Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Table of contents

1. Synthesis 3

1.1 Synthesis of GaCp 3

1.2 Synthesis of $Au_6(GaCl_2)_4(PEt_3)_6$ **1**: 3

1.3 Synthesis of $Au_7(GaCl_2)_3(P^nPr_3)_6$ **2:** 3

1.4 Synthesis of $Au_{13}(GaCl_2)_5(GaCl)(P^nPr_2{}^nBu)_9$ **3**: 4

1.5 Synthesis of $Au_{13}(GaCl_2)_5(P^nPr_3)_9$ **4**: 4

2. NMR-Data 5

3. Crystallographic data 7

4. Quantum chemical calculations 12

5. References 34

1. Synthesis

The reactions were partly done in an inert gas atmosphere performing standard Schlenk techniques, Toluene was pre-dried with sodium, pentane was dried with CaH_2. $^{n}Pr_3PAuCl$, Et_3PAuCl and $^{n}Pr_2{}^{n}Bu$ were synthesized as described earlier by our group.

1.1 Synthesis of GaCp

GaCp is generated in situ before each reduction and then used directly. 196 mg GaI (1 mmol) and 89 mg NaCp (1 mmol) are suspended in 20 ml toluene and stirred for one hour. The green solution turns gray after a few minutes. After one hour, stirring is stopped to allow the metathesis salt to settle. The GaCp dissolved in toluene is then filtered off and can be used for reduction.

1.2 Synthesis of $Au_6(GaCl_2)_4(PEt_3)_6$ 1:

351 mg of Et_3PAuCl (1 mmol) is dissolved in 20 ml of toluene. After one hour, a solution of 1 mmol GaCp dissolved in toluene is added. The dark red solution is stirred overnight before all volatiles are removed in vacuo. The crude product is washed with pentane, dissolved in toluene and stored at -30 °C. **1** crystallizes after one week.

Yield in respect to gold: 5 mg, 2 µmol, 1.3 %

^{31}P-NMR (C_6D_6): 45.2 (2P), 56.3 (4P)

1.3 Synthesis of $Au_7(GaCl_2)_3(P^{n}Pr_3)_6$ 2:

393 mg of $^{n}Pr_3PAuCl$ (1 mmol) is dissolved in 20 ml of toluene. After one hour, a solution of 1 mmol GaCp dissolved in toluene is added. The dark red solution is stirred overnight before all volatiles are removed in vacuo. The crude product is dissolved in pentane and stored at -18 °C. **2** crystallizes after a few days.

Yield in respect to gold: 55 mg, 19.9 µmol, 13.9 %

^{31}P-NMR (C_6D_6): 47.5 (2P), 60.8 (1P), 66.3 (1P), 76.7 (1P), 104.5 (1P)

1.4 Synthesis of $Au_{13}(GaCl_2)_5(GaCl)(P^nPr_2{}^nBu)_9$ **3**:

407 mg of $^nPr_2{}^n$BuPAuCl (1 mmol) is dissolved in 20 ml of toluene. After one hour, a solution of 1 mmol GaCp dissolved in toluene is added. The dark violet solution is stirred overnight before all volatiles are removed in vacuo. The crude product is dissolved in pentane and stored at -30 °C. **3** crystallizes after a few weeks.

Yield in respect to gold: 20 mg, 4.1 µmol, 5.2 %

^{31}P-NMR (C6D6): 34.8 pm (2P), 33.6, 35, 37.8, 39 (2P), 45.8 (2P), 60.9 (1P), 69 (2P)

1.5 Synthesis of $Au_{13}(GaCl_2)_5(P^nPr_3)_9$ **4**:

393 mg of $^nPr_3$PAuCl (1 mmol) is dissolved in 20 ml of toluene. After one hour, a solution of 1 mmol GaCp dissolved in toluene is added. The dark red solution is stirred overnight before all volatiles are removed in vacuo. The crude product is dissolved in pentane and stored at -18 °C. **4** crystallizes after one week.

Yield in respect to gold: 2 mg, 0.4 µmol, 0.55 %

2. NMR-Data

Device: Bruker AVIIIHD-300

The chemical shifts are given in ppm against the external standard 85% phosphoric acid. C_6D_6 was dried with 3 Å molecular sieves.

