Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Homoleptic Hexa and Penta Coordinated Gallium(I) Amide Complexes of Ruthenium and Molybdenum

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Table of Content

General Remarks

Unless stated otherwise, all synthetic manipulations were carried out using standard Schlenk techniques under an atmosphere of argon 4.6 purified by BTC-catalyst and dried over 3 Å molecular sieves or in a glovebox under an atmosphere of purified argon. All reactions were carried out in standardized Schlenk flasks and tubes which were rinsed with 1,1,1,3,3,3-hexamethyldisilyzane (HMDS), heated with a heat gun to 650 °C and cooled under vacuum argon. All synthesis of light sensitive compounds were performed under the red light. All solvents were carefully dried over molecular sieves and deuterated solvents were degassed prior to their use. All non-dried solvents used were distilled prior to their use. All the reagents were purchased from commercial sources and used as such without further purification.

Analytical Methods

NMR spectra were recorded on a Bruker Avance III 400US (1H, 400 MHz; 13C 101MHz). Chemical shifts are given relative to TMS and were referenced to the residual solvent peak as internal standards. Chemical shifts are reported in parts per million, downfield shifted from TMS, and are consecutively reported as position (δH or δC), relative integral, multiplicity (s = singlet, t = triplet, and m = multiplet) and assignment. FT-IR spectra were measured on an ATR setup with a Bruker Alpha FTIR spectrometer under an inert gas atmosphere in a glove-box. The mass spectra were taken using a Linden CMS LIFDI as ionization source and a ThermoFisher Scientific Exactive Plus Orbitrap as detector. The sample application was performed via a fumed silica capillary from a glovebox under an argon atmosphere to enable the measurement of highly air-sensitive compounds. The recorded mass spectra were evaluated using the FreeStyle 1.3 program from ThermoFisher Scientific and a fitting program developed by *Dr. Christian Gemel* details of which are outlined below. Reference isotope patterns were simulated using the enviPat Web application.[1]

Computerized Analysis of Mass Spectra

The general procedure for computerized peak identification in LIFDI-MS involves utilizing a Java computer program (Java 11, openjdk-1.11.0). The program's fundamental principles and workflow are outlined below.

To begin spectrum analysis, the program employs automated pattern recognition, identifying local maxima above a specified threshold value (which users can adjust, defaulting to 1% of the highest peak in the spectrum) as peaks. These peaks are then grouped automatically into peak groups and subsequently into isotopic patterns through a recursive process. The algorithm initiates at the highest remaining peak in the peak list and searches both left and right for peaks with an exact m/z shift of 1/z from each other, within a user-defined error range (ε). Users input the charge z of the ions (defaulting to 1) and the recursive process terminates when no peaks remain in the peak list.

The resulting list comprises peak groups, which are considered isotopic patterns if they contain a minimum number of peaks (defaulting to 5, user-adjustable).

For pattern analysis, users provide a list of potential fragments by loading a file containing all conceivable fragments the observed ions may consist of (such as metal atoms, ligands, solvents, etc.). The program generates weight matches for each pattern by recursively combining these fragments into ions. All possible fragment combinations up to the m/z value of the respective pattern are calculated, using the pattern centroid (intensity-weighted average, (m/z)centroid) as the experimental average weight. Acceptable fragment combinations have a molar weight (Mw) falling within the range: (m/z)centroid – 2.1 < Mw < (m/z)centroid + 4.1. The subtraction of 2.1 accounts for a possible loss of 2 hydrogen atoms and the addition of 4.1 accounts for the possibility of up to four additional hydrogens, which are not part of the input fragments (accounting for dehydrogenation or hydrogenation/protonation during ionization).

As the list of fragment formulas is often extensive, a "sieving" step is conducted. Isotopic patterns for each fragment are calculated, and an "offset" value is determined by comparing exact m/z values of calculated and experimental patterns. Only patterns with an average offset value below a specified threshold (defaulting to 0.2, user-adjustable) are further considered. The program then computes the goodness of fit (GoF) value between experimental and calculated patterns, and vice versa, using least squares fitting resulting in a total GoF, ranging between 0 (no common peaks) and 1 (identical patterns).

In the output file, each pattern is listed with possible pattern matches and their corresponding final GoF values. Additionally, users can visually compare patterns to their calculated counterparts.

Continuous Shape Measure[2]

The method of continuous shape measure uses the *N* vertices of an experimentally determined coordination polyhedron normalized and centered in the origin of a three-dimensional cartesian coordinate system as their position vectors Q_i (i = 1,2,3 …, *N*). These are compared to the position vectors P_i (i = 1,2,3, …, *N*) of the *N* vertices of an ideal reference polyhedron that is equally centered and normalized. This is expressed as

$$S_Q(P) = \frac{1}{N} min \sum_{i=1}^{N} \left|\overrightarrow{Q_i} - \overrightarrow{P_i}\right|^2 \times 100$$

A value of $S_Q(P) = 0$ thus represents the exact ideal shape, with increasing values indicating increasing distortions. This value was calculated from most ideal superimposition, determined by minimizing the distance between the superimposed polyhedral vertices by a numerical rotation algorithm. $S_Q(P)$ thus is the global minimum of these permutations.

In order to identify the cartesian coordinates of two polyhedra with minimized average distances of their vertices, a Java program has been used (Java 15, openjdk-15). The program takes as input the cartesian coordinates of two polyhedra, both centered at the origin. The program then freely rotates (and also stretches/shrinks on demand) one of the two polyhedra, finally locating the coordinates with minimized distances between the vertices of the two polyhedra in a recursive process.

The code for both programs can be obtained from the authors on request.

Comprehensive listing of homoleptic and closely related [M(ER*)$_n$] complexes known

In an endeavor to explore the then arising topic of isolobality between CO and E-R ligands (E = Al, Ga, In)(R = C(SiMe$_3$)$_3$, 1,2,3,4,5-pentamethylcyclopentadienyl (Cp*)) to gain access to a new class of mononuclear intermetallic complexes, *W. Uhl et. al.* in 1998 published the first mononuclear homoleptic transition metal (TM)-ER$_x$ compound Ni(InC(SiMe$_3$)$_3$)$_4$.[3] The homologous Ni(GaC(SiMe$_3$)$_3$)$_4$ followed shortly after further proving the concept beyond Indium.[4] Pt(InC(SiMe$_3$)$_3$)$_4$ provided the first example of a homoleptic 3rd row TM-ER$_{(x)}$ compound.[5] During this time *P. Jutzi et. al.* presented Ni(GaCp*)$_4$, thus providing a vital broadening of the field.[6] With Pd(GaCp*)$_4$, Pd(InC(SiMe$_3$)$_3$)$_4$ and Pt(GaCp*)$_4$ the homologous Ni-Pd-Pt row was completed by *R. A. Fischer et. al.* in 2003.[7] The homologous homoleptic, mononuclear compounds of AlCp*, Ni(AlCp*)$_4$ and Pd(AlCp*)$_4$ established Al within the row of E-R ligands.[8, 9] The more electron rich metals yielded the respective cationic, homoleptic compounds Zn(GaCp)$_4$[BArF]$_2$ ([BArF] = Tetrakis[3,5-bis(trifluoromethyl)phenyl]borate), Cu(GaCp*)$_4$[BArF] and Ag(GaCp*)$_4$[BPh$_4$].[10, 11] Fe(AlCp*)$_5$ and Ru(AlCp*)$_5$ are the first examples of homoleptic C-H activated isomers of TM-E-R complexes outside the d^{10} group with more than four group 13 metals coordinated.[12] Though not strictly homoleptic (GaCp*)$_4$Rh(MeGa(η^1-Cp*) and (GaCp*)$_4$Rh((OTf)Ga(η^1-Cp*) (OTf = trifluoromethanesulfonate) continue a trend of higher coordination numbers.[13, 14] The haptotropically shifted, halogen bridged (GaCp*)$_3$Ru(GaCl(η^1-Cp*))(Ga$_2$(μ-Cl)(η^1-Cp*))$_2$ provided the first hexa group 13 coordinated compound within the family.[15] The highest unhalogenated coordination number within the group stands at six provided by the only haptoropically shifted Mo(GaCp*)$_6$.[14, 16]

Another group of mononuclear homoleptic intermetallic TM-E-R compounds is based on Ga(DDP) (DDP = 2-((2,6-diisopropylphenyl)amino-4-((2,6-diisopropylphenyl)imino)-2-pentene). The first one Au(Ga·(THF)(DDP))$_2$[BArF] was also presented by *R. A. Fischer et. al.* in 2006.[17] This was followed up by Zn(Ga(Me)(DDP))$_2$.[10] With Hg(Ga(SC$_6$F$_5$)(DDP))$_2$ the first homoleptic TM-E-R compound of Mercury was obtained.[18] Cu(Ga(DDP))$_2$[OTf] then was the first and as of now only homoleptic complex of the series where the Ga(DDP) was only bound to the central TM atom.[19] Interest in this

class of compounds has not abated, just in 2022, *J. Okuda et. al.* published their work around $Zn(GaH(DDP))_2$.[20] This group of compounds generally does not exceed a coordination number of two E-R. However *C. Jones et. al.* reported a coordination number of three with their NHC-analogous $Ga[N(Ar)]_2CNCy_2$ (Ar = $C_6H_3{}^iPr_2$-2,6) (Cy = cyclohexyl) in the homoleptic $Pt(Ga[N(Ar)]_2CNCy_2)_3$.[21]

Table S 1: List of homoleptic and closely related $[M(ER^*)_n]$ compounds known and sorted by coordination number of central atom M and element E

Compounds with central atom coordination number = 2	
$Au(Ga{\cdot}(THF)(DDP))_2[BArF]$	A. Kempter, C. Gemel, N. J. Hardman, R. A. Fischer, *Inorg. Chem.*, 2006, **45**, 3133
$Hg(Ga(SC_6F_5)(DDP))_2$	G. Prabusankar, C. Gemel, M. Winter, R. W. Seidel, R. A. Fischer, *Chem. Eur. J.*, 2010, **16**, 6041
$Zn(GaH(DDP))_2$	L. J. Morris, T. Rajeshkumar, L. Maron, J. Okuda, *Chem. Eur. J.*, 2022, **28**, e202201480,
$Cu(Ga(DDP))_2[OTf]$	G. Prabusankar, S. Gonzalez-Gallardo, A. Doddi, C. Gemel, M. Winter, R. A. Fischer, *Eur. J. Inorg. Chem.*, 2010, 4415
$Zn(Ga(Me)(DDP))_2$	A. Kempter, C. Gemel, T. Cadenbach, R. A. Fischer, *Inorg. Chem.*, 2007, **46**, 9481
Compounds with central atom coordination number = 3	
$Pt(Ga[N(Ar)]_2CNCy_2)_3$	S. P. Green, C. Jones, A. Stasch, *Inorg. Chem.*, 2007, **46**, 11
Compounds with central atom coordination number = 4	
$Pt(GaCp^*)_4$	C. Gemel, T. Steinke, D. Weiss, M. Cokoja, M. Winter, R. A. Fischer, *Organometallics*, 2003, **22**, 2705
$Pd(GaCp^*)_4$	C. Gemel, T. Steinke, D. Weiss, M. Cokoja, M. Winter, R. A. Fischer, *Organometallics*, 2003, **22**, 2705
$Ni(GaCp^*)_4$	P. Jutzi, B. Neumann, L. O. Schebaum, A. Stammler, H.-G. Stammler, *Organometallics*, 1999, **18**, 4462
$Ag(GaCp^*)_4[BPh_4]$	T. Bollermann, A. Puls, C. Gemel, T. Cadenbach, R. A. Fischer, *Dalton Trans.*, 2009, 1372
$Zn(GaCp^*)_4[BAr^F]_2$	A. Kempter, C. Gemel, T. Cadenbach, R. A. Fischer, *Inorg. Chem.*, 2007, **46**, 9481

$Cu(GaCp^*)_4[BAr^F]$	T. Bollermann, A. Puls, C. Gemel, T. Cadenbach, R. A. Fischer, *Dalton Trans.*, 2009, 1372
$Ni(GaC(TMS)_3)_4$	W. Uhl, M. Benter, S. Melle, W. Saak, G. Frenking, J. Uddin, *Organometallics*, 1999, **18**, 3778
$Pd(AlCp^*)_4$	B. Buchin, T. Steinke, C. Gemel, T. Cadenbach, R. A. Fischer, *Z. anorg. allg. Chem.*, 2005, **631**, 2756
$Ni(AlCp^*)_4$	B. Buchin, T. Steinke, C. Gemel, T. Cadenbach, R. A. Fischer, *Z. anorg. allg. Chem.*, 2005, **631**, 2756
$Ni(InC(TMS)_3)_4$	W. Uhl, M. Pohlmann, R. Wartchow, *Angew. Chem. Int. Ed.*, 1998, **37**, 961 W. Uhl, M. Benter, S. Melle, W. Saak, G. Frenking, J. Uddin, *Organometallics*, 1999, **18**, 3778
$Pt(InC(TMS)_3)_4$	W. Uhl, S. Melle, *Z. anorg. allg. Chem.*, 2000, **626**, 2043
$Pd(InC(TMS)_3)_4$	C. Gemel, T. Steinke, D. Weiss, M. Cokoja, M. Winter, R. A. Fischer, *Organometallics*, 2003, **22**, 2705
Compounds with central atom coordination number = 5	
$(GaCp^*)_4Rh(Ga(O_3SCF_3)Cp^*)$	T. Bollermann, T. Cadenbach, C. Gemel, K. Freitag, M. Molon, V. Gwildies, R. A. Fischer, *Inorg. Chem.*, 2011, **50**, 5808
$(GaCp^*)_4Rh(MeGa(\eta^1\text{-}Cp^*)$	T. Cadenbach, C. Gemel, D. Zacher, R. A. Fischer, *Angew. Chem. Int. Ed.*, 2008, **47**, 3438
$Fe(AlCp^*)_5$ (C-H activated)	T. Steinke, M. Cokoja, C. Gemel, A. Kempter, A. Krapp, G. Frenking, U. Zennek, R. A. Fischer, *Angew. Chem. Int. Ed.*, 2005, **44**, 2943
$Ru(AlCp^*)_5$ (C-H activated)	T. Steinke, M. Cokoja, C. Gemel, A. Kempter, A. Krapp, G. Frenking, U. Zennek, R. A. Fischer, *Angew. Chem. Int. Ed.*, 2005, **44**, 2943
Compounds with central atom coordination number = 6	
$Ru(GaCp^*)_4)(ClGaCp^*)_2$	B. Buchin, C. Gemel, A. Kempter, T. Cadenbach, R. A. Fischer, *Inorg. Chimi. Acta*, 2006, **359**, 4833
$Mo(GaCp^*)_6$ (Haptotropic Shifted)	T. Cadenbach, T. Bollermann, C. Gemel, I. Fernandez, M. von Hopffgarten, G. Frenking, R. A. Fischer, *Angew. Chem. Int. Ed.*, 2008, **47**, 9150, T. Bollermann, T. Cadenbach, C. Gemel, K. Freitag, M. Molon, V. Gwildies, R. A. Fischer, *Inorg. Chem.*, 2011, **50**, 5808

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4. W. Uhl, M. Benter, S. Melle, W. Saak, G. Frenking and J. Uddin, *Organometallics*, 1999, **18**, 3778-3780.
5. W. Uhl and S. Melle, *Z. anorg. allg. Chem.*, 2000, **626**, 2043-2045.
6. P. Jutzi, B. Neumann, L. O. Schebaum, A. Stammler and H.-G. Stammler, *Organometallics*, 1999, **18**, 4462-4464.
7. C. Gemel, T. Steinke, D. Weiss, M. Cokoja, M. Winter and R. A. Fischer, *Organometallics*, 2003, **22**, 2705-2710.
8. T. Steinke, C. Gemel, M. Cokoja, M. Winter and R. A. Fischer, *Angew. Chem. Int. Ed.*, 2004, **43**, 2299-2302.
9. B. Buchin, T. Steinke, C. Gemel, T. Cadenbach and R. A. Fischer, *Z. anorg. allg. Chem.*, 2005, **631**, 2756-2762.
10. A. Kempter, C. Gemel, T. Cadenbach and R. A. Fischer, *Inorg. Chem.*, 2007, **46**, 9481-9487.
11. T. Bollermann, A. Puls, C. Gemel, T. Cadenbach and R. A. Fischer, *Dalton Trans.*, 2009, DOI: 10.1039/B815319A, 1372-1377.
12. T. Steinke, M. Cokoja, C. Gemel, A. Kempter, A. Krapp, G. Frenking, U. Zenneck and R. A. Fischer, *Angew. Chem. Int. Ed.*, 2005, **44**, 2943-2946.
13. T. Cadenbach, C. Gemel, D. Zacher and R. A. Fischer, *Angew. Chem. Int. Ed.*, 2008, **47**, 3438-3441.
14. T. Bollermann, T. Cadenbach, C. Gemel, K. Freitag, M. Molon, V. Gwildies and R. A. Fischer, *Inorg. Chem.*, 2011, **50**, 5808-5814.
15. B. Buchin, C. Gemel, A. Kempter, T. Cadenbach and R. A. Fischer, *Inorg. Chim. Acta.*, 2006, **359**, 4833-4839.
16. T. Cadenbach, T. Bollermann, C. Gemel, I. Fernandez, M. von Hopffgarten, G. Frenking and R. A. Fischer, *Angew. Chem. Int. Ed.*, 2008, **47**, 9150-9154.
17. A. Kempter, C. Gemel, N. J. Hardman and R. A. Fischer, *Inorg. Chem.*, 2006, **45**, 3133-3138.
18. G. Prabusankar, C. Gemel, M. Winter, R. W. Seidel and R. A. Fischer, *Chem. Eur. J.*, 2010, **16**, 6041-6047.
19. G. Prabusankar, S. Gonzalez-Gallardo, A. Doddi, C. Gemel, M. Winter and R. A. Fischer, *Eur. J. Inorg. Chem.*, 2010, **2010**, 4415-4418.
20. L. J. Morris, T. Rajeshkumar, L. Maron and J. Okuda, *Chem. Eur. J.*, 2022, **28**, e202201480.
21. S. P. Green, C. Jones and A. Stasch, *Inorg. Chem.*, 2007, **46**, 11-13.

