104	a	495.31	5.31856	YES	YES
105	a	495.53	8.07357	YES	YES
106	a	495.68	7.31043	YES	YES
107	a	495.75	2.85287	YES	YES
108	a	495.93	0.67971	YES	YES
109	a	525.21	1.51429	YES	YES
110	a	525.49	0.39434	YES	YES
111	a	525.74	101.52304	YES	YES

112	a	525.95	87.78452	YES	YES
113	a	526.33	90.55552	YES	YES
114	a	529.37	0.08973	YES	YES
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116	a	566.38	63.88117	YES	YES
117	a	566.79	11.71029	YES	YES
118	a	566.85	7.95859	YES	YES
119	a	567.50	62.82242	YES	YES
120	a	567.94	2.61679	YES	YES
121	a	574.92	33.86978	YES	YES
122	a	576.15	28.63052	YES	YES
123	a	576.48	120.91855	YES	YES
124	a	576.59	34.17394	YES	YES
125	a	577.71	22.15962	YES	YES
126	a	577.76	77.51434	YES	YES
127	a	579.17	64.09985	YES	YES
128	a	579.63	85.33611	YES	YES
129	a	579.90	76.80751	YES	YES
130	a	579.90	56.17899	YES	YES
131	a	580.64	95.59193	YES	YES
132	a	586.10	0.09476	YES	YES
133	a	593.80	2.47961	YES	YES
134	a	594.39	0.09783	YES	YES
135	a	596.00	16.56775	YES	YES
136	a	596.57	21.27592	YES	YES
137	a	597.61	66.01788	YES	YES
138	a	599.25	0.83470	YES	YES
139	a	649.51	7.67307	YES	YES
140	a	649.55	6.79060	YES	YES
141	a	650.41	43.94874	YES	YES
142	a	650.46	11.22200	YES	YES
143	a	651.44	53.71789	YES	YES
144	a	651.53	26.33595	YES	YES
145	a	809.88	6.54160	YES	YES
146	a	810.56	12.33783	YES	YES
147	a	811.04	38.21902	YES	YES
148	a	811.09	1.55265	YES	YES
149	a	812.28	22.40705	YES	YES
150	a	812.35	6.80488	YES	YES
151	a	812.98	22.66539	YES	YES
152	a	813.19	2.95677	YES	YES
153	a	813.52	7.10099	YES	YES
154	a	813.68	31.53338	YES	YES
155	a	814.41	0.04849	YES	YES
156	a	814.57	0.87214	YES	YES
157	a	816.80	32.60376	YES	YES
158	a	817.18	50.86666	YES	YES
159	a	817.22	5.22579	YES	YES
160	a	817.61	56.85240	YES	YES
161	a	817.87	96.86906	YES	YES
162	a	818.04	0.55114	YES	YES
163	a	823.55	19.74432	YES	YES
164	a	823.67	3.14894	YES	YES
165	a	826.10	1.89962	YES	YES
166	a	826.79	25.04398	YES	YES
167	a	830.96	26.80941	YES	YES

168	a	831.01	12.29905	YES	YES
169	a	847.80	5.21529	YES	YES
170	a	847.81	1.24366	YES	YES
171	a	852.18	4.67737	YES	YES
172	a	852.25	3.90704	YES	YES
173	a	854.07	4.59265	YES	YES
174	a	854.49	2.78141	YES	YES
175	a	894.85	0.70469	YES	YES
176	a	894.94	0.24614	YES	YES
177	a	896.52	1.53573	YES	YES
178	a	896.58	0.46807	YES	YES
179	a	897.28	1.12731	YES	YES
180	a	897.32	1.14495	YES	YES
181	a	904.16	0.58192	YES	YES
182	a	904.61	0.47983	YES	YES
183	a	904.79	0.44404	YES	YES
184	a	905.09	0.83587	YES	YES
185	a	905.98	0.24792	YES	YES
186	a	906.24	0.90626	YES	YES
187	a	986.88	1.50102	YES	YES
188	a	986.90	8.69883	YES	YES
189	a	987.97	0.31075	YES	YES
190	a	988.09	9.00642	YES	YES
191	a	988.28	1.83957	YES	YES
192	a	988.51	0.13298	YES	YES
193	a	1008.60	13.45866	YES	YES
194	a	1008.62	4.29759	YES	YES
195	a	1009.45	1.48909	YES	YES
196	a	1009.49	16.53907	YES	YES
197	a	1009.75	8.08883	YES	YES
198	a	1009.82	10.64817	YES	YES
199	a	1043.75	3.87259	YES	YES
200	a	1043.79	0.95871	YES	YES
201	a	1045.18	1.14358	YES	YES
202	a	1045.31	1.71423	YES	YES
203	a	1045.56	3.80474	YES	YES
204	a	1046.33	1.25852	YES	YES
205	a	1047.63	0.20785	YES	YES
206	a	1047.70	2.57219	YES	YES
207	a	1048.33	0.12058	YES	YES
208	a	1049.23	1.20846	YES	YES
209	a	1049.75	1.77426	YES	YES
210	a	1050.23	1.35711	YES	YES
211	a	1116.27	2.61610	YES	YES
212	a	1116.28	0.22442	YES	YES
213	a	1116.60	1.38818	YES	YES
214	a	1116.64	2.30694	YES	YES
215	a	1116.70	0.27934	YES	YES
216	a	1116.72	3.36382	YES	YES
217	a	1247.48	0.09107	YES	YES
218	a	1247.49	0.13451	YES	YES
219	a	1248.73	0.15379	YES	YES
220	a	1248.74	0.13888	YES	YES
221	a	1248.77	0.07641	YES	YES
222	a	1248.79	0.02024	YES	YES
223	a	1370.49	2.69927	YES	YES