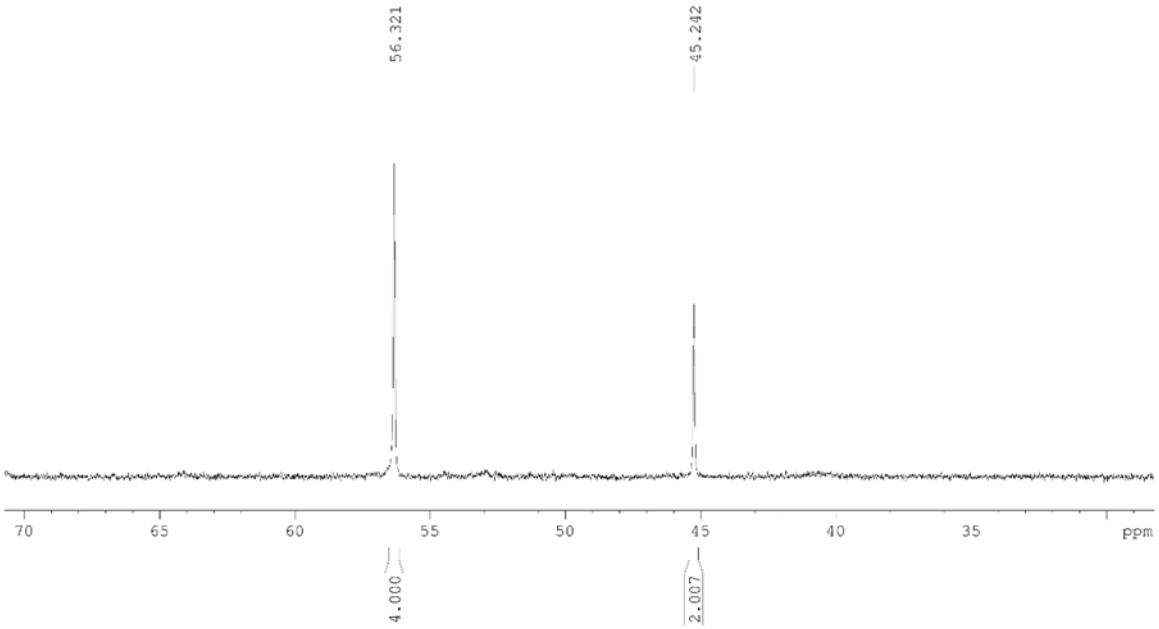


*Figure 1: ^{31}P-NMR spectra of $Au_6(GaCl_2)_4(PEt_3)_6$ **1***

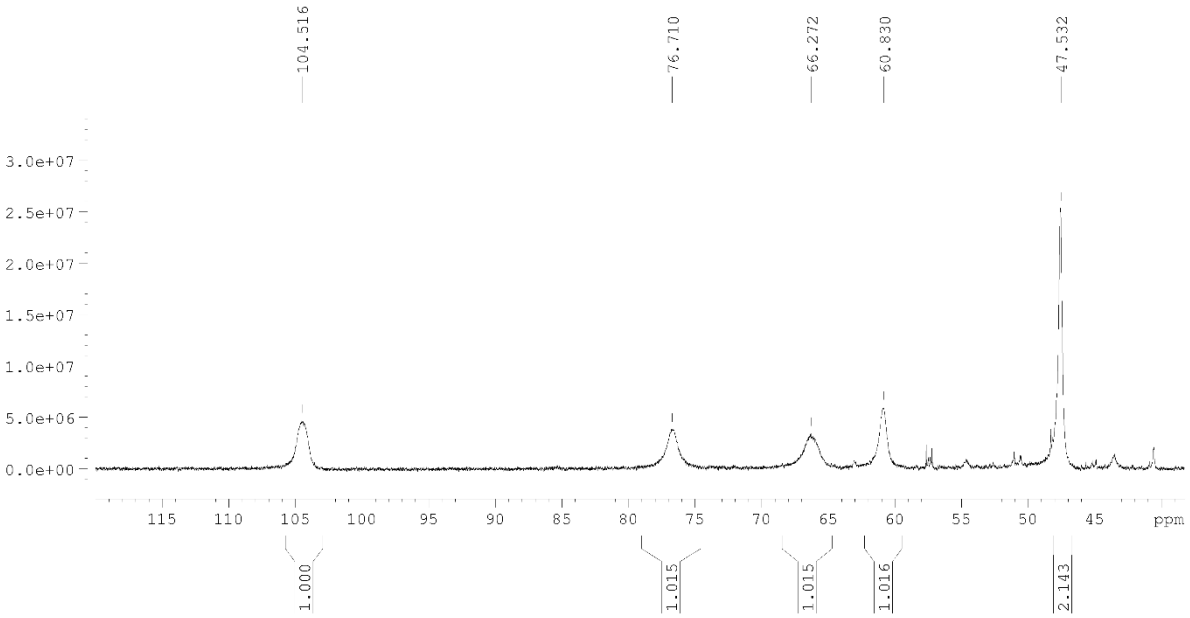


*Figure 2: ^{31}P-NMR spectra of $Au_7(GaCl_2)_3(P^nPr_3)_6$ **2***

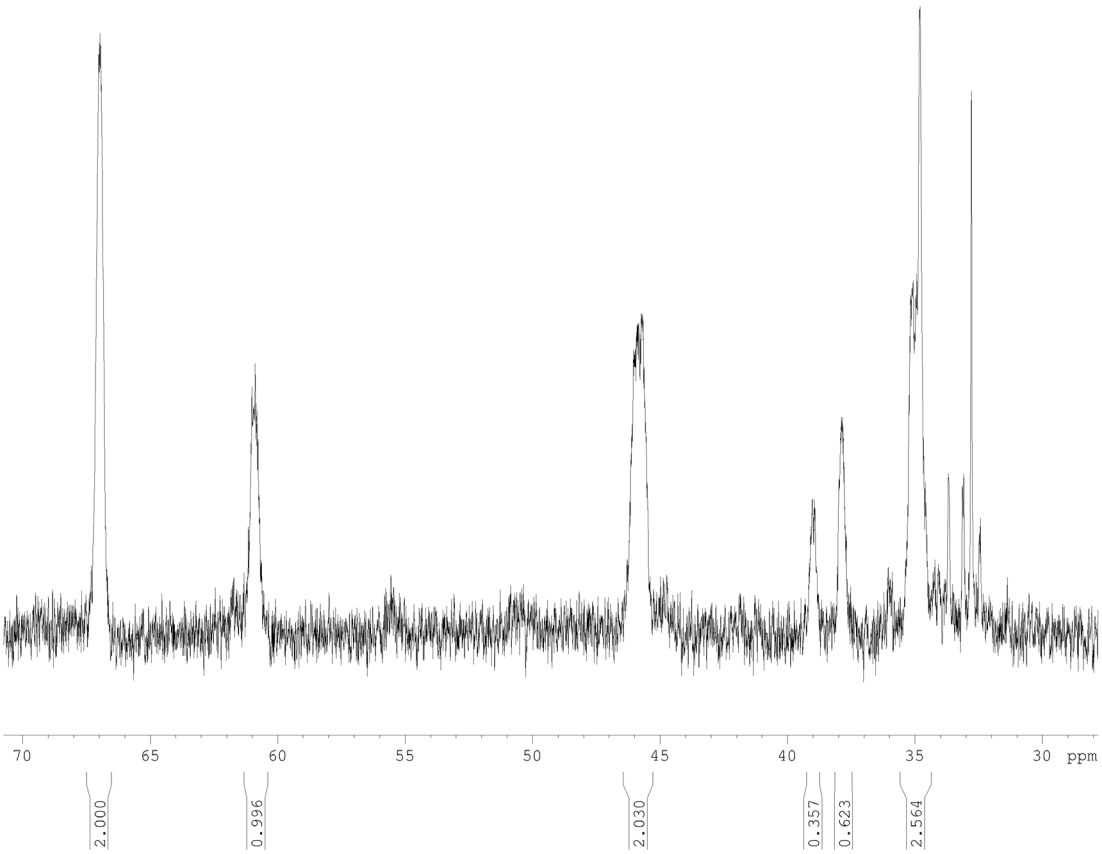


*Figure 3: ^{31}P-NMR spectra of $Au_{13}(GaCl_2)_5(GaCl)(P^nPr_2{}^nBu)_9$ **3***

3. Crystallographic data

Crystals of **1**,**2** and **4** were mounted on the diffractometer at 150 K (200 K for **4**). 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 data of **3** were collected on a Rigaku XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction at 100 K equipped with a PhotonJet-S microfocus sealed tube for monochromated CuKα radiation (λ = 1.54184 Å) and equipped with an Oxford Cryosystems cryostat. A numerical absorption correction based on gaussian integration over a multifaceted crystal model was applied using the program CrysAlisPro. The structures were solved by direct methods and refined against F2 for all observed reflections. Programs used: SHELXS and SHELXL[1] within the Olex2 program package.[2] The supplementary crystallographic data (for CCDC numbers 2226515 (**1**), 2226516 (**2**), 2226517 (**3**) and 2226518 (**4**)) 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.

$Au_6(GaCl_2)_4(PEt_3)_6$ **1**

CCDC Number	2226515
Empirical formula:	$C_{50}H_{106}Au_6Cl_8Ga_4P_6$
Formula weight:	2637.44
Temperature/K:	150.01
Crystal system:	monoclinic
Space group:	C2/m
a/A	16.034(2)
b/A	23.766(3)
c/A	11.388(3)
α/°	90
β/°	108.155(2)
γ/°	90
Volume/A_3	4123.8(13)
Z	2
$\rho_{calc}g/cm_3$	2.124
μ/mm^{-1}	12.315
F(000)	2460.0
Crystal size/mm_3	0.21 × 0.08 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.24 to 51.998
Index ranges	-19 ≤ h ≤ 19, -29 ≤ k ≤ 29, -14 ≤ l ≤ 14
Reflections collected	24715
Independent reflections	4168 [R_{int} = 0.0773, R_{sigma} = 0.0553]
Data/restraints/parameters	4168/164/244
Goodness-of-fit on F_2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0391, wR_2 = 0.0882
Final R indexes [all data]	R_1 = 0.0637, wR_2 = 0.1025
Largest diff. peak/hole / e A^{-3}	1.10/-1.65