NMR Data

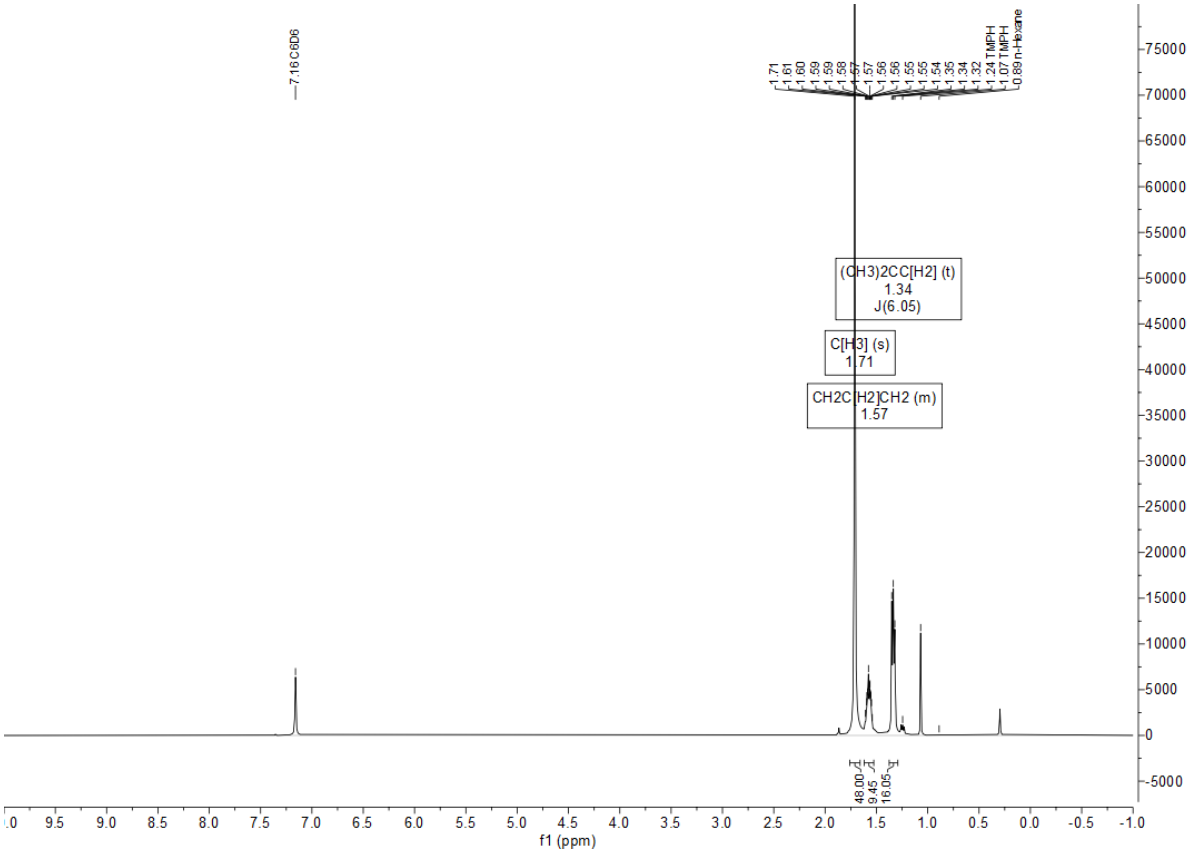

Figure S 1: ^{1}H-NMR Spectrum of **1** in benzene-d_6.

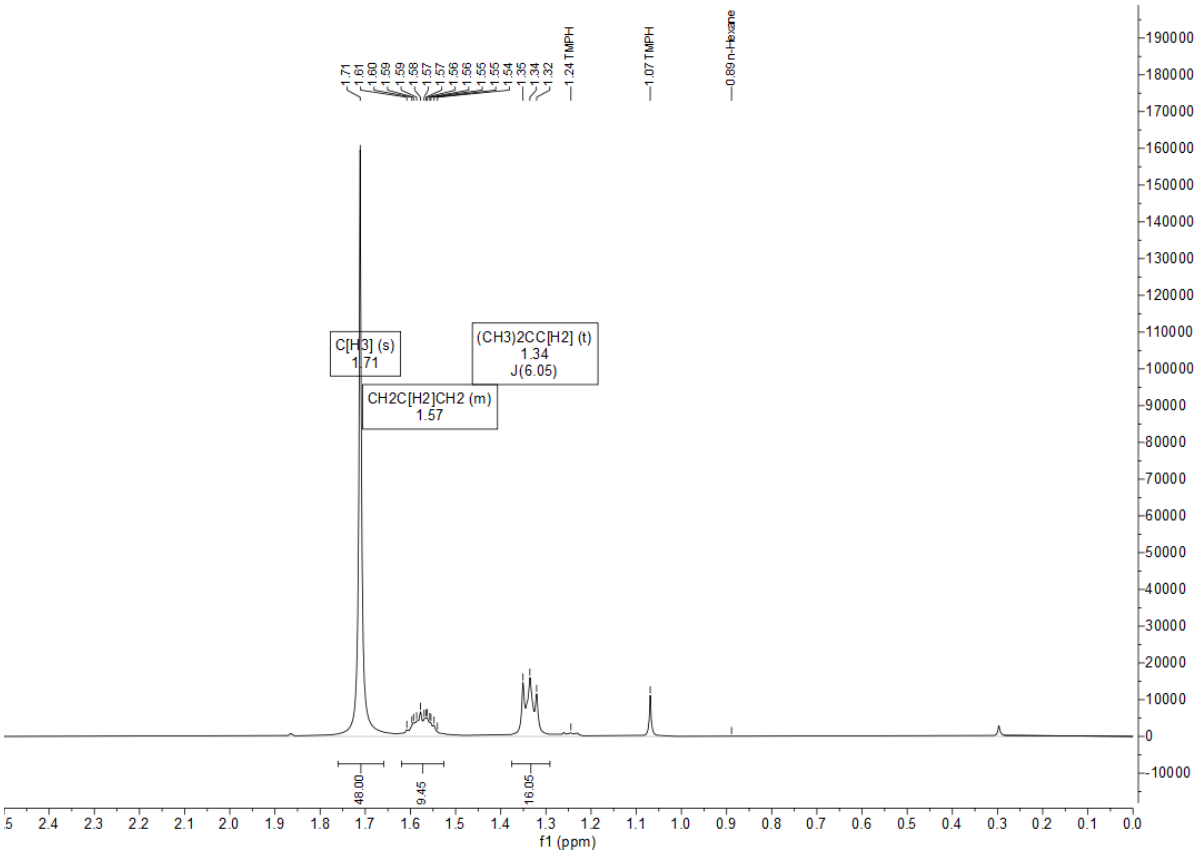

Figure S 2: ^{1}H-NMR Spectrum of **1** in benzene-d_6 from 2.50 ppm to 0.00 ppm.

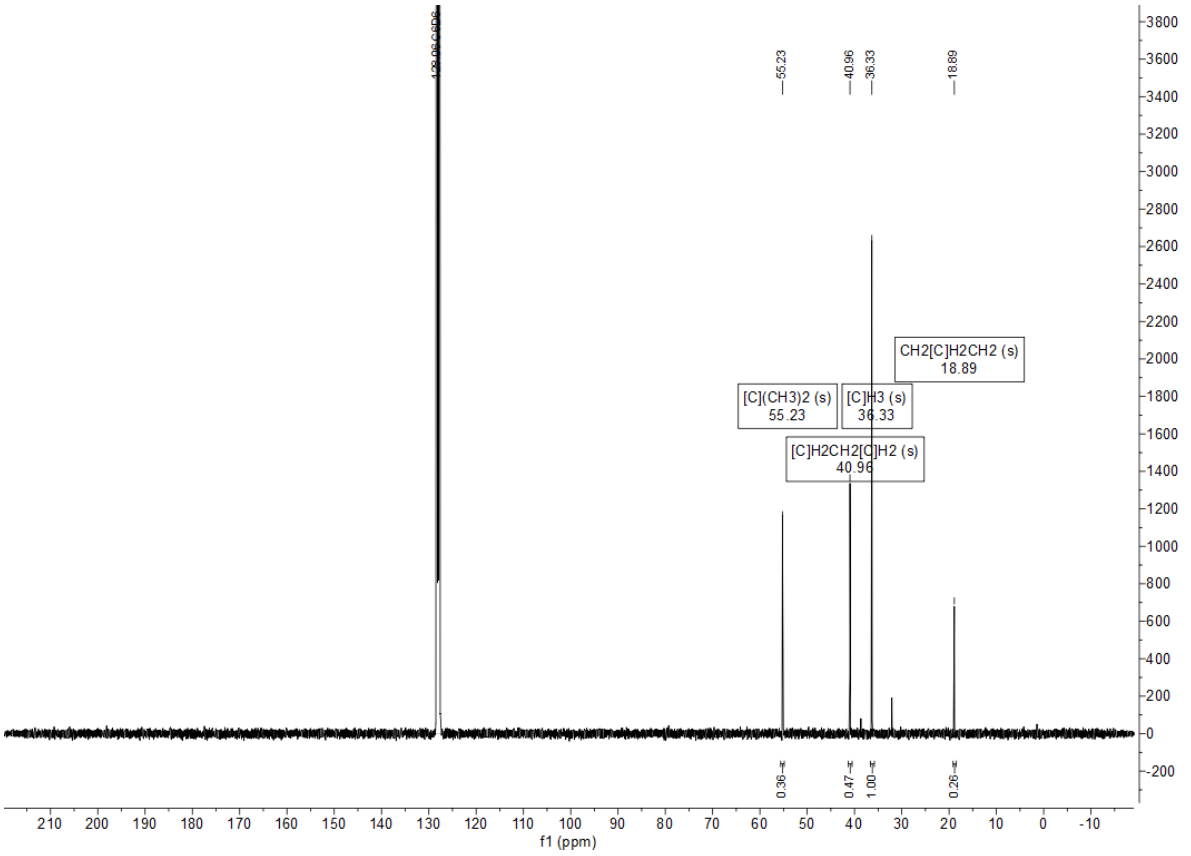

Figure S 3: ^{13}C-NMR Spectrum of **1** in benzene-d_6.

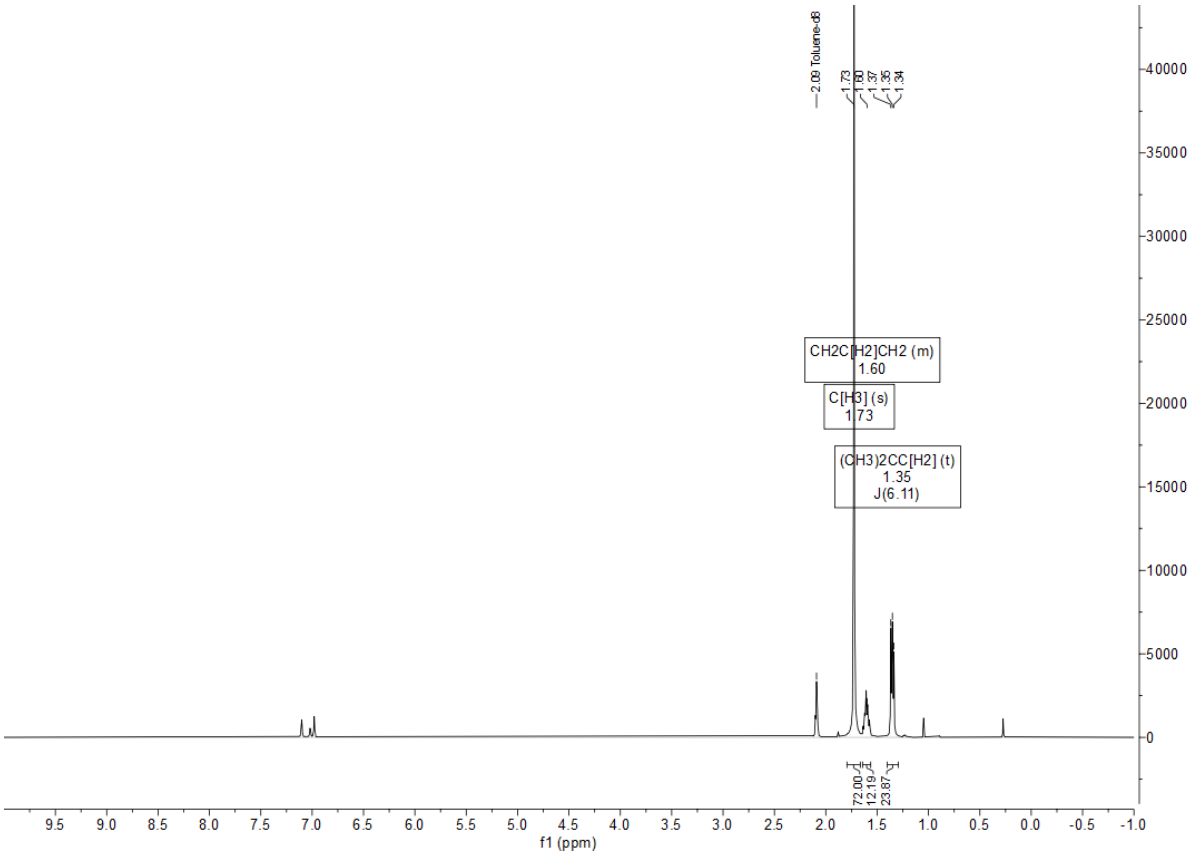

Figure S 4: ^{1}H-NMR Spectrum of **2** in toluene-d_8 from 2.50 ppm to 0.00 ppm.

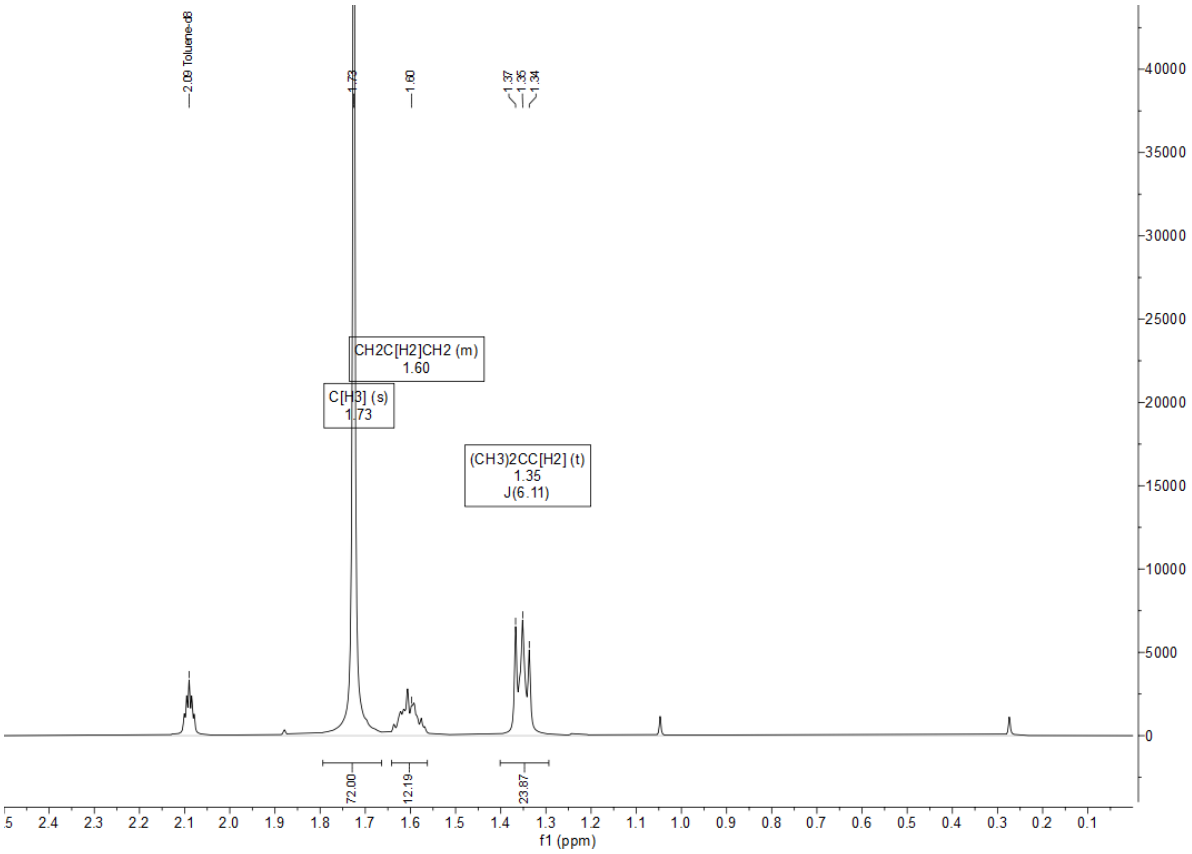

Figure S 5: ^{1}H-NMR Spectrum of **2** in toluene-d_8.