224	a	1370.57	0.05247	YES	YES
225	a	1372.45	3.70409	YES	YES
226	a	1372.52	0.34043	YES	YES
227	a	1372.87	3.49454	YES	YES
228	a	1372.90	0.07554	YES	YES
229	a	1377.01	1.12631	YES	YES
230	a	1377.17	0.83807	YES	YES
231	a	1377.62	1.60610	YES	YES
232	a	1377.68	1.20028	YES	YES
233	a	1377.84	0.48045	YES	YES
234	a	1378.00	0.46424	YES	YES
235	a	1415.90	4.89351	YES	YES
236	a	1415.90	2.92013	YES	YES
237	a	1416.40	1.70958	YES	YES
238	a	1416.42	4.63321	YES	YES
239	a	1416.48	1.44248	YES	YES
240	a	1416.64	0.21055	YES	YES
241	a	1435.39	14.08538	YES	YES
242	a	1435.52	0.87638	YES	YES
243	a	1435.60	12.90401	YES	YES
244	a	1435.61	3.61205	YES	YES
245	a	1435.90	2.84984	YES	YES
246	a	1435.95	8.78548	YES	YES
247	a	1956.99	6.56199	YES	YES
248	a	1957.21	131.70936	YES	YES
249	a	1958.94	590.83785	YES	YES
250	a	1959.09	520.55261	YES	YES
251	a	1966.20	559.90900	YES	YES
252	a	1966.86	1.61831	YES	YES
253	a	1997.00	67.15054	YES	YES
254	a	1997.09	29.93180	YES	YES
255	a	2000.65	929.47322	YES	YES
256	a	2000.71	824.98258	YES	YES
257	a	2006.19	1473.73305	YES	YES
258	a	2010.55	0.25622	YES	YES
259	a	3153.10	1.05965	YES	YES
260	a	3153.16	1.27537	YES	YES
261	a	3153.23	1.06840	YES	YES
262	a	3153.32	1.65164	YES	YES
263	a	3153.38	0.54044	YES	YES
264	a	3153.38	1.34686	YES	YES
265	a	3157.09	1.41987	YES	YES
266	a	3157.25	1.62043	YES	YES
267	a	3157.29	0.63162	YES	YES
268	a	3157.39	2.06307	YES	YES
269	a	3159.41	1.25424	YES	YES
270	a	3159.46	1.45724	YES	YES
271	a	3167.58	1.29816	YES	YES
272	a	3167.61	2.24355	YES	YES
273	a	3167.63	0.03974	YES	YES
274	a	3167.72	1.11626	YES	YES
275	a	3168.07	2.45550	YES	YES
276	a	3168.10	1.00914	YES	YES
277	a	3170.93	0.36618	YES	YES
278	a	3171.12	7.68554	YES	YES
279	a	3171.89	4.95184	YES	YES

280	a	3171.94	3.30118	YES	YES
281	a	3175.09	3.48858	YES	YES
282	a	3175.13	4.28674	YES	YES
283	a	3180.42	2.61292	YES	YES
284	a	3180.45	0.26105	YES	YES
285	a	3180.71	1.37713	YES	YES
286	a	3180.77	1.35446	YES	YES
287	a	3181.78	1.95392	YES	YES
288	a	3181.81	1.08643	YES	YES

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