$Au_7(GaCl_2)_3(P^nPr_3)_6$ **2**

CCDC Number	2226516
Empirical formula:	$C_{54}H_{126}Au_7Cl_6Ga_3P_6$
Formula weight:	2761.99
Temperature/K :	150.0
Crystal system :	triclinic
Space group:	P-1
a/A	13.0624(10)
b/A	15.2056(11)
c/A	21.0776(16)
α/°	92.022(2)
β/°	98.393(2)
γ/°	91.024(2)
Volume/A_3	4137.9(5)
Z	2
ρcalcg/cm_3	2.217
μ/mm-1	13.656
F(000)	2576.0
Crystal size/mm^3	0.276 × 0.162 × 0.038
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.09 to 55.998
Index ranges	-17 ≤ h ≤ 17, -20 ≤ k ≤ 20, -27 ≤ l ≤ 27
Reflections collected	237222
Independent reflections	19942 [R_{int} = 0.0722, R_{sigma} = 0.0348]
Data/restraints/parameters	19942/42/767
Goodness-of-fit on F_2	1.076
Final R indexes [I>=2σ (I)]	R_1 = 0.0313, wR_2 = 0.0681
Final R indexes [all data]	R_1 = 0.0472, wR_2 = 0.0786
Largest diff. peak/hole / e A_{-3}	1.55/-1.08

$Au_{13}(GaCl_2)_5(GaCl)(P^nPr_2{}^nBu)_9$ **3**

CCDC Number	2226517
Empirical formula:	$C_{90}H_{207}Au_{13}Cl_{11}Ga_6P_9$
Formula weight:	4937.11
Temperature/K :	100.00(13)
Crystal system:	monoclinic
Space group:	$P2_1/n$
a/Å	17.9369(2)
b/Å	29.9431(3)
c/Å	26.0812(3)
α/°	90
β/°	99.9143(12)
γ/°	90
Volume/A_3	13798.7(3)
Z	4
ρcalcg/cm_3	2.377
μ/mm^{-1}	29.702
F(000)	9128.0
Crystal size/mm^3	0.146 × 0.08 × 0.023
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.532 to 129.998
Index ranges	-21 ≤ h ≤ 21, -20 ≤ k ≤ 35, -30 ≤ l ≤ 30
Reflections collected	115496
Independent reflections	23236 [R_{int} = 0.0711, R_{sigma} = 0.0474]
Data/restraints/parameters	23236/549/1147
Goodness-of-fit on F_2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0526, wR_2 = 0.1270
Final R indexes [all data]	R_1 = 0.0745, wR_2 = 0.1436
Largest diff. peak/hole / e A^{-3}	1.74/-1.70

$Au_{13}(GaCl_2)_5(P^nPr_3)_9$ **4**

CCDC Number	2226518
Empirical formula:	$C_{81}H_{189}Au_{13}Cl_{10}Ga_5P_9$
Formula weight.	4705.71
Temperature/K:	200
Crystal system:	monoclinic
Space group:	P21/n
a/Å	16.1624(5)
b/Å	27.8938(8)
c/Å	28.6686(10)
α/°	90
β/°	94.5860(10)
γ/°	90
Volume/A^3	12883.3(7)
Z	4
$\rho_{calc}g/cm^3$	2.426
μ/mm^{-1}	16.114
F(000)	8648.0
Crystal size/mm^3	0.093 × 0.081 × 0.044
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.046 to 49.5
Index ranges	-19 ≤ h ≤ 19, -32 ≤ k ≤ 32, -33 ≤ l ≤ 33
Reflections collected	224751
Independent reflections	22016 [R_{int} = 0.1032, R_{sigma} = 0.0519]
Data/restraints/parameters	22016/193/1220
Goodness-of-fit on F_2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0338, wR_2 = 0.0637
Final R indexes [all data]	R_1 = 0.0619, wR_2 = 0.0771
Largest diff. peak/hole / e A-3	1.27/-0.98

4. Quantum chemical calculations

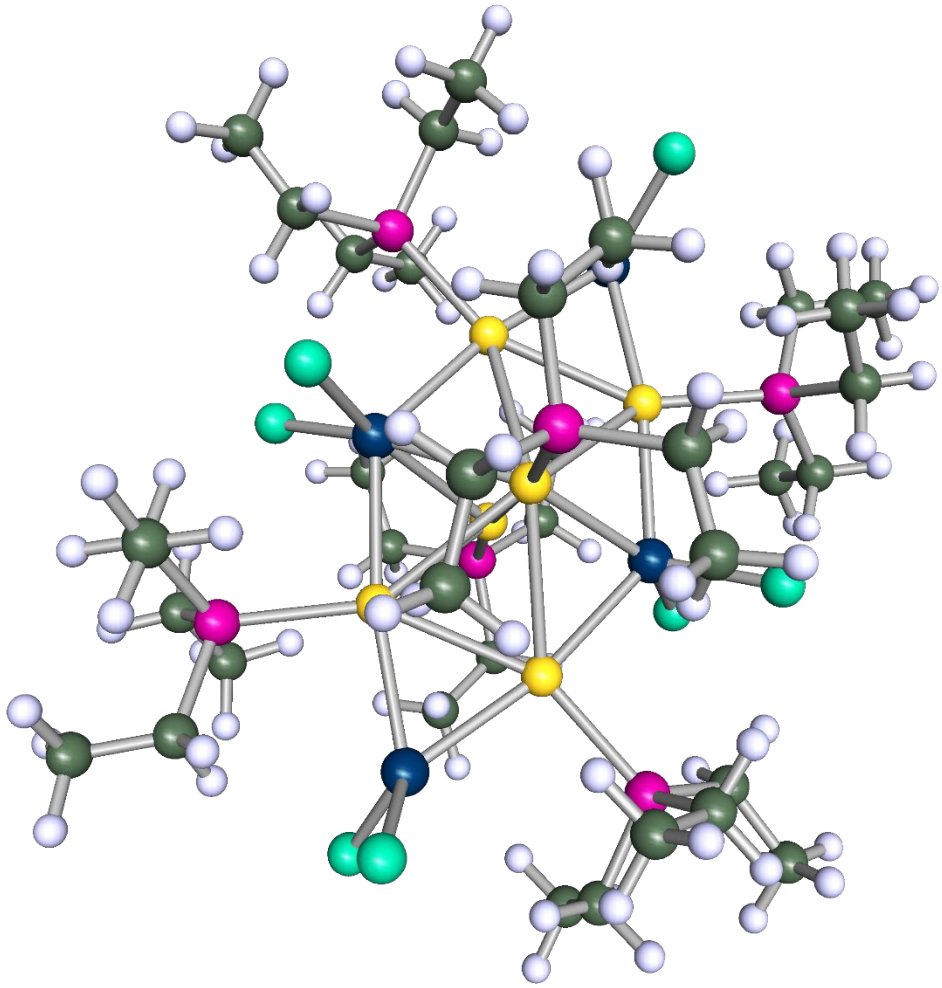


Figure S1: Geometry optimized structure of $\mathbf{1}^3$

Point group: C_1

Energy: -15669.38746354991 Hartree

HOMO-LUMO-gap: 1.917 eV

Atomic coordinates:

Au 3.660147 14.400983 6.912071	Au 4.335799 11.915599 8.647803	Ga 5.719402 15.722459 5.969620
Au 6.244827 13.271392 6.715668	Au 3.641924 11.284513 6.132132	Ga 1.859420 12.674811 7.945715