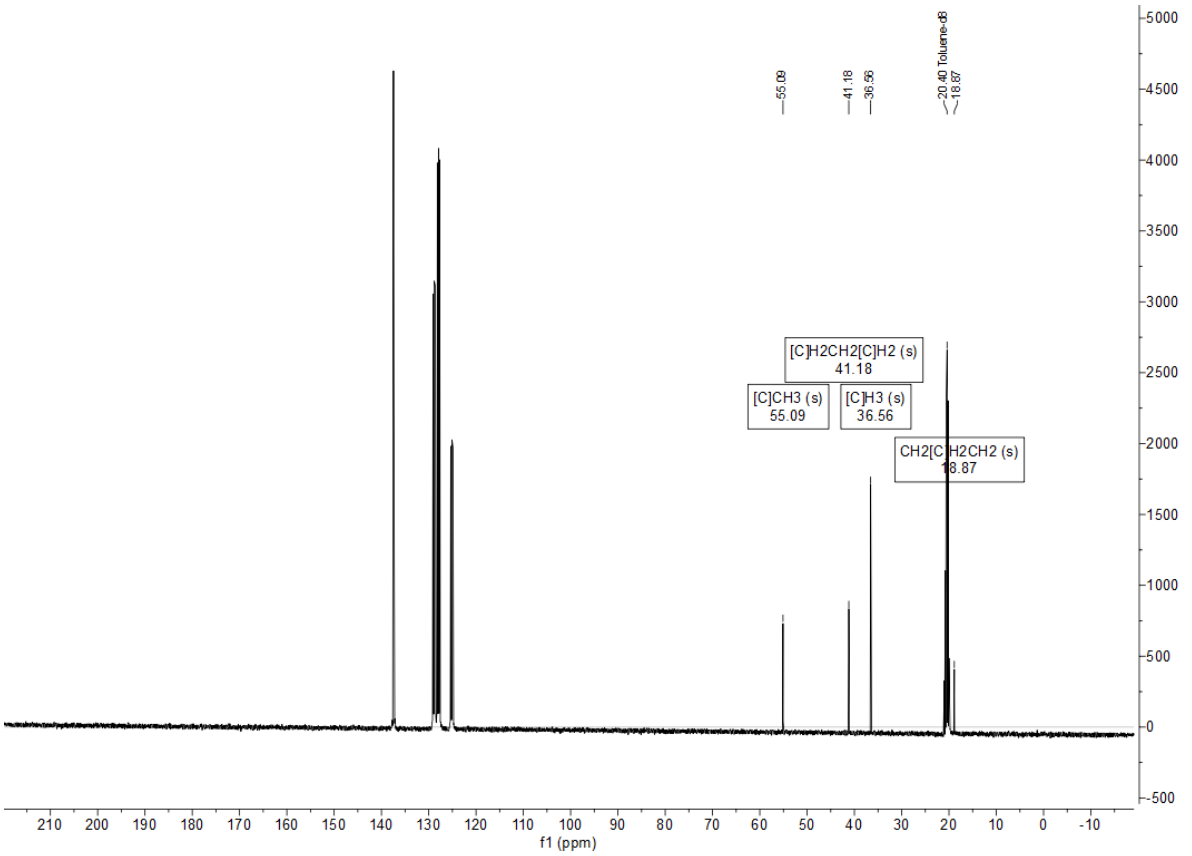

Figure S 6: ^{13}C-NMR Spectrum of **2** in toluene-d_8.

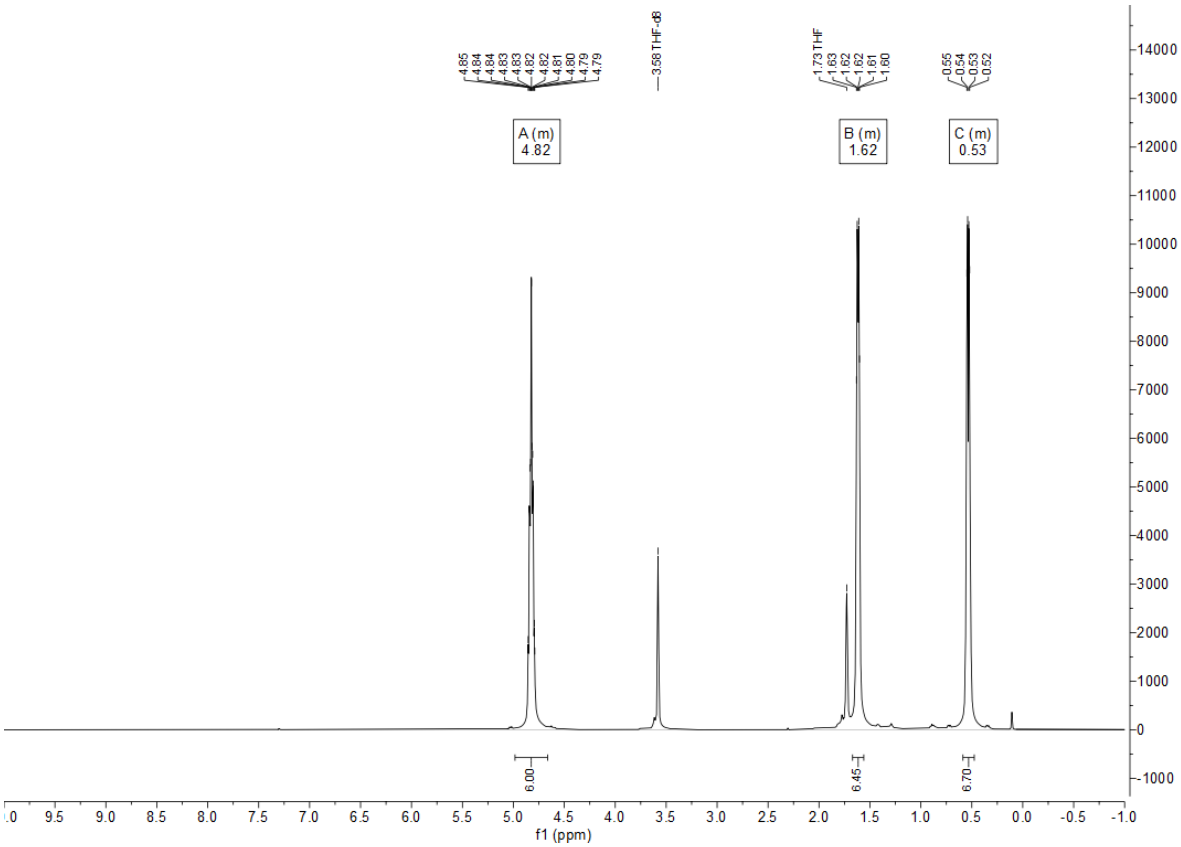

Figure S 7: ^{1}H-NMR Spectrum of [Mo(η^4-C_4H_6)$_3$] in thf-d_8.

IR Data

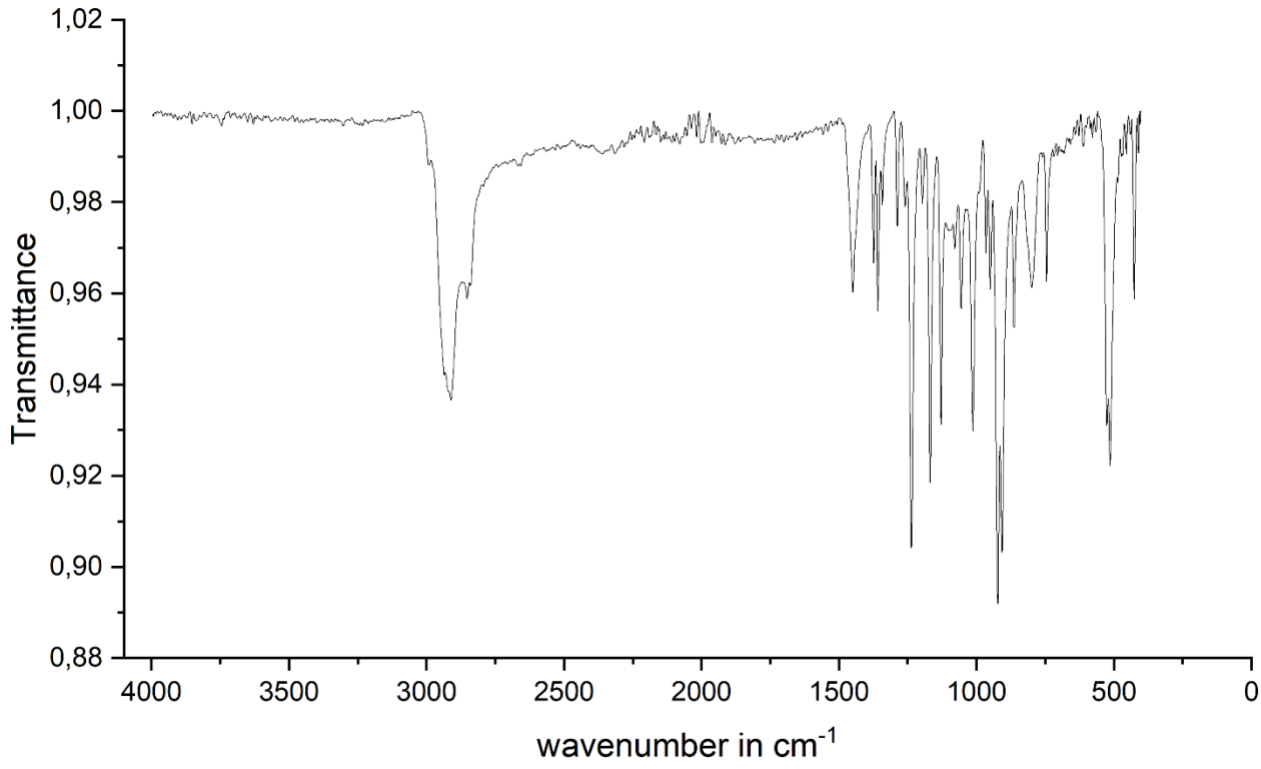

Figure S 8: IR Spectrum of **1**.

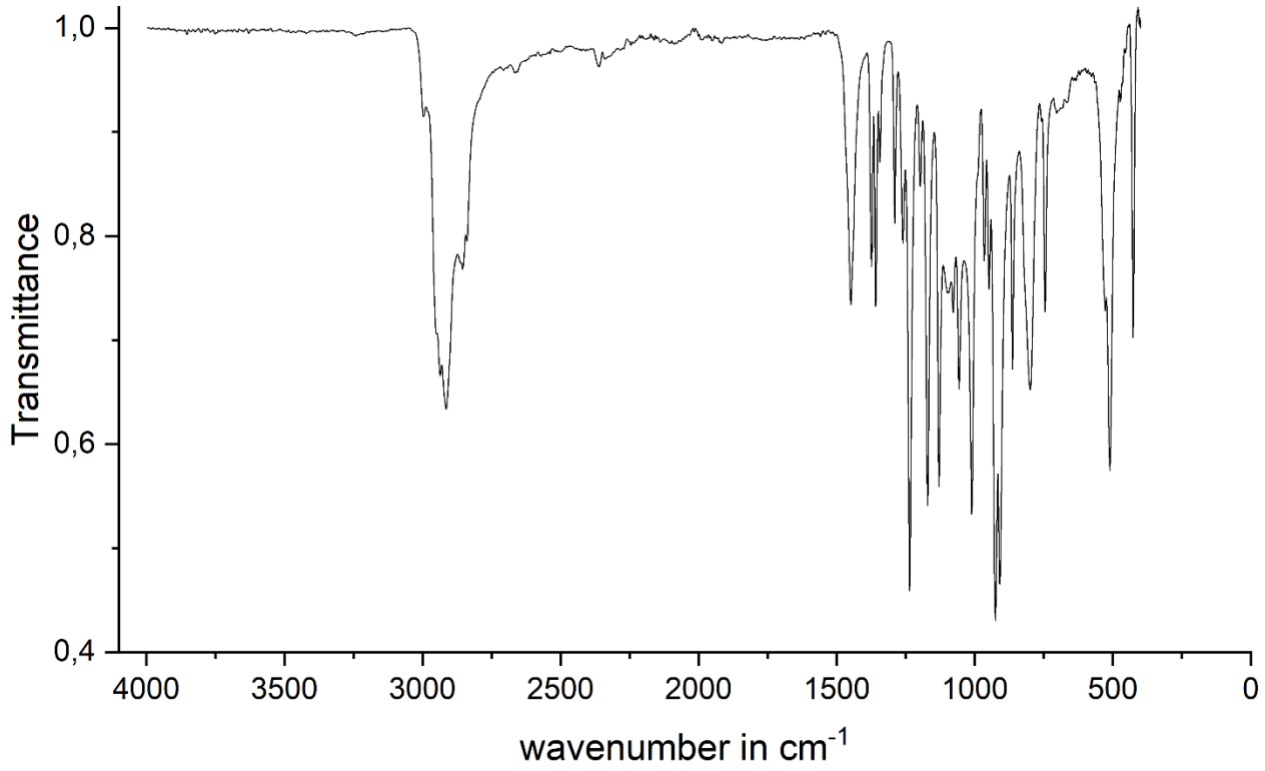

Figure S 9: IR-Spectrum of **2**.

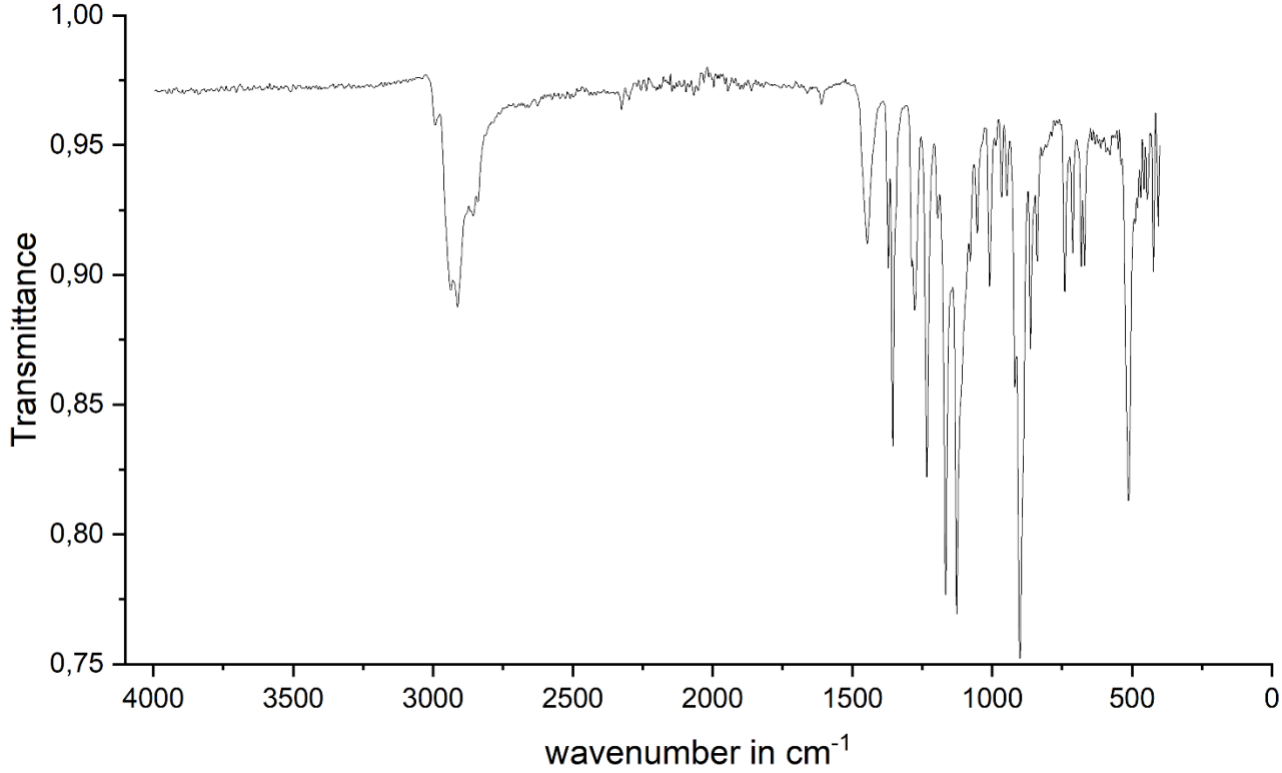

Figure S 10: IR-Spectrum of $[GaTMP]_4$.