P 2.026776 16.211033 6.590987

Ga 6.318041 10.661874 7.375175

P 8.648117 13.478875 6.239780

Au 4.517368 8.884398 8.289950

Au 1.925077 10.016149 8.441495

P 4.705379 12.654971 10.901700

P 3.385828 10.534904 3.910571

C 4.474764 14.487977 11.132680

Cl 5.869100 16.369238 3.808186

Cl 6.733511 17.389765 7.133326

Cl 1.056221 13.657823 9.885666

Cl 0.034267 12.956606 6.533060

C 0.598666 16.351449 7.776948

C 2.806566 17.905197 6.611251

C 1.199136 16.101311 4.928874

Cl 6.902699 9.674119 5.351517

Cl 8.258569 10.335986 8.621220

C 9.091541 15.051392 5.340498

C 9.650136 13.520728 7.802831

C 9.452869 12.128087 5.248608

Ga 2.414310 7.492614 8.958072

P 6.154409 7.073619 8.578843

P -0.491381 9.768202 8.798529

C 1.707755 10.759633 3.134456

C 4.619435 11.254773 2.714247

C 6.418406 12.364292 11.581266

C 3.522541 11.986402 12.179269

C 3.699121 8.711329 3.722322

C 2.731499 7.800901 4.484113

C 1.241235 12.206666 2.941958

C 5.488161 15.372654 10.402225

C 6.737278 10.922497 11.989387

C -0.322779 17.568345 7.613959

C 3.310473 18.344527 7.991432

C 2.142951 16.066304 3.722845

C 10.577366 15.272056 5.025250

C 9.187295 14.568889 8.820861

C 9.014360 12.079172 3.780655

Cl 2.246422 6.684987 11.063375

Cl 1.408990 5.923012 7.656678

C 7.596413 6.974730 7.406206

C 5.399469 5.368625 8.530367

C 6.957731 7.169821 10.253805

C -0.950050 8.147165 9.599684

C -1.431861 9.797645 7.197380

C -1.348309 11.057484 9.826220

C 4.915666 12.749916 2.871702

C 3.171436 10.499499 12.070338

C 8.526446 5.762123 7.551348

C 4.926650 4.930273 7.138710

C 5.997517 7.106291 11.446710

C -2.440026 7.910863 9.882591

C -0.862419 8.871186 6.117358

C -0.945497 11.051243 11.305214

H 2.845930 15.208517 3.780861

H 2.760655 16.985022 3.636309

H 10.714478 13.678435 7.513800

H 9.565763 12.495671 8.227888

H 3.691005 8.488951 2.629297

H 4.741516 8.569084 4.085790

H 3.946503 12.235879 13.180238

H 2.603382 12.599391 12.044087

H 5.288784 12.977789 3.894752

H 4.023451 13.386292 2.697186

H -1.228210 10.105060 11.816621

H -1.448712 11.887706 11.837664

H 5.232249 16.446137 10.537104

H 6.522647 15.231675 10.783476

H -0.801753 17.608014 6.611425

H 0.205721 18.532402 7.779313

H 4.052039 9.837478 12.202520

H 2.732975 10.267055 11.073447

H 10.554817 12.269416 5.335644

H 9.197354 11.175234 5.760721

H -2.444622 10.898264 9.705206

H -1.099301 12.037800 9.365010

H 10.995796 14.479511 4.367218

H 11.201284 15.319037 5.944373

H 8.992927 5.701867 8.558812

H 8.009224 4.797678 7.355625

H 6.547757 13.057113 12.445389

H 7.120144 12.692497 10.783464

H 0.584064 15.175429 4.984380

H 0.496837 16.962867 4.854630

H 2.721210 8.035006 5.571127

H 1.688625 7.877605 4.107578

H 9.221531 15.604689 8.420081

H 8.139574 14.375527 9.137033

H 1.027151 16.303285 8.800460

H 0.032539 15.402905 7.654895

H 7.177801 7.045369 6.379835

H 8.152730 7.925057 7.560089

H -0.548403 7.351583 8.932844

H -0.350739 8.073671 10.533820

H 0.175622 9.171724 5.856655

H -0.825700 7.806820 6.434146

H -2.493919 9.552118 7.427172

H -1.393864 10.856679 6.858786

H 7.812359 10.833820 12.259346

H 6.549343 10.218702 11.151517

H 2.051823 18.622492 6.213757

H 3.646086 17.886643 5.880943

H 0.996955 10.219805 3.798382

H 1.730007 10.210717 2.163726

H -2.862521 8.656398 10.590825

H -3.054873 7.931168 8.956320

H 3.807624 19.335906 7.916845

H 2.482399 18.432297 8.728389

H 6.158192 4.659795 8.935817

H 4.548941 5.371946 9.248435

H 8.479193 15.067873 4.412044

H 8.695785 15.884709 5.963232

H 4.163456 5.626854 6.731033

H 5.767865 4.863827 6.414637

H 4.263756 11.010455 1.685938

H 5.547979 10.667870 2.893063

H 6.562821 7.236995 12.396034

H 5.459467 6.136547 11.505719

H 4.496320 14.678434 12.231620

H 3.438461 14.690954 10.781380

H 7.706115 6.346517 10.309258

H 7.525117 8.127354 10.238761

H 1.217495 12.749066 3.911306

H 1.890438 12.763702 2.233218

H 7.913472 11.959440 3.697912

H 9.312409 12.992101 3.220003

H 0.149016 11.199113 11.420210

H -2.574413 6.906333 10.341719

H -1.481446 8.933813 5.194707

H 4.448128 3.928613 7.198163

H 9.356333 5.844455 6.814359

H 9.480349 11.204727 3.275843

H 10.703379 16.242009 4.494841

H 5.697612 13.069355 2.149109

H 1.553898 15.966021 2.784137

H 0.208747 12.218330 2.527785

H 3.039632 6.737969 4.379327

H -1.143244 17.511578 8.363751

H 4.066096 17.634780 8.390379

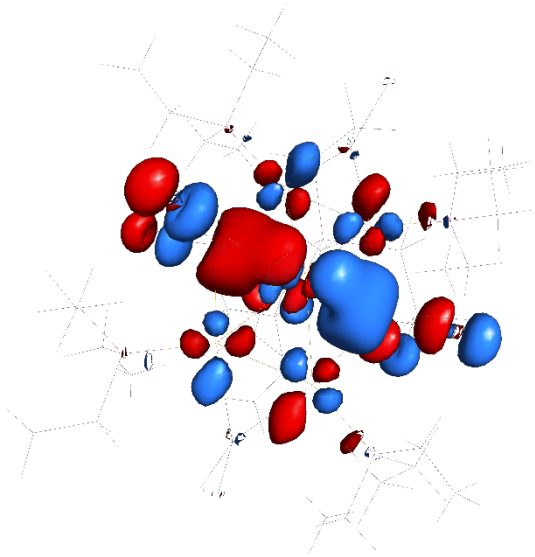
H 5.494499 15.169212 9.308210

H 9.831449 14.531943 9.727377

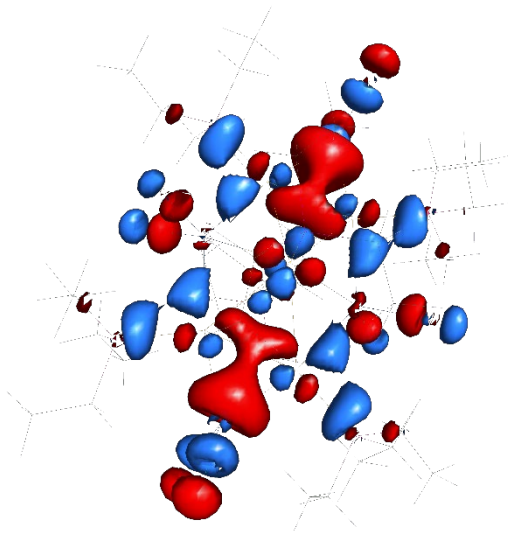
H 6.140916 10.598742 12.869382

H 5.223136 7.901052 11.395144

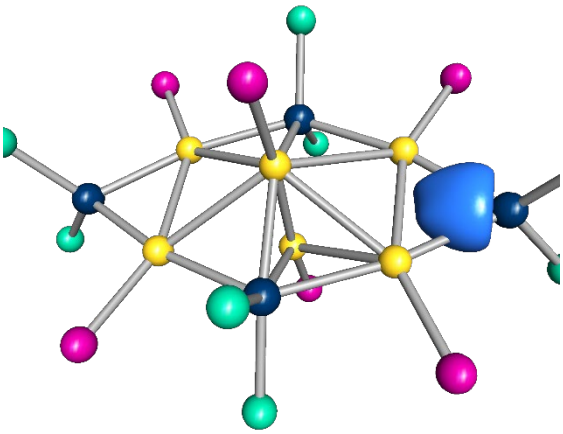
H 2.422952 10.220077 12.843623



HOMO-1



HOMO-2



LMO382

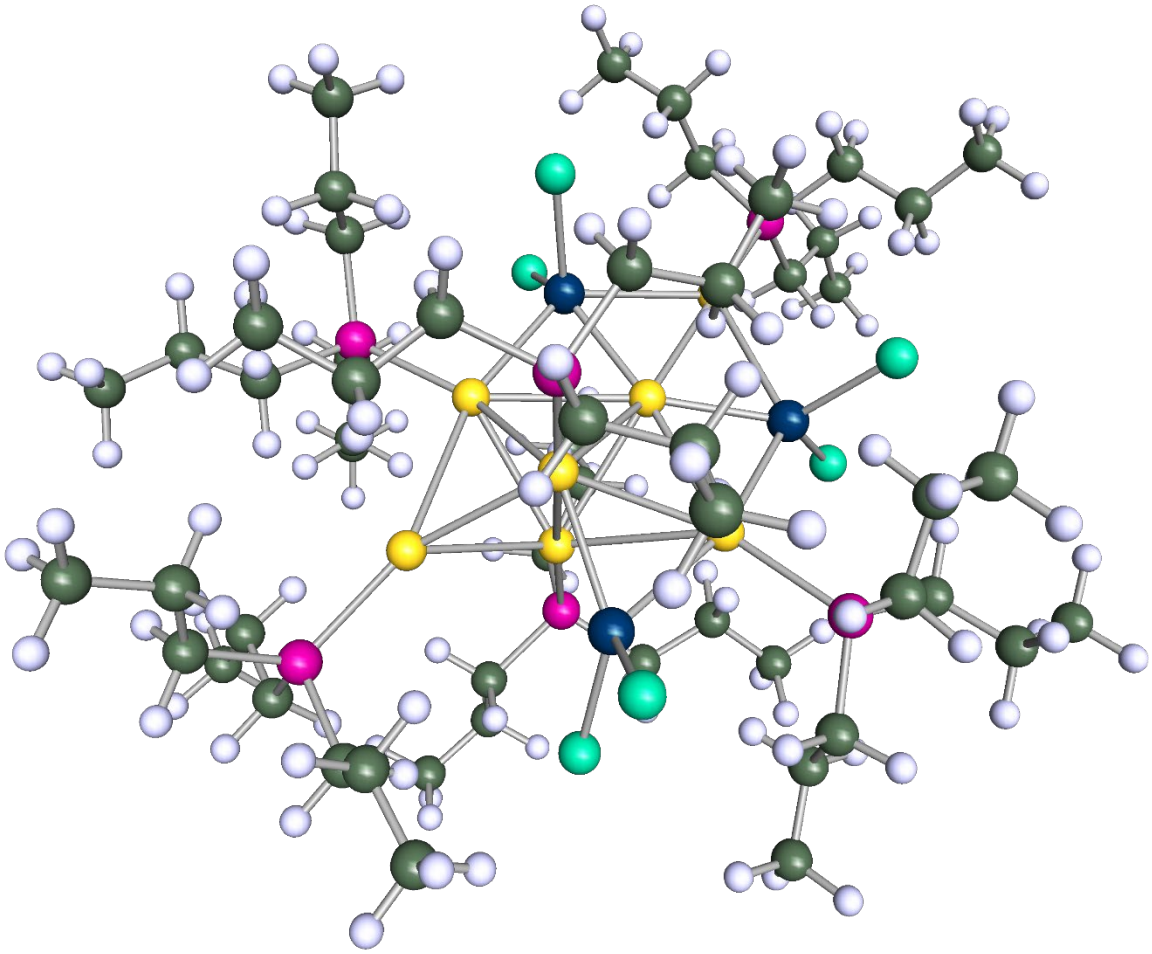


Figure S2: Geometry optimized structure of 2^3

Point group: C_1

Energy: -26647.62315677302 Hartree

HOMO-LUMO-gap: 1.569 eV

Atomic coordinates:

Au 0.645049 10.211717 16.996844	Ga 1.226665 7.708616 17.563041	Au 4.301291 12.906188 13.682747
Au -1.753719 9.024781 15.941220	P 0.431969 11.812520 18.747515	Ga 5.043102 10.613369 15.252020
Au -0.398380 11.385853 14.647468	P -3.576746 7.445848 16.297020	H 3.146830 12.387093 17.416725
Au 2.617428 11.171687 14.968315	H -2.472890 11.060392 18.166025	P 5.031704 7.636517 17.879576
Au 3.410362 8.970134 16.603412	Ga 1.473590 13.090574 13.863977	H 5.010696 10.366733 19.292337
Au 0.902283 8.728143 14.742373	P -2.248975 12.470648 13.524143	H 4.054515 7.359298 14.144506