LIFDI-Mass Spectra

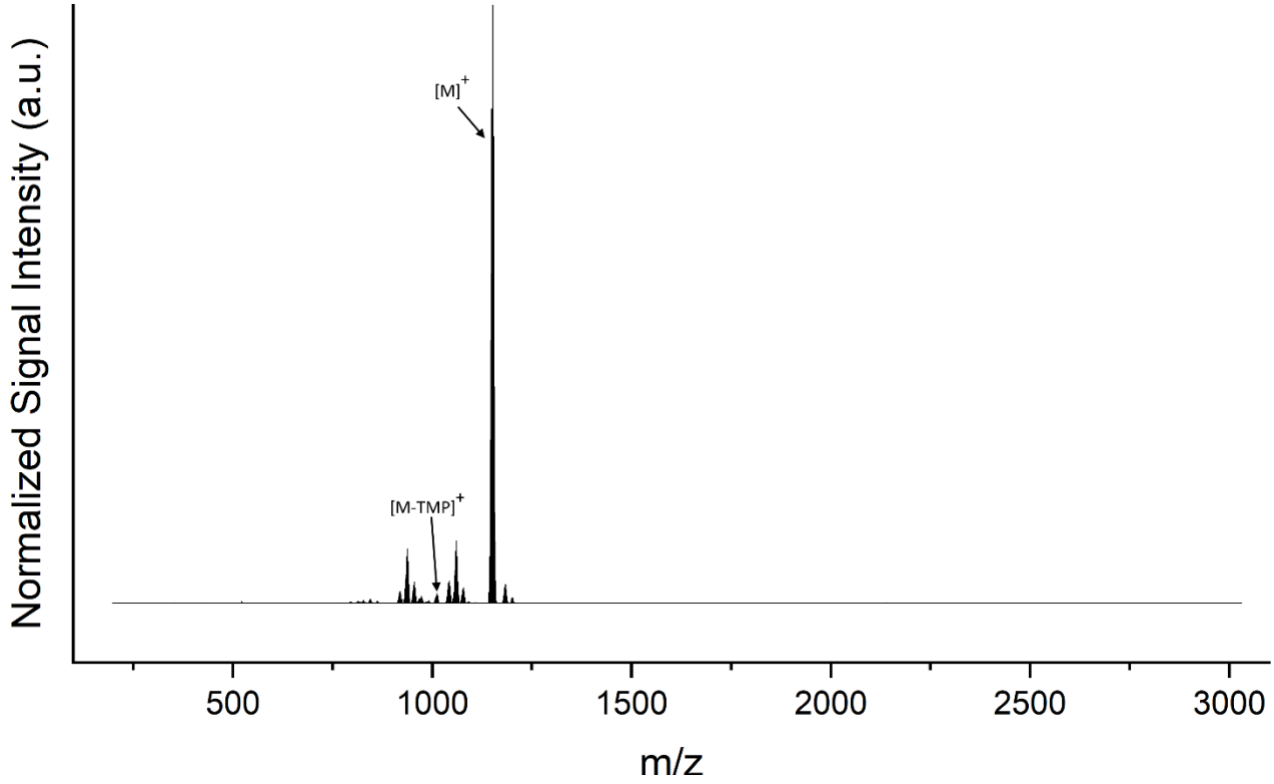

Figure S 11: Mass Spectrum of **1** from 200 – 3000 m/z.

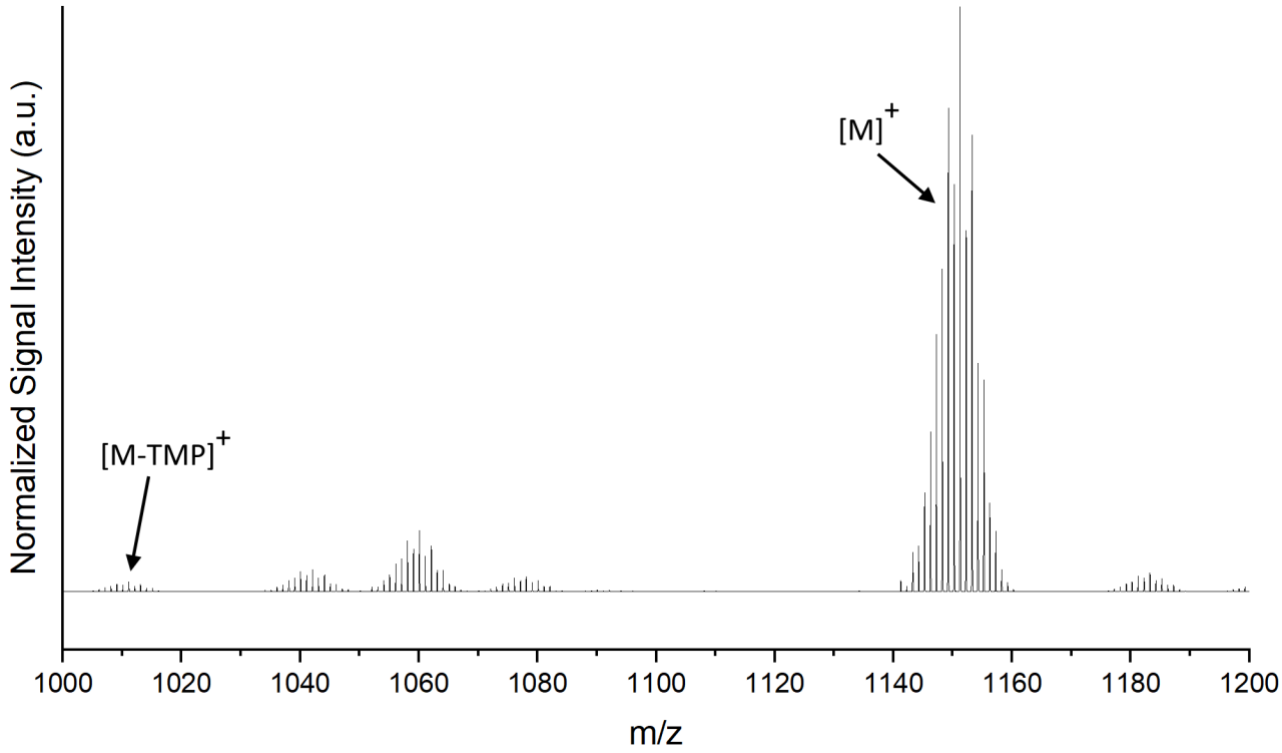

Figure S 12: Mass Spectrum of **1** from 1000 – 1200 m/z.

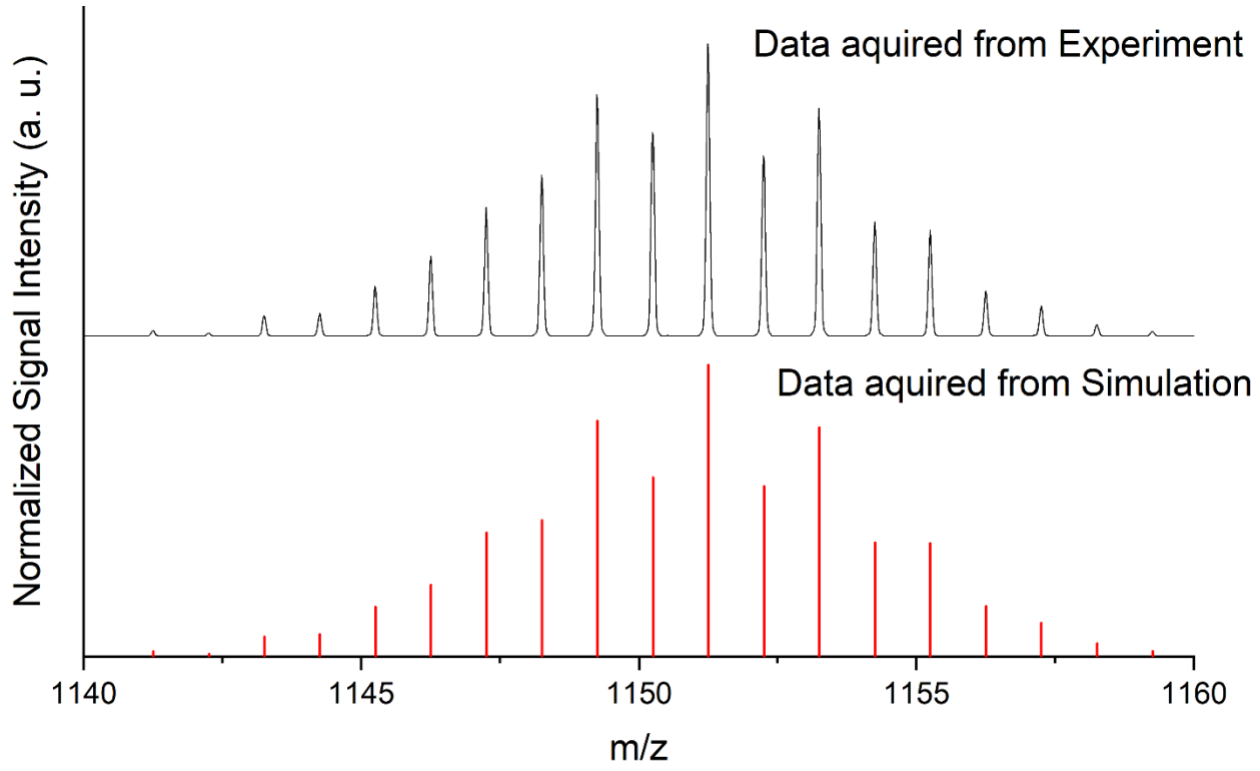

Figure S 13: Isotopic pattern of **1** and simulated isotopic pattern for $RuGa_5N_5C_{45}H_{90}$ (red).

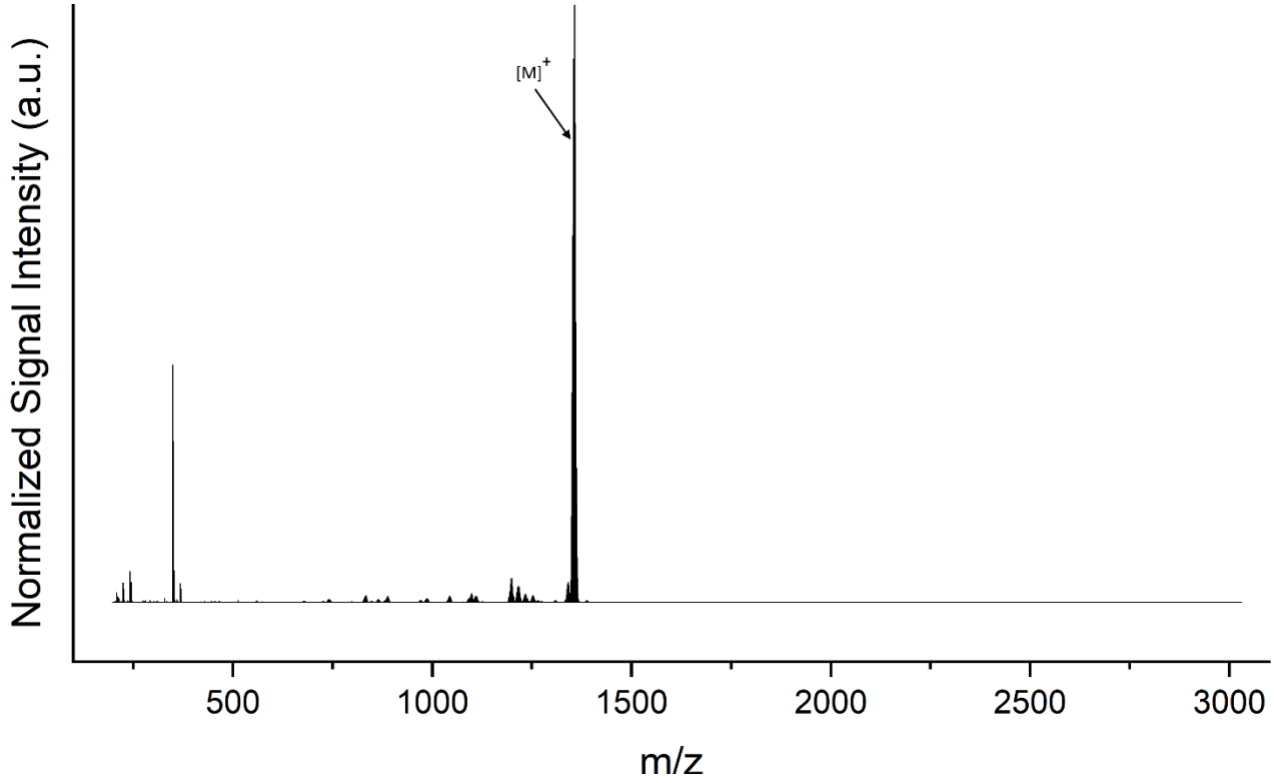

Figure S 14: Mass Spectrum of **2** from 200 – 3000 m/z

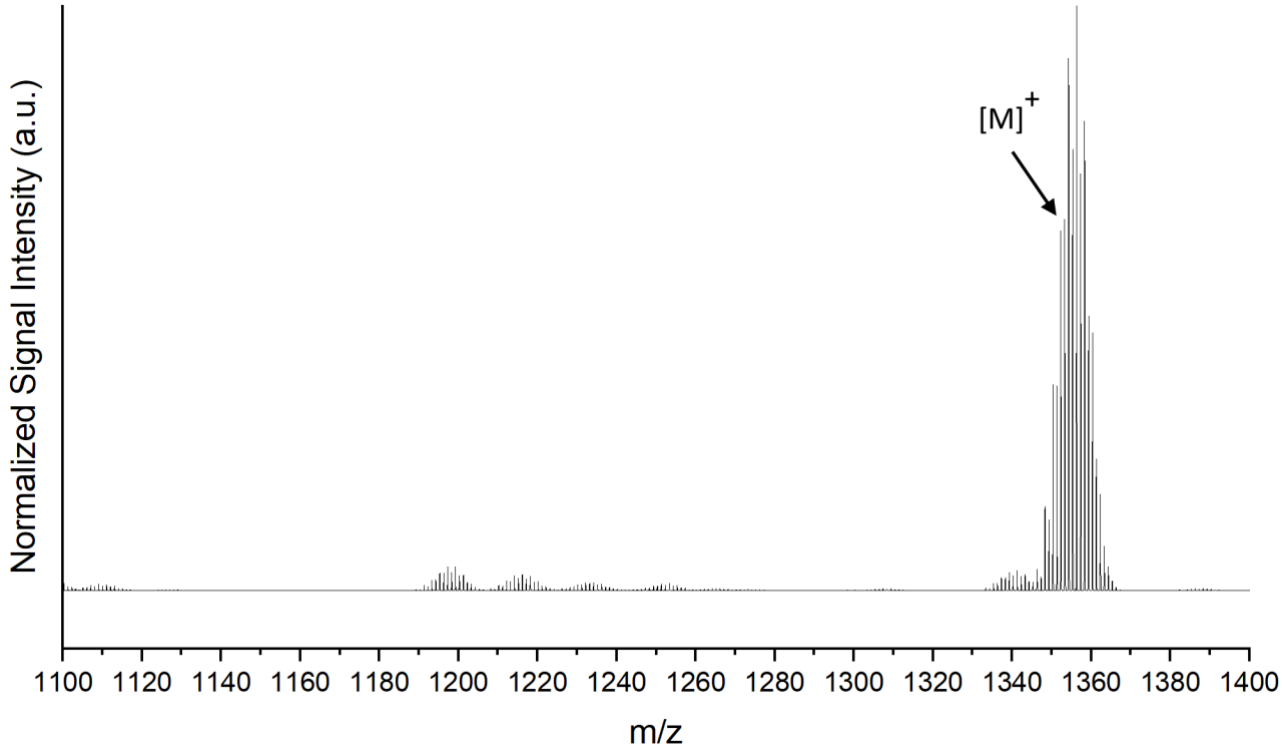

Figure S 15: Mass Spectrum of **2** from 1100 – 1400 m/z

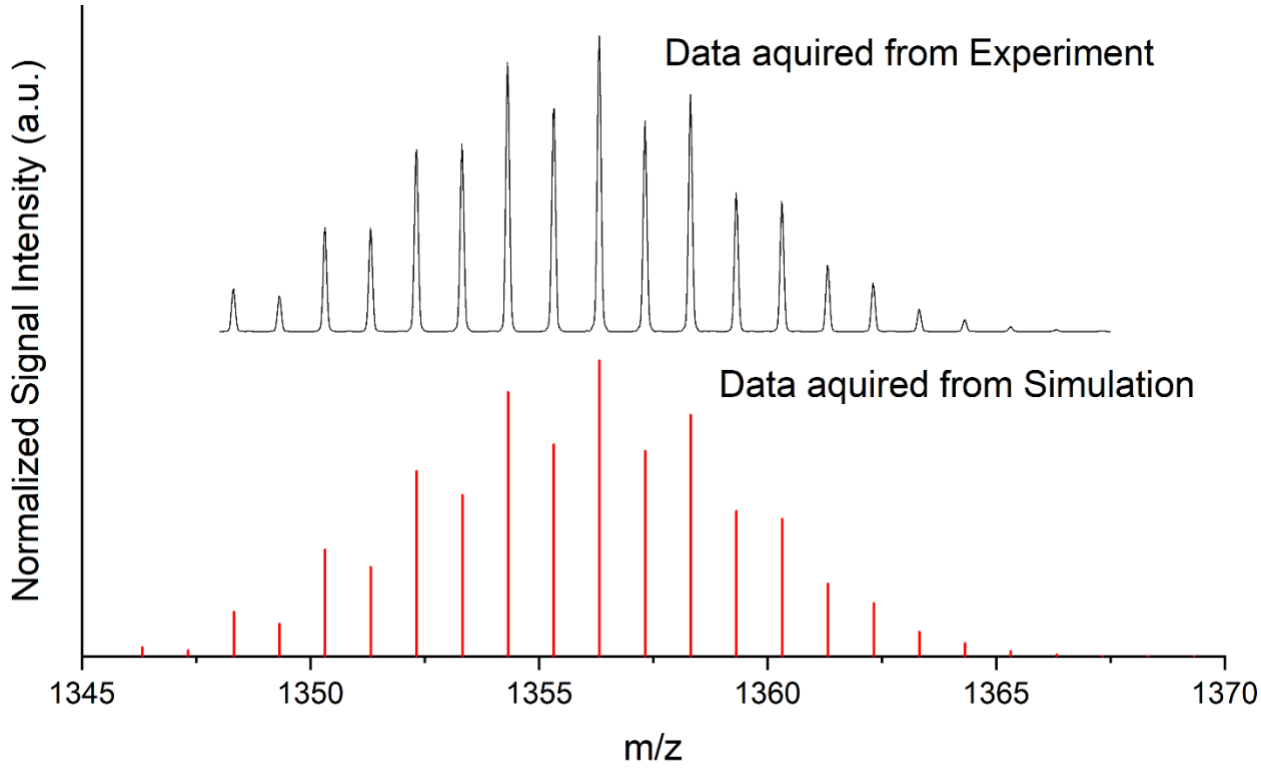

Figure S 16: Isotopic pattern of **2** and simulated isotopic pattern for $MoGa_6N_6C_{54}H_{108}$ (red).

Crystallography

SC-XRD structure report for compound **1**.

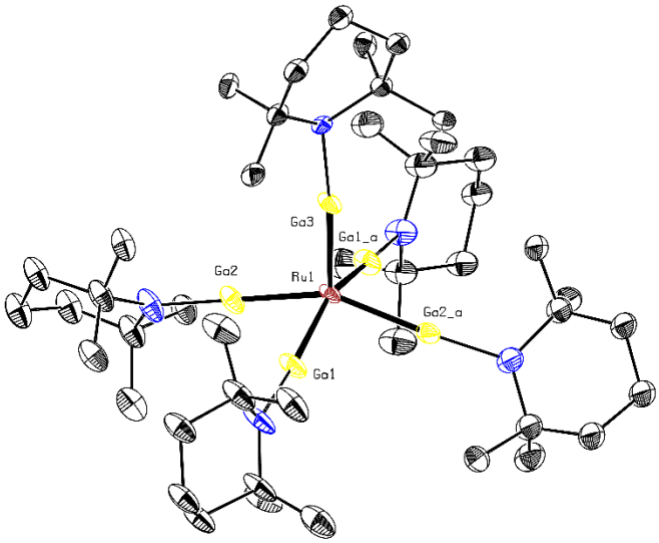

Figure S 17: Molecular structure of [Ru(GaTMP)$_5$] (**1**) in the solid state determined by single crystal X-ray diffraction. Ru: orange, Ga: yellow, N: blue and C: black. Hydrogen atoms and disordered molecule fragments are omitted. Thermal ellipsoids are shown at the 50% probability level.

A yellow, block-shaped crystal of $C_{45}H_{90}Ga_5N_5Ru$ coated with perfluorinated ether and fixed on top of a Kapton micro sampler was used for X-ray crystallographic analysis. The X-ray intensity data were collected at 100(2) K on a Bruker D8 VENTURE Duo three-angle diffractometer with an IMS microsource with MoK_α radiation (λ=0.71073 Å) using APEX4.[1C1] The diffractometer was equipped with a Helios optic monochromator, a Bruker PHOTON II detector, and a low temperature device.

A matrix scan was used to determine the initial lattice parameters. All data were integrated with the Bruker SAINT V8.40B software package using a narrow-frame algorithm and the reflections were corrected for Lorentz and polarisation effects, scan speed, and background.[2C1] The integration of the data using a monoclinic unit cell yielded a total of 5479 reflections within a 2θ range [°] of 3.82 to 52.83 (0.80 Å), of which 5479 were independent. Data were corrected for absorption effects including odd and even ordered spherical harmonics by the multi-scan method (TWINABS 2012/1).[3C1] Space group assignment was based upon systematic absences, E statistics, and successful refinement of the structure.

The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ using SHELXL in conjunction with SHELXLE.[4C1-6C1] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and a C–H

distance of 0.98 Å. Non-methyl hydrogen atoms were refined using a riding model with methylene, aromatic, and other C–H distances of 0.99 Å, 0.95 Å, and 1.00 Å, respectively, and U_{iso} values constrained to 1.2 times the U_{eq} of their pivot atoms. Severe whole molecule and rotational disorder of the TMP moieties was modelled using the *DSR* tool plugin within SHELXLE.[7C1]

Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[8C1] Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[9C1] Supplementary crystallographic data reported in this paper have been deposited with the Cambridge Crystallographic Data Centre (CCDC 2341048) and can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.[9C1] This report and the CIF file were generated using FinalCif.[10C1] Figures showing the coordination polyhedra around the ruthenium centre were created using VESTA 3.[11C1]

Refinement details for compound **1**.

1 was refined as a two-component twin.

Table S 2: Crystal data and structure refinement for compound **1**.

CCDC number	2341048
Empirical formula	$C_{45}H_{90}Ga_5N_5Ru$
Formula weight	1150.88
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$\frac{C2}{c}$ (15)
a [Å]	23.4724(19)
b [Å]	11.9908(9)
c [Å]	18.9429(14)
α [°]	90
β [°]	93.343(3)
γ [°]	90
Volume [Å^3]	5322.5(7)
Z	4
ρ_{calc} [gcm^{-3}]	1.436
μ [mm^{-1}]	2.804
F(000)	2376
Crystal size [mm^3]	0.113×0.120×0.312
Crystal colour	yellow
Crystal shape	fragment
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.82 to 52.83 (0.80 Å)
Index ranges	−29 ≤ h ≤ 29 0 ≤ k ≤ 14

	0 ≤ l ≤ 23
Reflections collected (HKLF4)	9221
Reflections collected (HKLF5)	5479
Independent reflections	5479 R_{int} = 0.0617 R_{sigma} = 0.0456
Completeness to θ = 25.242° (HKLF4)	99.6 %
Data / Restraints / Parameters	5479 / 1051 / 493
Goodness-of-fit on F^2	1.154
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0562 wR_2 = 0.0928
Final *R* indexes [all data]	R_1 = 0.0745 wR_2 = 0.0989
Largest peak/hole [eÅ^{-3}]	0.56/−0.85

Table S 3*: Atomic coordinates and Ueq [Å^2] for compound **1**.*

Atom	***x***	***y***	***z***	U_{eq}
Ru1	0.500000	0.62210(5)	0.250000	0.02208(15)
Ga1	0.54972(3)	0.66491(5)	0.35415(4)	0.03276(17)
Ga2	0.58257(3)	0.67017(5)	0.19995(4)	0.02960(16)
Ga3	0.500000	0.43247(7)	0.250000	0.0291(2)
N1	0.5932(9)	0.6901(17)	0.4384(8)	0.041(2)
C1	0.5972(7)	0.8026(13)	0.4684(9)	0.041(2)
C2	0.6580(9)	0.8257(16)	0.5006(10)	0.040(2)
H2A	0.658150	0.897449	0.526483	0.048
H2B	0.684447	0.832707	0.462032	0.048
C3	0.6794(8)	0.7323(13)	0.5517(10)	0.038(2)
H3A	0.719147	0.748050	0.569220	0.045
H3B	0.655297	0.729391	0.592794	0.045
C4	0.6769(10)	0.6216(15)	0.5133(12)	0.039(2)
H4A	0.688781	0.561740	0.546980	0.047
H4B	0.704345	0.622822	0.475570	0.047
C5	0.6179(9)	0.5942(15)	0.4804(13)	0.042(2)
C6	0.5850(8)	0.8876(12)	0.4073(9)	0.047(3)
H6A	0.587460	0.963650	0.426192	0.070
H6B	0.546673	0.874656	0.385587	0.070
H6C	0.613242	0.878024	0.371643	0.070
C7	0.5519(6)	0.8297(14)	0.5222(9)	0.051(3)
H7A	0.556279	0.907314	0.537795	0.077
H7B	0.557187	0.779979	0.563142	0.077
H7C	0.513654	0.818878	0.499738	0.077
C8	0.6266(10)	0.5004(19)	0.4318(11)	0.048(4)
H8A	0.643388	0.437233	0.458478	0.071
H8B	0.652374	0.523534	0.395649	0.071
H8C	0.589818	0.478035	0.409011	0.071
C9	0.5779(7)	0.5612(15)	0.5421(9)	0.047(3)
H9A	0.592847	0.493955	0.566039	0.071
H9B	0.539162	0.546769	0.522041	0.071
H9C	0.576997	0.622536	0.576220	0.071

N1A	0.5983(12)	0.706(2)	0.4301(11)	0.040(2)
C1A	0.6047(9)	0.8248(18)	0.4473(11)	0.041(2)
C2A	0.6620(12)	0.847(2)	0.4865(13)	0.040(3)
H2AA	0.692444	0.840795	0.452648	0.048
H2AB	0.662358	0.923890	0.504984	0.048
C3A	0.6753(10)	0.7674(17)	0.5471(13)	0.038(3)
H3AA	0.647526	0.777662	0.583928	0.046
H3AB	0.714029	0.782508	0.568585	0.046
C4A	0.6720(13)	0.648(2)	0.5188(16)	0.039(3)
H4AA	0.681585	0.595472	0.558038	0.047
H4AB	0.700717	0.638341	0.482984	0.047
C5A	0.6110(12)	0.619(2)	0.4844(17)	0.042(2)
C6A	0.6022(9)	0.8935(17)	0.3796(11)	0.041(4)
H6AA	0.614037	0.970279	0.390516	0.062
H6AB	0.563118	0.893498	0.358416	0.062
H6AC	0.627930	0.860971	0.346195	0.062
C7A	0.5581(9)	0.8675(19)	0.4945(12)	0.053(4)
H7AA	0.559700	0.949103	0.497036	0.079
H7AB	0.564387	0.836327	0.542181	0.079
H7AC	0.520534	0.844317	0.474445	0.079
C8A	0.6113(12)	0.502(2)	0.4464(15)	0.044(4)
H8AA	0.628414	0.445931	0.478954	0.066
H8AB	0.633723	0.506809	0.404444	0.066
H8AC	0.572102	0.479980	0.432218	0.066
C9A	0.5672(10)	0.605(2)	0.5387(13)	0.051(4)
H9AA	0.579426	0.545748	0.571978	0.077
H9AB	0.530420	0.584703	0.515012	0.077
H9AC	0.563269	0.675034	0.564466	0.077
N2	0.6524(2)	0.7043(4)	0.1650(3)	0.0368(11)
C10	0.6515(9)	0.819(2)	0.1320(12)	0.039(2)
C11	0.7010(8)	0.822(2)	0.0799(11)	0.041(2)
H11A	0.690824	0.772220	0.039188	0.049
H11B	0.705054	0.898292	0.061478	0.049
C12	0.7575(8)	0.7846(19)	0.1140(11)	0.041(3)
H12A	0.769394	0.835346	0.153365	0.049
H12B	0.787205	0.785707	0.079012	0.049
C13	0.7497(9)	0.6647(19)	0.1422(12)	0.038(2)
H13A	0.738295	0.614730	0.102204	0.046
H13B	0.786530	0.637535	0.163816	0.046
C14	0.7055(14)	0.660(2)	0.1958(17)	0.035(2)
C15	0.5967(9)	0.840(2)	0.0897(12)	0.039(4)
H15A	0.566325	0.854872	0.121778	0.059
H15B	0.586802	0.773750	0.061138	0.059
H15C	0.601091	0.904138	0.058599	0.059
C16	0.6573(11)	0.917(2)	0.1829(14)	0.043(4)
H16A	0.652021	0.986753	0.156741	0.065
H16B	0.695416	0.915590	0.207063	0.065
H16C	0.628359	0.910564	0.217918	0.065
C17	0.6923(14)	0.537(3)	0.211(2)	0.033(4)
H17A	0.724477	0.504077	0.238777	0.049
H17B	0.686007	0.496921	0.166340	0.049
H17C	0.657858	0.532817	0.237848	0.049

C18	0.7298(13)	0.715(2)	0.2626(13)	0.035(4)
H18A	0.759930	0.667459	0.284472	0.053
H18B	0.699438	0.724452	0.295472	0.053
H18C	0.745692	0.787679	0.251256	0.053
N2A	0.6524(2)	0.7043(4)	0.1650(3)	0.0368(11)
C10A	0.6627(8)	0.8017(16)	0.1190(10)	0.037(2)
C11A	0.7135(7)	0.7851(17)	0.0738(9)	0.040(2)
H11C	0.703185	0.730181	0.036226	0.048
H11D	0.722167	0.856634	0.050614	0.048
C12A	0.7663(7)	0.7451(18)	0.1155(10)	0.042(2)
H12C	0.778136	0.801217	0.151791	0.050
H12D	0.797864	0.735985	0.083473	0.050
C13A	0.7546(8)	0.6351(17)	0.1508(10)	0.038(2)
H13C	0.789297	0.611213	0.178975	0.046
H13D	0.746098	0.577999	0.113925	0.046
C14A	0.7029(12)	0.642(2)	0.2008(15)	0.035(2)
C15A	0.6075(7)	0.8121(16)	0.0697(10)	0.034(3)
H15D	0.611861	0.873574	0.036323	0.050
H15E	0.574862	0.826961	0.098240	0.050
H15F	0.601131	0.742361	0.043450	0.050
C16A	0.6699(10)	0.9092(19)	0.1643(11)	0.044(4)
H16D	0.668057	0.974615	0.133188	0.066
H16E	0.706996	0.907597	0.190933	0.066
H16F	0.639368	0.913355	0.197251	0.066
C17A	0.6845(13)	0.523(2)	0.2160(18)	0.036(4)
H17D	0.718084	0.478067	0.230889	0.054
H17E	0.665952	0.490178	0.173086	0.054
H17F	0.657678	0.523166	0.253707	0.054
C18A	0.7211(11)	0.694(2)	0.2740(11)	0.038(4)
H18D	0.753080	0.651506	0.296018	0.056
H18E	0.688822	0.691660	0.304519	0.056
H18F	0.732788	0.771492	0.267376	0.056
N3	0.4948(6)	0.2783(6)	0.2606(6)	0.0199(17)
C19	0.552(3)	0.222(4)	0.277(3)	0.0236(18)
C20	0.5625(5)	0.1045(9)	0.2457(6)	0.0275(18)
H20A	0.577562	0.112768	0.198186	0.033
H20B	0.591748	0.065380	0.276252	0.033
C21	0.5094(6)	0.0360(8)	0.2399(7)	0.0296(19)
H21A	0.496829	0.019344	0.287794	0.036
H21B	0.517101	−0.035641	0.216300	0.036
C22	0.4620(5)	0.0988(9)	0.1974(6)	0.0271(18)
H22A	0.472904	0.105249	0.147835	0.033
H22B	0.426635	0.053724	0.197066	0.033
C23	0.449(3)	0.215(4)	0.225(3)	0.0233(18)
C24	0.6073(5)	0.2904(9)	0.2642(7)	0.030(2)
H24A	0.640895	0.246930	0.280671	0.045
H24B	0.606635	0.360761	0.290410	0.045
H24C	0.609144	0.306023	0.213605	0.045
C25	0.5491(5)	0.2139(9)	0.3582(6)	0.028(2)
H25A	0.587368	0.199039	0.379577	0.042
H25B	0.523386	0.153058	0.369864	0.042
H25C	0.534832	0.284307	0.376554	0.042

C26	0.4176(5)	0.2794(9)	0.1664(6)	0.027(2)
H26A	0.382069	0.240506	0.151958	0.041
H26B	0.441553	0.285107	0.125830	0.041
H26C	0.408741	0.354294	0.183223	0.041
C27	0.4136(5)	0.2104(9)	0.2887(6)	0.026(2)
H27A	0.377318	0.172859	0.276234	0.039
H27B	0.406147	0.286245	0.305040	0.039
H27C	0.434520	0.168760	0.326450	0.039

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor

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SC-XRD structure report for compound **2**.

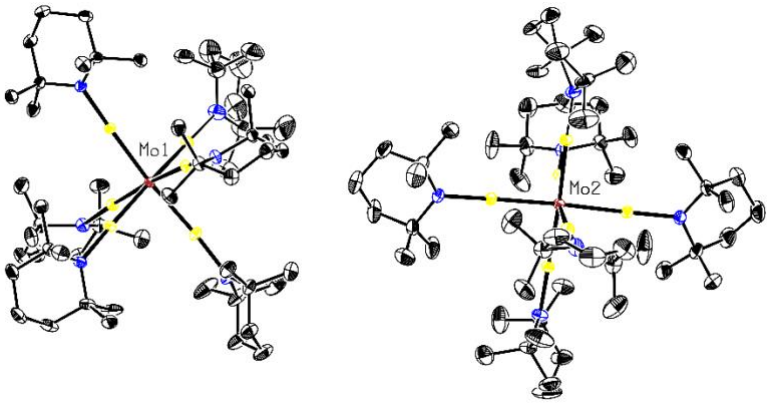

Figure S 18: Molecular structure of [Mo(GaTMP)$_6$] (**2**) in the solid state determined by single crystal X-ray diffraction. Mo: red, Ga: yellow, N: blue and C: black. Hydrogen atoms and disordered molecule fragments are omitted. Thermal ellipsoids are shown at the 50% probability level.

A colourless, block-shaped crystal of $C_{54}H_{108}Ga_6MoN_6$ coated with perfluorinated ether and fixed on top of a Kapton micro sampler was used for X-ray crystallographic analysis. The X-ray intensity data were collected at 100(2) K on a Bruker D8 VENTURE Duo three-angle diffractometer with an IMS microsource with MoK_α radiation (λ=0.71073 Å) using APEX4.[1C2] The diffractometer was

equipped with a Helios optic monochromator, a Bruker PHOTON II detector, and a low temperature device.

A matrix scan was used to determine the initial lattice parameters. All data were integrated with the Bruker SAINT V8.40B software package using a narrow-frame algorithm and the reflections were corrected for Lorentz and polarisation effects, scan speed, and background.[2C2] The integration of the data using a monoclinic unit cell yielded a total of 776202 reflections within a 2θ range [°] of 4.08 to 52.83 (0.80 Å), of which 26306 were independent. Data were corrected for absorption effects including odd and even ordered spherical harmonics by the multi-scan method (SADABS 2016/2).[3C2] Space group assignment was based upon systematic absences, E statistics, and successful refinement of the structure.