P 1.200051 7.232823 12.951146

Cl 1.173873 7.229789 19.816950

Cl 0.748927 5.595501 16.706989

C 1.612564 13.256447 18.681308

C 0.451274 11.193037 20.507046

C -1.190437 12.732779 18.679441

C -5.237756 7.935608 17.018092

C -4.102685 6.559936 14.736786

C -3.022646 6.008372 17.347321

C -2.450514 11.888939 18.913008

Cl 1.259121 15.080076 14.941415

Cl 1.209492 13.592661 11.650524

C -2.304203 14.331147 13.560648

C -3.911002 11.919263 14.172273

C -2.283581 12.122176 11.696997

P 5.756153 14.287937 12.383590

Cl 6.536356 11.620204 16.631661

Cl 6.318029 9.652438 13.649180

C 3.085663 12.940806 18.383177

C 4.613283 5.841187 18.150252

C 6.747297 7.665533 17.153899

C 5.214677 8.228230 19.635940

C 5.717617 9.671052 19.796764

C 4.037823 6.814721 13.172403

C 1.284056 8.058342 11.276261

C 2.683183 6.109108 13.012770

C -0.223157 6.034943 12.808999

H 1.215725 13.915294 17.874235

H 1.507418 13.815136 19.642392

H 0.016910 11.996245 21.149335

H -0.254722 10.332404 20.526622

C 1.812562 10.742820 21.058732

H 2.271028 10.017268 20.350483

H -1.130956 13.562632 19.423633

H -1.224327 13.200927 17.669053

H -2.404465 11.406148 19.915796

H -5.879330 8.241216 16.159788

H -5.700361 7.015614 17.448863

C -5.202642 9.067571 18.056861

H -3.231416 5.940548 14.424150

H -4.924338 5.852256 15.000808

C -4.530497 7.488201 13.588495

H -3.802983 5.212665 17.278401

H -2.098463 5.622038 16.858494

C -2.711067 6.338244 18.817211

C -3.734038 12.726355 18.815185

H -1.348218 14.661472 13.094346

H -3.128213 14.672149 12.890581

C -2.448787 14.945180 14.961907

H -3.890221 10.805627 14.138444

H -3.909323 12.173191 15.257109

C -5.169834 12.473286 13.483969

H -3.124924 12.693986 11.239902

H -1.335990 12.562879 11.308851

C -2.370800 10.632841 11.328803

C 4.822024 15.580310 11.425516

C 7.072706 15.220506 13.308592

C 6.636797 13.268652 11.097198

H 3.501278 12.254166 19.153741

C 3.945054 14.208864 18.296536

H 5.358672 5.418463 18.864254

H 3.629900 5.843119 18.674668

C 4.538798 4.988100 16.875767

H 6.641547 7.334981 16.095793

H 7.023207 8.743278 17.091539

C 7.842386 6.861330 17.874749

H 4.204348 8.106316 20.090795

H 5.891554 7.514923 20.162767

H 6.686356 9.802495 19.265971

C 5.888642 10.071251 21.268864

H 4.162751 7.599321 12.395192

C 5.223800 5.845575 13.087446

H 1.741844 7.338262 10.558189

H 0.227233 8.204704 10.951726

C 2.023829 9.408786 11.243227

H 2.499142 5.419256 13.868581

H 2.674389 5.494322 12.082433

H -0.278244 5.545151 13.808593

H -1.136071 6.668281 12.724049

C -0.177103 4.988871 11.680980

H 2.499595 11.616663 21.122664

C 1.680895 10.085508 22.439929

H -4.755717 9.971959 17.586119

H -4.520407 8.795322 18.892904

C -6.594171 9.399127 18.614467

H -5.331634 8.180901 13.937936

H -3.667283 8.135882 13.311007

C -5.034025 6.724480 12.355301

H -3.629774 6.709232 19.328258

H -1.965442 7.164436 18.860300

C -2.155629 5.124078 19.574994

H -4.638198 12.106106 19.002693

H -3.736905 13.555468 19.558727

H -3.840156 13.185409 17.806081

H -1.633846 14.554175 15.611714

H -3.413098 14.623799 15.420850

C -2.376348 16.478386 14.936432

H -5.169737 13.586018 13.533781

H -5.154150 12.213141 12.400953

C -6.467916 11.941319 14.110918