The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ using SHELXL in conjunction with SHELXLE.[4C2-6C2] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and a C–H distance of 0.98 Å. Non-methyl hydrogen atoms were refined using a riding model with methylene, aromatic, and other C–H distances of 0.99 Å, 0.95 Å, and 1.00 Å, respectively, and U_{iso} values constrained to 1.2 times the U_{eq} of their pivot atoms. Whole molecule disorder and rotational disorder, e.g. of TMP moieties, was modelled using the *DSR* tool plugin within SHELXLE.[[7C2]

Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[8C2] Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[9C2] Supplementary crystallographic data reported in this paper have been deposited with the Cambridge Crystallographic Data Centre (CCDC 2341049) and can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.[9C2] This report and the CIF file were generated using FinalCif.[10C2] Figures showing the coordination polyhedra around the molybdenum centre were created using VESTA 3.[11C2]

Table S 4: Crystal data and structure refinement for compound **2**.

CCDC number	2341049
Empirical formula	$C_{54}H_{108}Ga_6MoN_6$
Formula weight	1355.72
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$\frac{P2_1}{c}$ (14)
a [Å]	26.9295(18)
b [Å]	21.9030(15)

c [Å]	24.2260(15)
α [°]	90
β [°]	116.221(2)
γ [°]	90
Volume [Å^3]	12819.0(15)
Z	8
ρ_{calc} [gcm^{-3}]	1.405
μ [mm^{-1}]	2.709
F(000)	5616
Crystal size [mm^3]	0.278×0.339×0.428
Crystal colour	colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.08 to 52.83 (0.80 Å)
Index ranges	−33 ≤ h ≤ 33 −27 ≤ k ≤ 27 −30 ≤ l ≤ 30
Reflections collected	776202
Independent reflections	26306 R_{int} = 0.0429 R_{sigma} = 0.0122
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	26306 / 739 / 1436
Goodness-of-fit on F^2	1.028
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0198 wR_2 = 0.0441
Final *R* indexes [all data]	R_1 = 0.0255 wR_2 = 0.0466
Largest peak/hole [eÅ^{-3}]	0.55/−0.46

Table S 5*: Atomic coordinates and Ueq [Å^2] for compound **2**.*

Atom	***x***	***y***	***z***	U_{eq}
Mo1	0.38238(2)	0.74227(2)	0.23060(2)	0.01366(3)
Mo2	0.11461(2)	0.23662(2)	0.34993(2)	0.01461(3)
Ga1	0.32971(2)	0.72828(2)	0.28718(2)	0.01931(4)
Ga2	0.32465(2)	0.67490(2)	0.15029(2)	0.02012(4)
Ga3	0.45061(2)	0.74184(2)	0.19234(2)	0.01487(4)
Ga4	0.43058(2)	0.81839(2)	0.30507(2)	0.01559(4)
Ga5	0.32948(2)	0.82742(2)	0.17237(2)	0.01659(4)
Ga6	0.43626(2)	0.66305(2)	0.29688(2)	0.01627(4)
Ga7	0.17039(2)	0.31657(2)	0.33955(2)	0.01780(4)
Ga8	0.05019(2)	0.23283(2)	0.24396(2)	0.01641(4)
Ga9	0.06052(2)	0.15865(2)	0.36589(2)	0.01725(4)
Ga10	0.17637(2)	0.22566(2)	0.45628(2)	0.02001(4)
Ga11	0.16747(2)	0.16462(2)	0.32425(2)	0.01861(4)
Ga12	0.06146(2)	0.31313(2)	0.36953(2)	0.01758(4)
N1	0.29434(6)	0.72121(8)	0.33751(7)	0.0263(3)
N3	0.50659(6)	0.73802(6)	0.16701(7)	0.0174(3)

N4	0.46444(6)	0.87955(7)	0.36181(7)	0.0194(3)
N5	0.28979(6)	0.89690(7)	0.13216(7)	0.0201(3)
N6	0.47526(6)	0.60219(6)	0.35206(7)	0.0192(3)
N7	0.21475(6)	0.37883(7)	0.33388(7)	0.0249(3)
N8	0.00095(6)	0.22435(7)	0.16147(7)	0.0215(3)
N9	0.01804(6)	0.09709(7)	0.37621(7)	0.0237(3)
N10	0.22489(7)	0.21346(8)	0.53826(7)	0.0297(4)
N12	0.01959(6)	0.37220(7)	0.38440(7)	0.0237(3)
C1	0.23537(9)	0.73903(12)	0.31267(10)	0.0377(5)
C2	0.22532(10)	0.77367(12)	0.36204(11)	0.0444(6)
H2A	0.243627	0.814038	0.368915	0.053
H2B	0.185091	0.780681	0.346790	0.053
C3	0.24697(10)	0.73964(12)	0.42285(11)	0.0421(6)
H3A	0.226736	0.700635	0.417299	0.051
H3B	0.241021	0.764449	0.453562	0.051
C4	0.30852(9)	0.72711(10)	0.44553(9)	0.0339(5)
H4A	0.322256	0.703565	0.484364	0.041
H4B	0.328707	0.766428	0.454504	0.041
C5	0.32101(8)	0.69143(9)	0.39859(8)	0.0256(4)
C6	0.22264(10)	0.78276(14)	0.25888(11)	0.0521(7)
H6A	0.184035	0.796219	0.242405	0.078
H6B	0.228561	0.761795	0.226543	0.078
H6C	0.247180	0.818304	0.273221	0.078
C7	0.19534(9)	0.68477(14)	0.28765(12)	0.0545(7)
H7A	0.157326	0.699981	0.265770	0.082
H7B	0.198428	0.658743	0.321925	0.082
H7C	0.204756	0.661015	0.259309	0.082
C8	0.38354(8)	0.69198(10)	0.42046(9)	0.0307(4)
H8A	0.402001	0.675794	0.462440	0.046
H8B	0.395957	0.733939	0.419926	0.046
H8C	0.392833	0.666552	0.393050	0.046
C9	0.30443(10)	0.62397(10)	0.39771(11)	0.0401(5)
H9A	0.328994	0.604630	0.436808	0.060
H9B	0.307645	0.602779	0.363811	0.060
H9C	0.266099	0.621596	0.391963	0.060
N2	0.27960(7)	0.62157(8)	0.08901(8)	0.0349(4)
C10	0.3029(11)	0.5847(11)	0.0551(11)	0.0364(10)
C11	0.2653(2)	0.5913(3)	−0.0148(2)	0.0575(11)
H11A	0.266396	0.634142	−0.027383	0.069
H11B	0.279534	0.564952	−0.037783	0.069
C12	0.20507(18)	0.5736(3)	−0.0316(2)	0.0659(12)
H12A	0.181951	0.576998	−0.076578	0.079
H12B	0.203153	0.531120	−0.018832	0.079
C13	0.18584(19)	0.6161(2)	0.0011(3)	0.0626(12)
H13A	0.146786	0.606624	−0.009114	0.075
H13B	0.187099	0.658064	−0.013345	0.075
C14	0.2206(2)	0.6138(3)	0.0722(3)	0.0454(10)
C15	0.3611(2)	0.6059(3)	0.0684(3)	0.0413(12)
H15A	0.375016	0.581172	0.044519	0.062
H15B	0.385568	0.601152	0.112365	0.062
H15C	0.359954	0.648909	0.056808	0.062
C16	0.3103(3)	0.5173(3)	0.0706(3)	0.0547(13)

H16A	0.334648	0.499190	0.054657	0.082
H16B	0.274211	0.496940	0.051942	0.082
H16C	0.326916	0.512129	0.115415	0.082
C17	0.2010(2)	0.6722(3)	0.0926(3)	0.0661(16)
H17A	0.161698	0.668300	0.082728	0.099
H17B	0.206200	0.707611	0.070952	0.099
H17C	0.222638	0.677838	0.137081	0.099
C18	0.2073(2)	0.5550(3)	0.0960(3)	0.0683(14)
H18A	0.167733	0.554073	0.085610	0.102
H18B	0.229035	0.552911	0.140731	0.102
H18C	0.216390	0.520096	0.076862	0.102
N2A	0.27960(7)	0.62157(8)	0.08901(8)	0.0349(4)
C10A	0.302(2)	0.584(2)	0.055(2)	0.0370(18)
C11A	0.2620(5)	0.5657(5)	−0.0058(5)	0.064(2)
H11C	0.278599	0.534945	−0.022701	0.077
H11D	0.251095	0.601578	−0.033557	0.077
C12A	0.2077(4)	0.5369(6)	−0.0018(5)	0.073(2)
H12C	0.218161	0.501218	0.026113	0.088
H12D	0.179698	0.523969	−0.043000	0.088
C13A	0.1823(4)	0.5951(6)	0.0266(5)	0.062(2)
H13C	0.176649	0.632577	0.001704	0.074
H13D	0.146523	0.583148	0.025772	0.074
C14A	0.2248(5)	0.6056(6)	0.0911(4)	0.0411(16)
C15A	0.3473(5)	0.6245(6)	0.0523(5)	0.044(2)
H15D	0.363682	0.603996	0.028385	0.067
H15E	0.376072	0.632194	0.094145	0.067
H15F	0.331011	0.663437	0.032686	0.067
C16A	0.3266(5)	0.5244(5)	0.0967(5)	0.053(2)
H16D	0.343453	0.497756	0.077192	0.080
H16E	0.296690	0.502485	0.100818	0.080
H16F	0.354670	0.536638	0.137499	0.080
C17A	0.2094(4)	0.6519(5)	0.1238(5)	0.055(2)
H17D	0.169384	0.650146	0.110636	0.082
H17E	0.219370	0.692309	0.114551	0.082
H17F	0.229049	0.644285	0.168144	0.082
C18A	0.2292(4)	0.5579(6)	0.1343(6)	0.070(3)
H18D	0.193717	0.553577	0.136138	0.105
H18E	0.258137	0.568533	0.175132	0.105
H18F	0.238611	0.519306	0.120779	0.105
C19	0.51820(7)	0.79215(8)	0.13789(8)	0.0196(4)
C20	0.52709(8)	0.77282(9)	0.08185(9)	0.0272(4)
H20A	0.491310	0.759234	0.048595	0.033
H20B	0.539732	0.808635	0.066550	0.033
C21	0.56921(9)	0.72171(9)	0.09642(9)	0.0298(4)
H21A	0.606124	0.736057	0.126670	0.036
H21B	0.571854	0.709207	0.058538	0.036
C22	0.55100(8)	0.66763(9)	0.12271(9)	0.0251(4)
H22A	0.579100	0.634881	0.133592	0.030
H22B	0.515711	0.651432	0.090653	0.030
C23	0.54311(7)	0.68420(8)	0.17998(8)	0.0185(3)
C24	0.46758(8)	0.83436(9)	0.11477(9)	0.0269(4)
H24A	0.472927	0.868209	0.091493	0.040

H24B	0.463018	0.850562	0.149964	0.040
H24C	0.434433	0.811269	0.088080	0.040
C25	0.56786(8)	0.82959(8)	0.18306(9)	0.0255(4)
H25A	0.570468	0.867667	0.163256	0.038
H25B	0.601931	0.805910	0.194889	0.038
H25C	0.562843	0.839046	0.219814	0.038
C26	0.51522(8)	0.62998(8)	0.19461(9)	0.0241(4)
H26A	0.537459	0.593127	0.199685	0.036
H26B	0.478207	0.623952	0.160796	0.036
H26C	0.512097	0.638092	0.232742	0.036
C27	0.59985(8)	0.69257(9)	0.23643(9)	0.0273(4)
H27A	0.618156	0.652832	0.248911	0.041
H27B	0.594346	0.710234	0.270483	0.041
H27C	0.623001	0.719955	0.225650	0.041
C28	0.43591(8)	0.90769(9)	0.39572(8)	0.0245(4)
C29	0.44225(9)	0.97736(9)	0.39691(9)	0.0314(5)
H29A	0.419117	0.993657	0.355205	0.038
H29B	0.428324	0.994850	0.425096	0.038
C30	0.50149(9)	0.99782(9)	0.41740(9)	0.0325(5)
H30A	0.524339	0.985431	0.460640	0.039
H30B	0.502906	1.042868	0.415028	0.039
C31	0.52428(9)	0.96906(9)	0.37626(9)	0.0309(4)
H31A	0.563313	0.981763	0.390591	0.037
H31B	0.503015	0.984301	0.333717	0.037
C32	0.52130(7)	0.89904(8)	0.37603(8)	0.0220(4)
C33	0.37425(9)	0.89261(11)	0.36199(10)	0.0384(5)
H33A	0.354416	0.914032	0.381744	0.058
H33B	0.369018	0.848488	0.363617	0.058
H33C	0.359781	0.905646	0.318976	0.058
C34	0.45670(9)	0.88248(9)	0.46152(9)	0.0316(5)
H34A	0.431697	0.895581	0.478814	0.047
H34B	0.494022	0.898037	0.487153	0.047
H34C	0.457609	0.837781	0.460473	0.047
C35	0.53536(8)	0.87578(9)	0.32518(9)	0.0271(4)
H35A	0.571621	0.891587	0.331841	0.041
H35B	0.507131	0.889766	0.285160	0.041
H35C	0.536338	0.831047	0.325908	0.041
C36	0.56549(8)	0.87318(10)	0.43711(9)	0.0313(4)
H36A	0.602412	0.881481	0.440257	0.047
H36B	0.560344	0.828995	0.438363	0.047
H36C	0.561840	0.892599	0.471574	0.047
C37	0.32059(8)	0.95043(8)	0.12662(8)	0.0233(4)
C38	0.28620(9)	1.00868(9)	0.11634(10)	0.0340(5)
H38A	0.283365	1.018844	0.154670	0.041
H38B	0.305480	1.042827	0.107175	0.041
C39	0.22840(9)	1.00251(10)	0.06410(11)	0.0381(5)
H39A	0.207251	1.040562	0.060184	0.046
H39B	0.230616	0.995555	0.024873	0.046
C40	0.19938(8)	0.94928(10)	0.07730(10)	0.0324(5)
H40A	0.162238	0.944405	0.042362	0.039
H40B	0.194205	0.958731	0.114382	0.039
C41	0.23088(7)	0.88885(9)	0.08755(8)	0.0228(4)

C42	0.37251(8)	0.95758(9)	0.18803(10)	0.0330(5)
H42A	0.391383	0.995742	0.187732	0.050
H42B	0.397487	0.923066	0.193777	0.050
H42C	0.361818	0.958485	0.221790	0.050
C43	0.33947(9)	0.94339(10)	0.07555(10)	0.0332(5)
H43A	0.363154	0.977943	0.077061	0.050
H43B	0.306980	0.942492	0.035380	0.050
H43C	0.360280	0.905253	0.081688	0.050
C44	0.20537(8)	0.84438(10)	0.11618(10)	0.0325(5)
H44A	0.165907	0.839311	0.088610	0.049
H44B	0.209743	0.860448	0.155830	0.049
H44C	0.224042	0.804787	0.122505	0.049
C45	0.22342(9)	0.86214(11)	0.02565(9)	0.0344(5)
H45A	0.184506	0.851125	0.000928	0.052
H45B	0.246580	0.825678	0.033047	0.052
H45C	0.234412	0.892614	0.003530	0.052
C46	0.45656(8)	0.53804(8)	0.33662(8)	0.0211(4)
C47	0.46760(8)	0.50261(8)	0.39547(9)	0.0254(4)
H47A	0.442399	0.517678	0.412301	0.030
H47B	0.459346	0.458862	0.385256	0.030
C48	0.52708(8)	0.50908(9)	0.44423(9)	0.0290(4)
H48A	0.552644	0.492463	0.428601	0.035
H48B	0.532468	0.485894	0.481539	0.035
C49	0.53934(8)	0.57630(9)	0.45991(8)	0.0277(4)
H49A	0.578235	0.580732	0.491234	0.033
H49B	0.515223	0.591588	0.478071	0.033
C50	0.53019(7)	0.61551(8)	0.40361(8)	0.0209(4)
C51	0.39382(8)	0.53840(9)	0.29622(9)	0.0300(4)
H51A	0.380113	0.496303	0.288420	0.045
H51B	0.385646	0.558575	0.257027	0.045
H51C	0.375617	0.560536	0.317375	0.045
C52	0.48286(9)	0.50489(9)	0.30007(9)	0.0305(4)
H52A	0.464100	0.465740	0.285073	0.046
H52B	0.522192	0.497658	0.326839	0.046
H52C	0.479052	0.530154	0.265033	0.046
C53	0.53139(8)	0.68243(9)	0.42189(9)	0.0279(4)
H53A	0.566188	0.690969	0.458282	0.042
H53B	0.500169	0.690659	0.431280	0.042
H53C	0.528591	0.708597	0.387816	0.042
C54	0.57812(8)	0.60617(9)	0.38612(9)	0.0285(4)
H54A	0.613135	0.617490	0.420997	0.043
H54B	0.572168	0.631855	0.350616	0.043
H54C	0.579569	0.563204	0.375624	0.043
C55	0.20120(10)	0.44307(10)	0.33975(12)	0.0382(5)
C56	0.21250(10)	0.48399(11)	0.29543(13)	0.0478(6)
H56A	0.184122	0.475959	0.252920	0.057
H56B	0.208950	0.527216	0.305088	0.057
C57	0.26963(10)	0.47416(11)	0.29850(12)	0.0458(6)
H57A	0.274039	0.499946	0.267393	0.055
H57B	0.298541	0.485831	0.339675	0.055
C58	0.27583(10)	0.40737(11)	0.28625(11)	0.0412(6)
H58A	0.313236	0.400660	0.289085	0.049

H58B	0.248479	0.397122	0.243826	0.049
C59	0.26748(8)	0.36473(9)	0.33125(10)	0.0293(4)
C60	0.13849(11)	0.44646(11)	0.32025(16)	0.0621(9)
H60A	0.126919	0.489314	0.316121	0.093
H60B	0.130244	0.426619	0.351514	0.093
H60C	0.118425	0.425616	0.280717	0.093
C61	0.23238(16)	0.46717(13)	0.40545(14)	0.0703(10)
H61A	0.217585	0.507239	0.408504	0.105
H61B	0.271799	0.471018	0.415935	0.105
H61C	0.227738	0.438709	0.434042	0.105
C62	0.26371(11)	0.29959(11)	0.30717(15)	0.0532(7)
H62A	0.296285	0.290825	0.300398	0.080
H62B	0.230169	0.295339	0.268269	0.080
H62C	0.262256	0.270805	0.337394	0.080
C63	0.31807(10)	0.36727(13)	0.39407(12)	0.0523(7)
H63A	0.350446	0.351223	0.390397	0.078
H63B	0.311113	0.342551	0.423651	0.078
H63C	0.325028	0.409673	0.408386	0.078
C64	−0.04103(8)	0.17506(9)	0.14135(8)	0.0253(4)
C65	−0.05258(9)	0.15229(10)	0.07698(9)	0.0346(5)
H65A	−0.019939	0.129433	0.079452	0.042
H65B	−0.084390	0.123810	0.062184	0.042
C66	−0.06525(10)	0.20423(11)	0.03088(10)	0.0429(6)
H66A	−0.071277	0.187825	−0.009676	0.051
H66B	−0.099291	0.225811	0.025879	0.051
C67	−0.01646(11)	0.24819(12)	0.05473(10)	0.0457(6)
H67A	−0.024368	0.282160	0.025065	0.055
H67B	0.016837	0.226565	0.057488	0.055
C68	−0.00438(9)	0.27456(9)	0.11835(9)	0.0315(5)
C69	−0.01728(10)	0.12078(10)	0.18522(10)	0.0396(5)
H69A	−0.042134	0.085655	0.169339	0.059
H69B	−0.013769	0.131764	0.226000	0.059
H69C	0.019238	0.110243	0.188343	0.059
C70	−0.09531(9)	0.19318(12)	0.14289(12)	0.0460(6)
H70A	−0.119252	0.157237	0.134398	0.069
H70B	−0.114040	0.224473	0.111630	0.069
H70C	−0.087386	0.209414	0.183644	0.069
C71	0.05074(10)	0.30848(12)	0.14301(11)	0.0521(7)
H71A	0.049637	0.338697	0.112655	0.078
H71B	0.080688	0.279303	0.150738	0.078
H71C	0.057296	0.329221	0.181471	0.078
C72	−0.04880(11)	0.32117(11)	0.11205(12)	0.0518(7)
H72A	−0.047036	0.355901	0.087471	0.078
H72B	−0.042452	0.335460	0.152978	0.078
H72C	−0.085396	0.302057	0.091665	0.078
C73	0.03434(8)	0.03234(9)	0.37763(9)	0.0276(4)
C74	−0.01559(9)	−0.00660(10)	0.33765(11)	0.0377(5)
H74A	−0.027495	0.003895	0.293866	0.045
H74B	−0.004723	−0.050182	0.343247	0.045
C75	−0.06394(10)	0.00268(11)	0.35331(13)	0.0469(6)
H75A	−0.053215	−0.009888	0.396342	0.056
H75B	−0.095825	−0.022540	0.325862	0.056

C76	−0.07983(9)	0.06997(11)	0.34505(13)	0.0459(6)
H76A	−0.111037	0.076500	0.355534	0.055
H76B	−0.092557	0.081286	0.301324	0.055
C77	−0.03136(9)	0.11180(10)	0.38551(10)	0.0328(5)
C78	0.07655(9)	0.02801(10)	0.35152(11)	0.0369(5)
H78A	0.085477	−0.014962	0.348991	0.055
H78B	0.110292	0.050015	0.378507	0.055
H78C	0.060945	0.046195	0.310336	0.055
C79	0.06286(10)	0.00571(10)	0.44324(10)	0.0424(6)
H79A	0.079146	−0.034022	0.442160	0.064
H79B	0.035513	0.000618	0.459327	0.064
H79C	0.092058	0.033608	0.469933	0.064
C80	−0.04799(10)	0.17755(11)	0.36528(13)	0.0461(6)
H80A	−0.083448	0.186440	0.365806	0.069
H80B	−0.051683	0.183222	0.323511	0.069
H80C	−0.019551	0.205282	0.393507	0.069
C81	−0.02065(12)	0.10718(12)	0.45312(12)	0.0519(7)
H81A	−0.051952	0.124893	0.457878	0.078
H81B	0.013255	0.129510	0.479042	0.078
H81C	−0.016405	0.064190	0.465583	0.078
C82	0.27721(8)	0.24819(10)	0.56663(9)	0.0335(5)
C83	0.32433(9)	0.20704(13)	0.61050(10)	0.0481(6)
H83A	0.333748	0.177170	0.585932	0.058
H83B	0.357511	0.232469	0.633617	0.058
C84	0.31003(10)	0.17306(14)	0.65551(11)	0.0532(7)
H84A	0.303248	0.202327	0.682580	0.064
H84B	0.341140	0.146171	0.681570	0.064
C85	0.25867(12)	0.13531(12)	0.61999(11)	0.0521(7)
H85A	0.248817	0.113077	0.649348	0.063
H85B	0.266629	0.104681	0.594911	0.063
C86	0.20942(10)	0.17456(11)	0.57773(9)	0.0403(5)
C87	0.29190(10)	0.26886(14)	0.51538(11)	0.0549(7)
H87A	0.328594	0.287940	0.533534	0.082
H87B	0.264352	0.298445	0.488960	0.082
H87C	0.292180	0.233444	0.490799	0.082
C88	0.27367(11)	0.30556(12)	0.60092(13)	0.0533(7)
H88A	0.307613	0.329588	0.613296	0.080
H88B	0.269366	0.293649	0.637560	0.080
H88C	0.241759	0.330126	0.573820	0.080
C89	0.16355(14)	0.13091(15)	0.53620(12)	0.0787(12)
H89A	0.157577	0.099570	0.561520	0.118
H89B	0.174546	0.111389	0.506901	0.118
H89C	0.129211	0.153900	0.513666	0.118
C90	0.18668(11)	0.21071(16)	0.61543(13)	0.0627(8)
H90A	0.170047	0.182561	0.633979	0.094
H90B	0.158519	0.239503	0.588553	0.094
H90C	0.216869	0.233279	0.647974	0.094
N11	0.2084(8)	0.1077(9)	0.3077(6)	0.0258(17)
C91	0.2496(4)	0.0715(5)	0.3456(4)	0.0376(15)
C92	0.3036(2)	0.0753(3)	0.3378(2)	0.0501(12)
H92A	0.319553	0.116681	0.349433	0.060
H92B	0.330736	0.045705	0.365995	0.060

C93	0.29378(19)	0.0618(2)	0.2721(2)	0.0419(11)
H93A	0.278950	0.019941	0.260268	0.050
H93B	0.329048	0.064718	0.268763	0.050
C94	0.2521(2)	0.1087(3)	0.2293(3)	0.0348(11)
H94A	0.267735	0.150293	0.240560	0.042
H94B	0.245203	0.100797	0.186262	0.042
C95	0.1977(4)	0.1050(4)	0.2342(4)	0.0256(13)
C96	0.2629(5)	0.0979(5)	0.4108(5)	0.063(3)
H96A	0.294784	0.076186	0.442104	0.094
H96B	0.230766	0.092445	0.419155	0.094
H96C	0.271631	0.141428	0.411990	0.094
C97	0.2307(3)	0.0043(3)	0.3390(3)	0.0609(15)
H97A	0.257565	−0.019488	0.373519	0.091
H97B	0.228033	−0.012251	0.300247	0.091
H97C	0.194354	0.002047	0.339101	0.091
C98	0.16093(18)	0.1583(2)	0.19836(18)	0.0353(10)
H98A	0.155274	0.156765	0.155554	0.053
H98B	0.178847	0.196935	0.217052	0.053
H98C	0.125083	0.155392	0.199512	0.053
C99	0.1642(2)	0.0476(2)	0.2019(3)	0.0539(14)
H99A	0.152643	0.050489	0.157573	0.081
H99B	0.131350	0.044651	0.209445	0.081
H99C	0.187216	0.011200	0.218295	0.081
N11A	0.2087(8)	0.1106(9)	0.2992(7)	0.0246(16)
C91A	0.1959(5)	0.0934(5)	0.2440(5)	0.0337(16)
C92A	0.2018(2)	0.0249(2)	0.2357(3)	0.0462(12)
H92C	0.170366	0.003483	0.237987	0.055
H92D	0.198754	0.018029	0.193901	0.055
C93A	0.2535(3)	−0.0032(3)	0.2805(3)	0.0575(14)
H93C	0.284811	0.012128	0.273421	0.069
H93D	0.251395	−0.047978	0.274627	0.069
C94A	0.2640(3)	0.0120(3)	0.3478(3)	0.0558(15)
H94C	0.236587	−0.010114	0.357113	0.067
H94D	0.301295	−0.002853	0.376523	0.067
C95A	0.2602(4)	0.0804(5)	0.3585(4)	0.0351(16)
C96A	0.1358(3)	0.1090(4)	0.2040(2)	0.069(2)
H96D	0.123972	0.090708	0.163198	0.104
H96E	0.131562	0.153468	0.199892	0.104
H96F	0.113026	0.093004	0.222939	0.104
C97A	0.2322(4)	0.1274(4)	0.2202(4)	0.0614(19)
H97D	0.216525	0.122865	0.175442	0.092
H97E	0.269681	0.110281	0.239291	0.092
H97F	0.233674	0.170776	0.230714	0.092
C98A	0.2521(5)	0.0829(5)	0.4161(6)	0.0430(19)
H98D	0.281904	0.060239	0.449010	0.064
H98E	0.216353	0.064610	0.408146	0.064
H98F	0.252809	0.125543	0.428721	0.064
C99A	0.3135(2)	0.1112(4)	0.3676(3)	0.0657(17)
H99D	0.344635	0.092460	0.402499	0.099
H99E	0.311642	0.154746	0.375807	0.099
H99F	0.318819	0.106419	0.330307	0.099
C100	0.04312(8)	0.40672(9)	0.44309(9)	0.0289(4)

C101	−0.00032(10)	0.41389(13)	0.46661(11)	0.0489(6)
H10A	−0.006929	0.373665	0.480786	0.059
H10B	0.014111	0.441745	0.502484	0.059
C102	−0.05435(10)	0.43851(16)	0.41900(14)	0.0667(9)
H10C	−0.048952	0.480501	0.407513	0.080
H10D	−0.081571	0.440162	0.436140	0.080
C103	−0.07628(9)	0.39785(12)	0.36227(12)	0.0446(6)
H10E	−0.110975	0.415635	0.330596	0.054
H10F	−0.085153	0.357150	0.373325	0.054
C104	−0.03495(8)	0.39025(9)	0.33516(9)	0.0239(4)
C105	0.09140(12)	0.36994(13)	0.49063(11)	0.0603(8)
H10G	0.106259	0.391035	0.530376	0.090
H10H	0.120514	0.365952	0.476983	0.090
H10I	0.078354	0.329273	0.494961	0.090
C106	0.06694(11)	0.46889(12)	0.43887(12)	0.0500(6)
H10J	0.086543	0.486406	0.480176	0.075
H10K	0.036787	0.496224	0.413041	0.075
H10L	0.092768	0.463911	0.420690	0.075
C107	−0.05646(9)	0.33879(11)	0.28784(10)	0.0370(5)
H10M	−0.093896	0.348740	0.256731	0.055
H10N	−0.057352	0.300617	0.308484	0.055
H10O	−0.031938	0.334007	0.267956	0.055
C108	−0.03275(12)	0.44783(12)	0.30095(13)	0.0570(7)
H10P	−0.068921	0.454604	0.265935	0.085
H10Q	−0.004543	0.442992	0.286059	0.085
H10R	−0.023362	0.482902	0.328871	0.085

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

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Computational Data

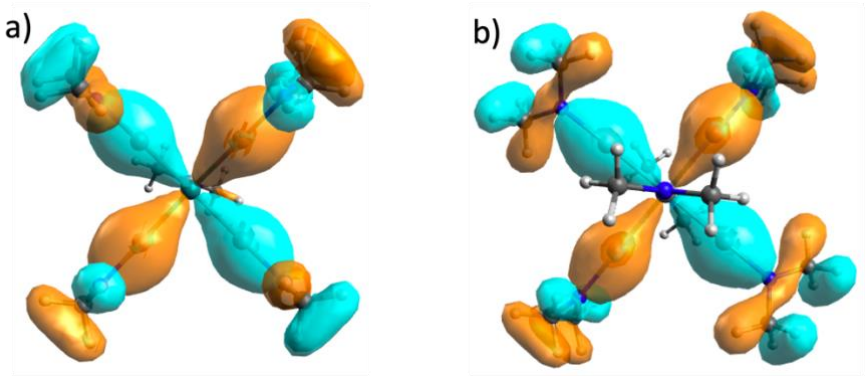

*Figure S 19: Excerpt of the occupied molecular orbitals of **1**$_{NMe2}$ (a) and **2**$_{NMe2}$ (b) showing σ bonding between the GaNMe$_2$ ligand and the transition metal (HOMO-14 and HOMO-15 respectivelly).*

[Ru(GaTMP)$_5$]:

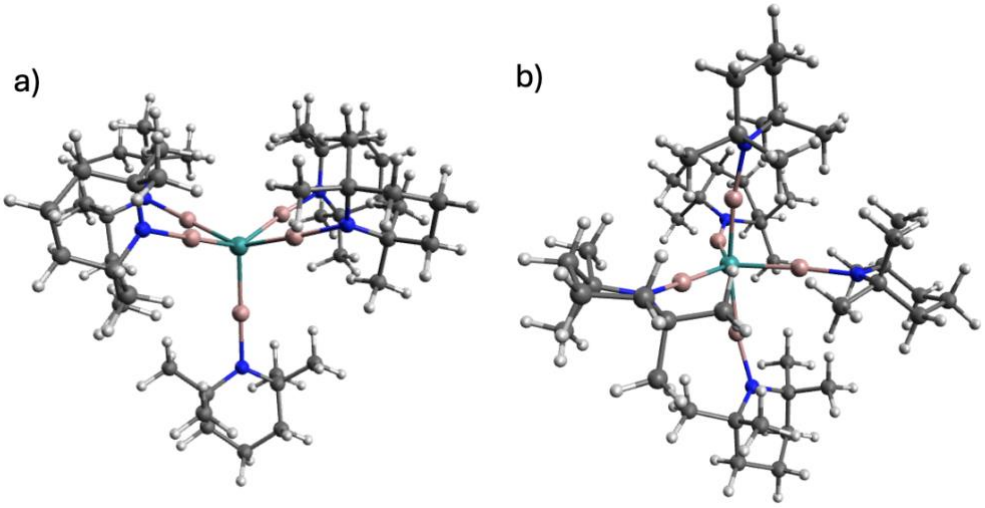

*Figure S 20: Optimized structure of a) **1**$_{SP}$ and b) **1**$_{TB}$.*

1$_{sp}$ xyz Coordinates:

Ru 10.9625336746 4.8135270062 14.0514953028
Ga 8.9579178587 4.2189633336 15.0126425439
Ga 9.8770435308 4.0789227423 12.1584183817
Ga 10.9386770320 7.1139679443 14.0382222113
N 7.2652546234 3.6652428843 15.5932863857
N 8.7726702528 3.4898159543 10.7665230187
N 10.9056697601 9.0005334848 14.1097230863
C 4.8301064920 4.1317936911 15.7352420791
C 5.8713449542 2.4080402624 17.2133004052
C 5.8600405684 3.4841309639 13.4978390880
C 6.3877457719 5.6884313486 14.5450005207
C 7.2395033664 1.1420891350 15.4789396073
C 8.3745323128 2.3658680583 17.3308440194
C 6.7269503017 4.0169690516 9.4723890665
C 7.3005757982 1.6429504311 10.0095849464
C 8.9966597734 4.7891277876 8.6109386698
C 8.0069629197 5.8108922599 10.6579394186
C 9.7579611560 1.6503612586 9.3411495329
C 9.0920813914 1.2570767085 11.7104041606
C 11.9601551507 9.7222856711 14.8645940913
C 10.7970217487 11.9725808586 14.3461227313
C 12.1092358699 11.1619727122 14.3254773931

C 10.1311397123 10.0411664024 11.9715884888
C 8.5193821530 8.9054217694 13.5098876655
Ga 12.9762646072 4.1807476768 13.1316079506
Ga 12.0165675792 4.1605201435 15.9903427778
N 14.6709382700 3.5625324678 12.6160072475
N 13.0698825507 3.6214094338 17.4389295818
C 17.1316882719 3.8901040023 12.5946050529
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C 15.9511821866 3.4066585609 14.7944389532
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C 9.7364573791 5.3062317068 9.1065748820
C 8.2288640347 5.9544547202 10.9780153884
C 11.0504638696 2.3497192913 9.9049345633
C 10.1121617717 1.7058383444 12.1185784118
C 11.4517973930 10.4822032574 15.0573435648
C 10.5573071926 12.1794782262 13.3238447906
C 11.7962790845 11.5408116625 13.9839752345
C 10.3224333920 9.3402959684 11.9843149240
C 8.3831369647 8.9355841143 13.5198222913
Ga 13.0269030191 5.3174201118 13.6761095294
Ga 11.9752558654 3.7392130791 16.1433800546
N 14.5661679606 5.1868654999 12.6183635416
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C 16.7538761436 4.1390831383 12.0922510939
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C 14.9843309525 1.7303315275 18.1235086535
C 13.9360125795 0.1174726624 16.5274945855
C 12.9248177362 2.3343157688 19.4953497329
C 14.0924595164 4.0700105005 18.1443352448
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C 12.0848257091 0.9725076643 15.0782880777
C 10.7507496573 11.1377428379 16.2750577105
C 12.7696116213 9.8530963573 15.5517095094
H 11.3841295131 11.9260693751 16.7348068968
H 10.5424103412 10.3651416475 17.0430587147
H 9.7824801525 11.5946790383 15.9965154446
H 13.3259180311 9.3930438738 14.7095011509
H 12.5764799579 9.0589038658 16.3080599075
H 13.4205457068 10.6094277021 16.0363142251
H 12.4439692758 12.3223044554 14.4345919233
H 12.4140373561 11.0327336122 13.2141715956
C 9.3317938168 11.2447041974 13.3478774781
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H 10.2945785083 13.1293671715 13.8341293128
C 9.6877233741 9.7419995389 13.3417536544
H 10.5665105901 8.2572144275 11.9953164414
H 11.2674658780 9.8854807218 11.7954993800
H 9.6351160632 9.5317774944 11.1329170473
H 8.5923035530 7.8437733342 13.5432653542
H 7.6780088085 9.1208774704 12.6832605946
H 7.8864735059 9.2052827692 14.4732017857
H 8.6629391314 11.4557018676 12.4871041596
H 8.7270448185 11.4378713793 14.2577168973
C 16.7205309251 4.8221619432 10.7239988158
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H 16.2077135842 4.1764048129 9.9782710931
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H 16.5756530117 6.8138170579 11.5483111758
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H 14.0546854739 8.1102176638 10.9200824266
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H 9.2158561476 6.0563718628 8.4756462481
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H 10.6087458308 5.7994343903 9.5804806745
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H 14.1279733995 -0.1985231607 18.6772188148
C 12.6119387336 0.9219522549 16.5242149113
H 12.8130801656 1.4708464245 14.4070641930
H 11.1274345538 1.5331948980 15.0135162182
H 11.8967891568 -0.0489646220 14.6918445707
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H 14.5725268959 0.5017776524 15.7001686811
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H 11.8817377786 -0.0009292530 18.4111485851
H 11.2640183396 -0.7737517900 16.9249761327
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H 15.5421975472 1.8600253215 19.0754141252
H 11.9610750723 2.8822821544 19.4809530939
H 13.5155820684 2.6900563897 20.3650517246
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H 7.0351018865 1.0137143975 15.0234422250
H 7.8898763486 0.3893188894 16.4638607983
H 9.3306348836 2.8364761868 17.4261192464
H 8.3060908427 1.8087909481 18.4640479796
H 8.0279708998 3.5892948213 18.4076921193
C 4.7678056944 2.3883848777 16.2230566480
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H 5.4427927731 5.8688094089 13.8911148259
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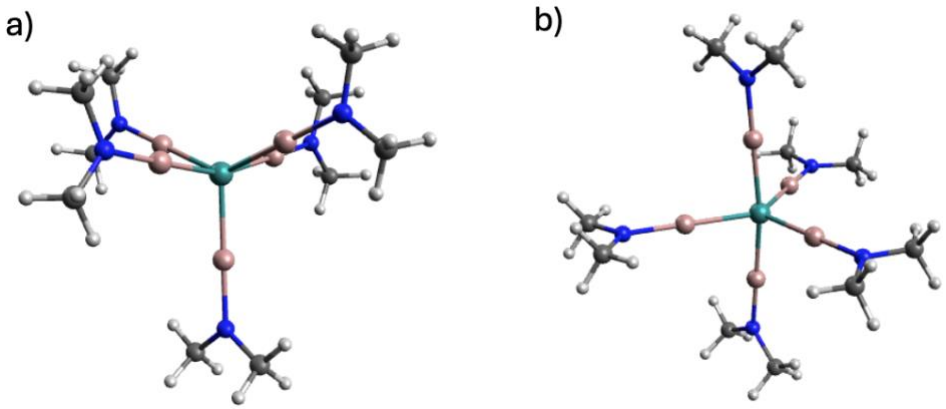

*Figure S 21: Optimized structure of a) **1**$_{NMe2\ SP}$ and b) **1**$_{NMe2\ TB}$.*

1$_{NMe2\ SP}$ **xyz Coordinates:**

Ru 10.9097358574 4.6220579939 14.1831367948
Ga 8.9098995421 3.8123330315 15.0168153896
Ga 10.0241848266 4.2400610219 12.0795669431
Ga 10.9083481843 6.9284299560 14.1880693506
N 7.3113955296 3.1623922225 15.6814441479
N 9.3120987181 3.8914865989 10.4135840070
N 10.9079192730 8.7889013009 14.1935084266
C 11.9931034639 9.5839961292 13.6503876482
Ga 12.9113134578 3.8185830582 13.3474117086
Ga 11.7941575450 4.2340036287 16.2860280201
N 14.5118322691 3.1730056029 12.6832350906
N 12.5040472232 3.8819937845 17.9521852793
C 9.8220277624 9.5802973578 14.7406120450
C 15.5931862892 4.0340911333 12.2448096291
C 14.7932701938 1.7564164804 12.5510796505
C 9.0377645151 2.5467663862 9.9448285943
C 8.9783485467 4.9329889811 9.4613869823
C 12.7808112046 2.5365883681 18.4175038119
C 12.8344258341 4.9215923528 18.9076396581
C 7.0305103406 1.7449560055 15.8053277799
C 6.2302336046 4.0205645186 16.1259793733
H 7.9023119141 4.9207716420 9.1999845041
H 9.5472229307 4.8239854287 8.5175937143
H 9.2083922870 5.9252107611 9.8758519142

H 7.9644534048 2.4037895406 9.7124382771
H 9.3134566020 1.8063238141 10.7098341566
H 9.6079961288 2.3073770468 9.0261731177
H 9.0308034741 8.9285745015 15.1403758710
H 9.3609281267 10.2349237707 13.9747400724
H 10.1640142708 10.2358070815 15.5658559343
H 11.6507686577 10.2432099378 12.8282360946
H 12.7850712185 8.9349749650 13.2477136055
H 12.4533643967 10.2353113315 14.4195749340
H 14.9945656890 1.4732342378 11.4994272331
H 13.9383400716 1.1580997878 12.8986927868
H 15.6771474026 1.4553569618 13.1467040550
H 15.8396767761 3.8732628622 11.1771052355
H 16.5196376864 3.8583317362 12.8255947393
H 15.3193367940 5.0920872683 12.3674610326
H 12.6026483052 5.9144491691 18.4956642235
H 13.9101782372 4.9110447955 19.1702847237
H 12.2646690002 4.8086650527 19.8504308146
H 12.5074971677 1.7976703013 17.6501789959
H 12.2101091770 2.2934776592 19.3348867449
H 13.8541762520 2.3952418618 18.6506504304
H 6.5035562732 5.0793347961 16.0089739656
H 5.9851444690 3.8536157911 17.1930612220
H 5.3031255699 3.8477345721 15.5453579742
H 7.8852183537 1.1490215412 15.4531049560
H 6.1460030236 1.4471748947 15.2089883757
H 6.8306301584 1.4553496971 16.8554988393

$1_{NMe2\ TB}$ xyz Coordinates:

Ru 10.7952760000 4.6513340000 13.9973720000
Ga 8.7759520000 3.7144370000 14.6245350000
Ga 9.9357500000 4.8118980000 11.8541710000
Ga 10.9358010000 6.9293790000 14.3357000000
N 7.1590560000 2.9699020000 15.1337100000
N 9.2390990000 4.9373470000 10.1512300000
N 11.0575650000 8.7659000000 14.6010700000
C 12.1934920000 9.5554420000 14.1624060000
Ga 12.7199180000 3.7437210000 13.0887050000
Ga 11.5964710000 4.0750480000 16.0908770000
N 14.2699700000 3.0303340000 12.3672030000
N 12.2210470000 3.5976490000 17.7591020000
C 10.0273060000 9.5434980000 15.2641730000
C 15.4492080000 3.8264590000 12.0848440000
C 14.4068160000 1.6298140000 12.0154750000
C 8.8782730000 3.7781230000 9.3579490000
C 9.0217610000 6.2068150000 9.4843620000
C 12.4546680000 2.2201630000 18.1479790000
C 12.5381200000 4.5691000000 18.7881960000
C 6.8869370000 1.5472830000 15.0588350000
C 6.0497220000 3.7575420000 15.6362370000
H 7.9576660000 6.3514290000 9.2143650000
H 9.6124470000 6.2870540000 8.5511900000
H 9.3152480000 7.0422960000 10.1364910000
H 7.8061270000 3.7885170000 9.0813020000
H 9.0679190000 2.8510500000 9.9181590000
H 9.4606340000 3.7262450000 8.4175020000
H 9.1948750000 8.8962840000 15.5777380000
H 9.6106500000 10.3267820000 14.6008070000
H 10.4142340000 10.0525900000 16.1687030000
H 11.8953100000 10.3401780000 13.4396490000
H 12.9414570000 8.9170650000 13.6691710000
H 12.6940480000 10.0634510000 15.0099670000
H 14.6130280000 1.4946980000 10.9356470000
H 13.4830960000 1.0802550000 12.2489040000
H 15.2341480000 1.1457770000 12.5703710000
H 15.7080310000 3.8121240000 11.0079950000
H 16.3346140000 3.4596170000 12.6398900000
H 15.2865020000 4.8750310000 12.3741260000
H 12.3392870000 5.5902650000 18.4317370000
H 13.6036050000 4.5202280000 19.0858560000
H 11.9332360000 4.4098880000 19.7018750000
H 12.1949870000 1.5363500000 17.3268470000
H 11.8456300000 1.9337130000 19.0273080000
H 13.5156520000 2.0411320000 18.4098470000
H 6.3157050000 4.8242340000 15.6677200000
H 5.7608050000 3.4538430000 16.6614030000
H 5.1503540000 3.6550950000 14.9980490000
H 7.7628880000 1.0056510000 14.6726700000
H 6.0337200000 1.3260460000 14.3881390000
H 6.6420710000 1.1227620000 16.0520630000

[Mo(GaTMP)$_6$]:

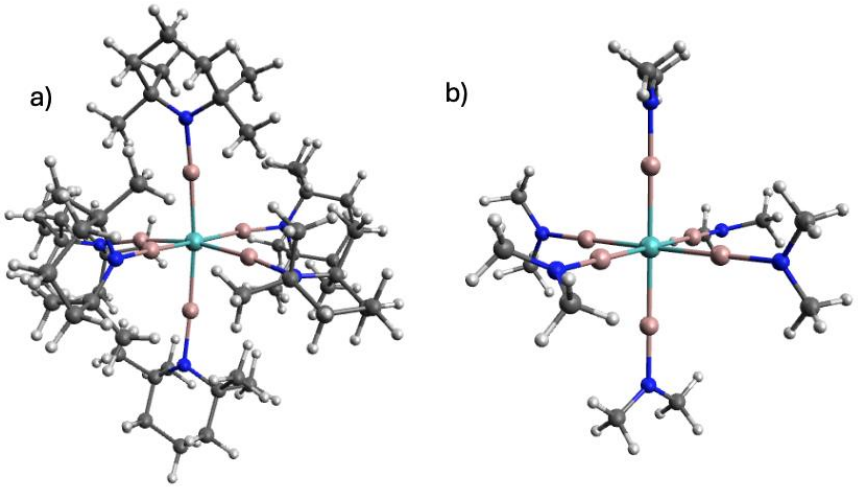

*Figure S 22: Optimized structure of a) **2** and b) **2**$_{NMe2}$.**2:***

2 xyz Coordinates:

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Ga 0.6236938715 6.7744001920 7.4118087707
Ga -1.4923485639 5.0588761973 5.6451842655
Ga -2.7117857684 3.4500624679 8.1140789332
Ga -0.3220855460 4.7320644589 10.2425172511
Ga 0.7355943818 3.5871958641 7.4304219203
Ga -2.4977513878 6.9781768936 8.3005511007
N 1.8560925146 8.0335399915 6.7436935581
N -1.7708883801 4.9305361204 3.7942314582
N -3.9920513729 2.0897476135 7.9009992579
N 0.5080917860 4.1878215122 11.8450945436
N -3.5528770584 8.5329823580 8.3569198368
C 1.4543788624 9.4575732199 6.8566246713
C 2.3571472315 10.3452228445 5.9665042697
H 2.0966632626 10.1423046603 4.9044477906
H 2.1164598097 11.4122814283 6.1596370400
C 3.8464111515 10.0635981143 6.1632499318
H 4.4531339361 10.7137923205 5.4985062959
H 4.1582527585 10.3100644062 7.2016075582
C 4.1167029706 8.5908522728 5.8573436452
H 5.1933779425 8.3434241291 5.9734773519
H 3.8549747957 8.3963778729 4.7940647947
C 3.2836748015 7.6298927027 6.7404694406
C 0.0096111850 9.5753585545 6.3311576949
H -0.3370827234 10.6281917720 6.3508188056
H -0.7035264212 8.9896706578 6.9516724422
H -0.0563279330 9.1970858702 5.2918688137
C 1.4723165074 9.9692868129 8.3210033854
H 1.0675143392 11.0002040339 8.3965481850
H 2.4917023915 9.9753179708 8.7520221180
H 0.8477103868 9.3076014793 8.9575748332
C 3.3704396756 6.2235483600 6.1151224361
H 4.4237846511 5.8849156361 6.0410017213
H 2.9249281763 6.2296601245 5.1006299419
H 2.8316610180 5.4577193906 6.7145362676
C 3.8854944809 7.5605997694 8.1682972678
H 4.9149497472 7.1452759555 8.1553850741
H 3.2576609760 6.9094131019 8.8112118534
H 3.9299112208 8.5560392616 8.6493898859
C -2.8596625703 4.0392921656 3.3271380984
C -2.6201122999 3.6360647305 1.8520753482
H -1.7475751588 2.9467855159 1.8234667931
H -3.4977553379 3.0622263995 1.4852696075
C -2.3242648856 4.8349557826 0.9504860262
H -2.1414509894 4.4973518587 -0.0913614617
H -3.2039715235 5.5133391596 0.9018154790
C -1.1016048048 5.5776129854 1.4889586828
H -0.8503312485 6.4545462985 0.8551713075
H -0.2265107912 4.8920206373 1.4528652356
C -1.2765781618 6.0485397887 2.9538409585
C -2.8254422211 2.7568576490 4.1828762726
H -3.5688479206 2.0202699946 3.8157991352
H -3.0790234715 2.9564150950 5.2467486106
H -1.8197500957 2.2912248199 4.1485230818
C -4.2675557554 4.6708009834 3.4913994067
H -5.0670134426 3.9341123322 3.2665948996
H -4.4197941523 5.5418119584 2.8269652802
H -4.4041856459 5.0215762188 4.5352026233
C 0.1110106971 6.4641480269 3.4815494273
H 0.5519880257 7.2587992686 2.8465411833
H 0.7986131548 5.5956093375 3.4920239123
H 0.0663799454 6.8708691885 4.5147513809
C -2.1983124339 7.2940152780 3.0148182393
H -1.7613851666 8.1471148798 2.4547856072
H -2.3368238928 7.6116239420 4.0692308775
H -3.2009021313 7.0939114971 2.5929436140
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C -4.3749626220 -0.1416194760 6.8923137796
H -4.0435516918 0.1698968075 5.8774796258
H -4.1254863508 -1.2193706595 6.9962352816
C -5.8828666164 0.0882126980 7.0085380471
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H -5.8785137332 1.9184721371 5.8584068931
C -5.4302063845 2.4411646595 7.9130584130
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C -3.6731240900 0.0329635493 9.3359555422
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H -3.1506645188 0.6680662153 10.0793515310
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H -6.6281919409 4.2197162373 7.4466071919
H -5.0988444120 4.1012771798 6.5104138454
H -5.0704121549 4.5917291815 8.2385197463
C -6.0780256401 2.2955823759 9.3139652065
H -7.1062313221 2.7135143616 9.3186385265
H -5.4739321772 2.8435448301 10.0649977955
H -6.1476157875 1.2423796953 9.6434361805
C 1.4182521295 5.1289326772 12.5369422783
C 2.6236973343 4.3556936930 13.1303059422
H 3.2596400700 4.0159920454 12.2836539833
H 3.2402545890 5.0514191969 13.7387938158
C 2.2014603481 3.1334935775 13.9475780941
H 1.6380576098 3.4482817766 14.8528759911
H 3.0969636170 2.5919760766 14.3187935731
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H 1.0196441945 1.3119138773 13.6518574291
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H 4.1873732974 2.5819743335 4.9466049774
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Ga -0.1789219872 4.9175233866 9.9499529581
Ga 0.8917827461 3.3760556775 7.0642883623
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H -2.4113375220 3.3090752287 3.37691854