H -1.526161 10.090644 11.813332

H -3.302418 10.189388 11.750705

C -2.342964 10.401727 9.810863

H 5.513864 16.080450 10.708135

H 4.071333 15.011707 10.830019

C 4.101763 16.620163 12.303946

H 7.598350 15.896641 12.593358

H 6.529422 15.873728 14.028776

C 8.070383 14.324631 14.063848

H 7.082001 12.405976 11.643352

H 5.824967 12.833347 10.469541

C 7.688381 13.968805 10.219069

H 4.995211 13.944886 18.046570

H 3.563880 14.887544 17.501205

H 3.945752 14.772030 19.258430

H 5.533961 4.972985 16.374306

H 3.827334 5.462417 16.163154

C 4.079842 3.551002 17.160499

H 7.932223 7.205163 18.930654

H 7.558036 5.785100 17.921795

C 9.208361 6.994678 17.183054

H 6.243493 11.121707 21.356735

H 4.929078 9.989056 21.827029

H 6.631744 9.420867 21.784058

H 6.179524 6.396904 13.222632

H 5.164846 5.055694 13.869288

H 5.262805 5.335369 12.097611

H 3.059047 9.292256 11.633471

H 1.524788 10.116404 11.943324

C 2.072772 10.019661 9.836712

H -0.099634 5.497709 10.692597

H 0.739140 4.365296 11.782179

C -1.405627 4.066561 11.683144

H 2.678746 9.810529 22.848229

H 1.192512 10.766526 23.173930

H 1.078615 9.153055 22.373663

H -6.545132 10.231891 19.350494

H -7.293902 9.706424 17.804367

H -7.045349 8.521973 19.130976

H -5.322435 7.422745 11.538798

H -4.250787 6.042171 11.954718

H -5.925194 6.102900 12.597855

H -1.924340 5.388877 20.629545

H -2.882780 4.279743 19.581915

H -1.211680 4.771000 19.106450

H -2.507073 16.901240 15.957077

H -1.387031 16.813698 14.555942

H -3.166850 16.915545 14.284684

H -7.363431 12.355321 13.596761

H -6.523544 10.831230 14.043525

H -6.539925 12.215753 15.187252

H -2.400690 9.317877 9.565993

H -3.198512 10.905953 9.306994

H -1.407118 10.801985 9.361300

H 4.853692 17.251764 12.830766

H 3.513349 16.100440 13.094228

C 3.158203 17.514565 11.487502

H 7.516345 13.628992 14.734073

H 8.621322 13.680767 13.340357

C 9.077897 15.137561 14.889276

H 8.500503 14.379978 10.860915

H 7.232347 14.841426 9.697827

C 8.301125 13.019801 9.177370

H 4.072138 2.943275 16.228456

H 4.752005 3.043374 17.889287

H 3.048296 3.545766 17.575324

H 9.988658 6.409479 17.718559

H 9.166946 6.625991 16.133811

H 9.540509 8.056033 17.149085

H 2.547924 11.023610 9.863972

H 2.648825 9.379654 9.129797

H 1.050044 10.150627 9.415678

H -1.348179 3.317114 10.862980

H -1.490040 3.510526 12.643641

H -2.347919 4.643961 11.545808

H 2.673076 18.274887 12.138113

H 3.699060 18.054696 10.677011

H 2.350993 16.907795 11.020906

H 9.782772 14.465071 15.425361

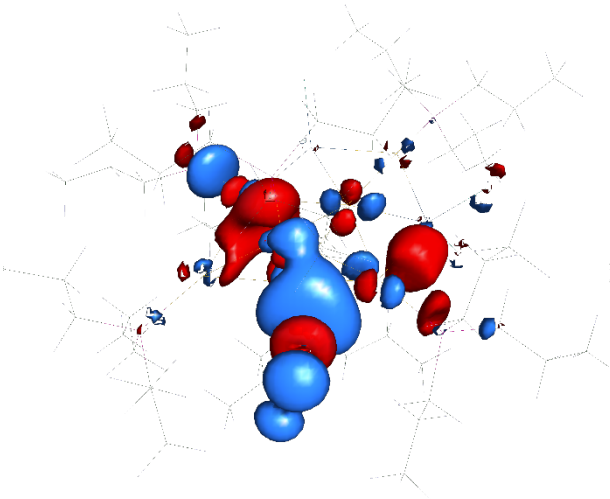
H 9.680831 15.820805 14.248499

H 8.562287 15.760148 15.654679

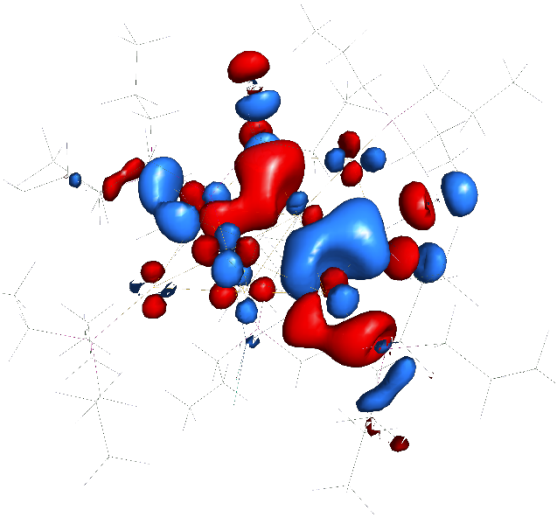
H 9.064897 13.541220 8.558995

H 8.795560 12.150406 9.665475

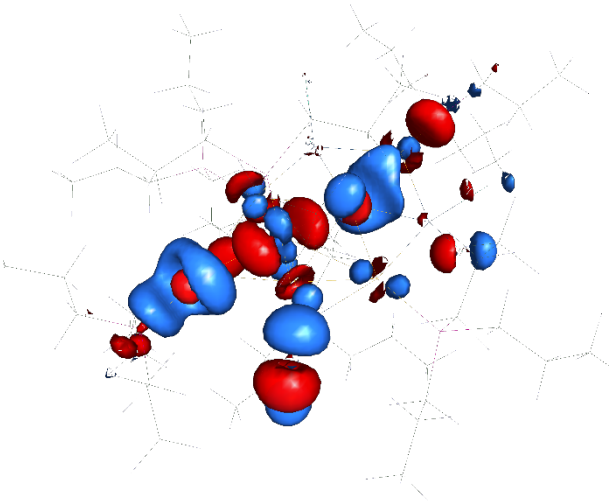
H 7.523931 12.619164 8.488522



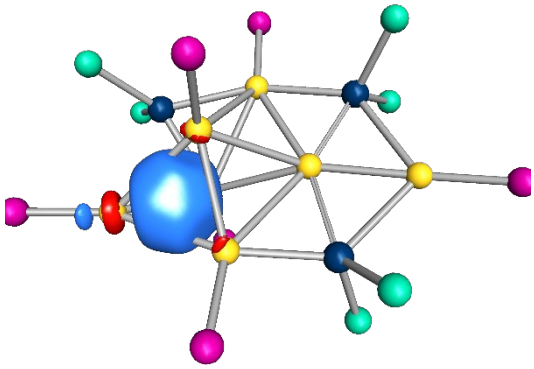
HOMO-1



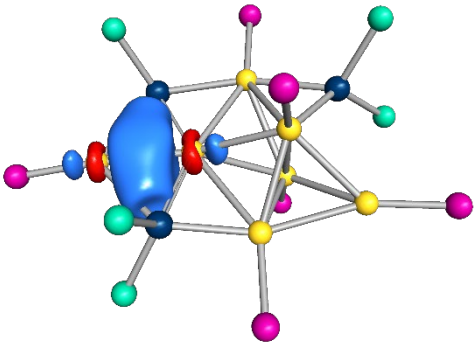
HOMO-2



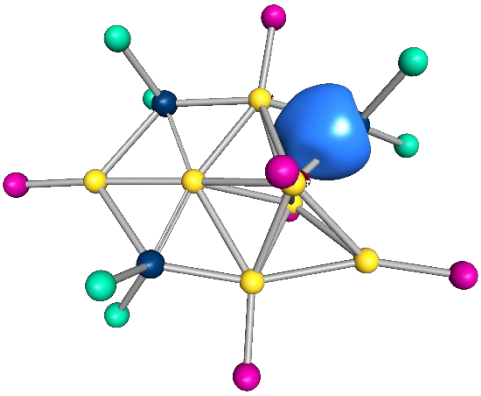
HOMO-5



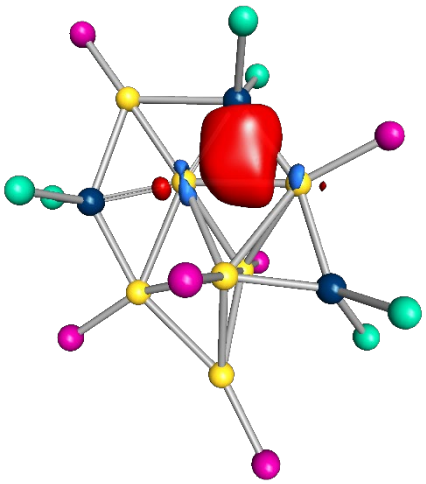
LMO434



LMO433



LMO431



LMO 430

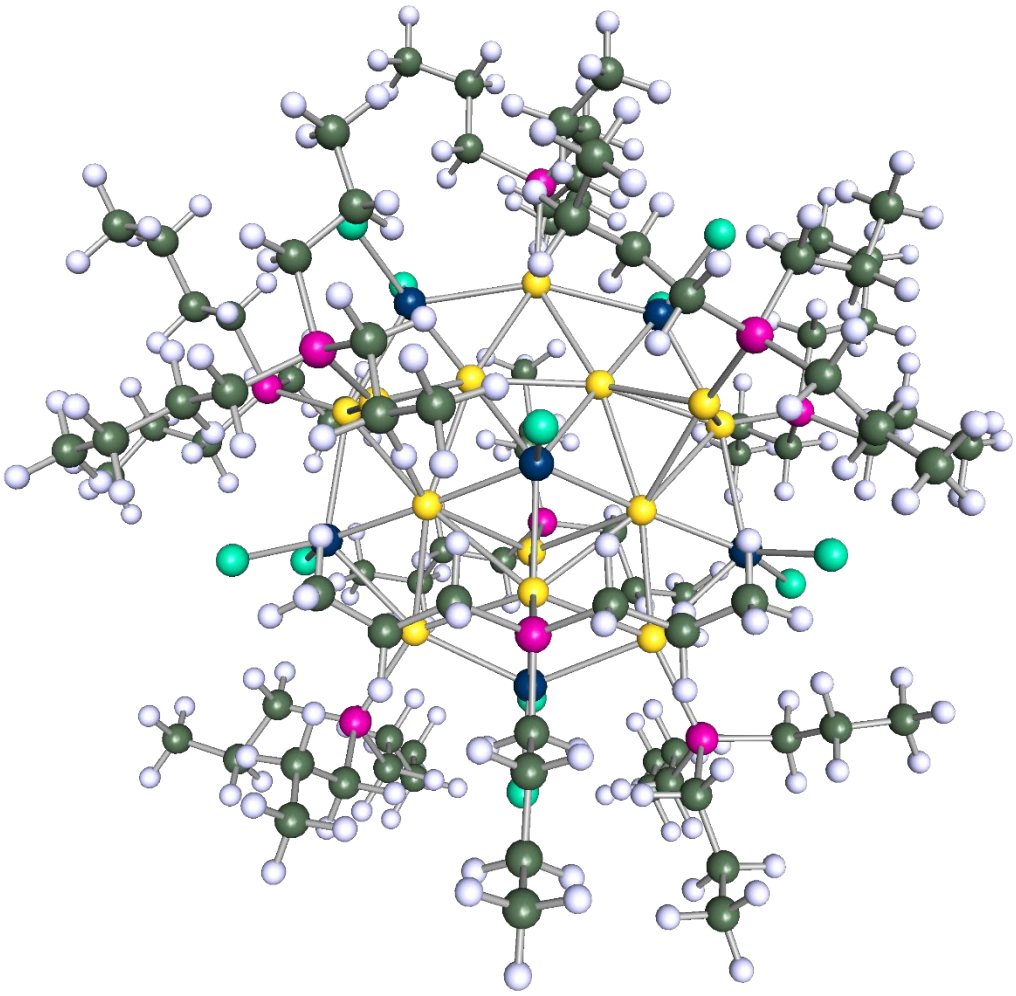


Figure S2: Geometry optimized structure of $\mathbf{3}^3$

Point group: C_1

Energy: -25001.85851252075 Hartree

HOMO-LUMO-gap: 1.536 eV

Atomic coordinates:

Au 2.045727 21.080687 14.647746	Au 5.001678 21.926996 14.376869	P 1.726132 18.812065 14.137638
Au 2.716738 23.600045 15.352490	Au 0.885328 23.404498 12.987535	Au 4.392542 21.804314 17.098088
Au -0.285570 23.262967 15.529067	Ga 1.617283 22.405683 17.393207	Ga 3.528265 23.447376 12.794967

P 3.293349 25.866269 15.967904

Ga -1.668427 23.398002 13.094421

P -2.112484 23.588186 17.109861

Au 7.115923 22.724768 12.592964

Au 6.768743 19.952243 13.084423

Au 4.781034 21.474069 11.518670

Ga 6.673513 20.722930 15.893075

Au 1.116024 25.092582 10.697859

Au -0.601507 22.801336 10.501943

Au 2.311137 22.491060 10.632943

Cl 0.773858 20.334503 17.981813

Cl 1.216620 23.546257 19.385862

C 0.182546 18.028538 14.814919

C 1.769448 18.453571 12.313875

C 3.068805 17.736688 14.848886

C 3.168897 17.747890 16.384778

P 4.782803 21.607087 19.491575

Cl 4.492455 25.488670 12.170350

C 2.887307 26.355901 17.717216

C 5.086866 26.297603 15.745604

C 2.418121 27.105971 14.894818

Cl -3.203851 21.701346 13.421353

Cl -2.929551 25.312355 12.956916

C -2.301268 22.338182 18.474662

C -1.916303 25.170652 18.074579

C -3.788174 23.714789 16.316537

C 0.894652 27.116696 15.086219

P 8.719388 24.144334 11.631709

Ga 6.092916 19.689868 10.299897

P 8.252317 18.069808 13.296671

Au 3.874120 20.917549 8.899111

Cl 7.070063 18.757476 17.040297

Cl 8.596627 21.917168 16.301167

P 1.204196 27.168937 9.593931

Ga 1.150164 21.728156 8.508584

P -2.636646 22.213520 9.362402

C -1.148509 18.408973 14.149519

C 1.517773 16.995923 11.885986

C 4.048347 16.613367 16.925297

C 3.515497 20.674600 20.482942

C 4.787499 23.315098 20.235113

C 6.388773 20.825716 20.029828

C 6.053799 25.489425 16.624139

C 3.198140 27.803411 18.131124

C -2.774720 20.939723 18.054382

C -2.113053 26.459349 17.262423

C -4.986995 23.966773 17.247374

C 0.152428 27.923645 14.014769

C 7.941854 25.511064 10.639277

C 9.839992 25.090288 12.781283

C 9.814457 23.298341 10.387430

Cl 7.991189 20.130493 9.066234

Cl 5.717390 17.449999 9.917016

C 8.978476 17.560934 11.664120

C 9.693970 18.440395 14.409235

C 7.554141 16.520815 14.049553

P 4.423072 20.171897 6.683088

C -0.226330 28.299759 9.960376

C 2.712579 28.221198 9.890876

C 1.181118 26.994060 7.739702

Cl 0.322998 19.719148 7.761650

Cl 0.900731 23.104471 6.676855

C -2.695664 22.837468 7.612259

C -4.169700 22.870666 10.182405

C -2.899093 20.393243 9.109468

C -2.327299 17.665783 14.807911

C 1.702273 16.795081 10.374929

C 3.412759 19.174123 20.171534

C 4.940094 23.427504 21.762815

C 7.646481 21.691400 19.851488

C 7.522351 25.844874 16.359589

C 2.761080 28.114331 19.575026

C -2.624609 19.491019 10.320590

C -2.894397 19.999074 19.267705

C -1.822999 27.720849 18.088420

C -6.304956 24.074590 16.463749

C 7.117491 25.038544 9.430830

C 10.424698 24.306478 13.967944

C 10.836028 22.289807 10.936247

C 10.073677 16.480644 11.689961

C 10.566070 19.624156 13.965206

C 6.433336 15.838114 13.250881

C 4.852094 18.374734 6.488920

C 5.962471 21.023488 6.087655

C 3.116645 20.512369 5.407499

C -1.618435 27.673388 9.781261

C 2.812270 28.888163 11.270803

C 2.469775 26.423552 7.123049

C -2.662642 24.362176 7.442652

C -5.500207 22.704358 9.427632

C -3.688827 17.951659 14.162931

C 2.352325 18.480432 21.045384

C 8.930992 20.905545 20.151729

C 3.082179 29.549547 20.011574

C -2.841032 18.010181 9.978590

C -3.413624 18.600256 18.914175

C 6.428467 26.189859 8.673120

C 11.290941 25.188086 14.878145

C 11.585307 21.561264 9.810987

C 10.584043 16.103640 10.281854

C 11.693267 19.921542 14.964090

C 5.951325 14.541330 13.916938

C 3.676733 17.400233 6.660066

C 5.898434 22.558700 6.116242

C 3.455216 20.176007 3.945101

C -2.751209 28.654172 10.135618

C 4.151542 29.612763 11.466750

C 2.387322 26.335678 5.592826

C -2.733096 24.776366 5.961428

C -6.690374 23.218996 10.253073

C 2.225043 16.976330 20.773104

C 7.378083 27.185886 7.992132

C 9.551333 15.399992 9.390181

C 4.122396 15.930614 6.554254

C 7.212642 23.201605 5.649885

C 2.270874 20.457087 3.006449

C -4.147770 28.031945 10.010109

C -2.733949 26.294810 5.745130

C 2.960238 14.935617 6.667663

C 5.071137 24.887240 22.224015

H 8.667411 16.041675 9.181897

H 9.998346 15.123014 8.409823

H 9.182021 14.462656 9.865842

H 3.318182 13.884899 6.591429

H 2.207596 15.094462 5.862185

H 2.432850 15.042502 7.641900

H 8.107928 17.244048 11.048068

H 9.349678 18.491186 11.179016

H 5.581404 16.544061 13.132583

H 6.776080 15.615893 12.216523

H 10.938443 16.834800 12.296120

H 9.695314 15.559935 12.193167

H 11.474139 15.443395 10.403214

H 10.951360 17.024753 9.771888

H 8.410177 15.821526 14.199623

H 7.203172 16.822627 15.062717

H 5.140011 14.067127 13.321726

H 5.557066 14.731899 14.939607

H 6.777417 13.799947 14.007979

H 9.923436 20.527550 13.861327

H 10.999951 19.419120 12.959093

H 12.333628 20.850904 10.227104

H 10.878448 20.982085 9.177456

H 12.130626 22.277252 9.154759

H 11.272842 20.210770 15.951736

H 12.328476 20.762900 14.608416

H 12.354865 19.037584 15.111204

H 10.308210 21.546869 11.575277

H 9.255049 18.629264 15.415109

H 10.300744 17.507962 14.487543

H 2.893838 17.602893 5.892908

H 3.193099 17.571885 7.647933

H 5.636002 18.161811 7.249636

H 5.322425 18.254137 5.484810

H 4.871534 15.727290 7.353167

H 4.651651 15.775587 5.583730

H 2.756313 16.990200 10.078567

H 1.053808 17.481329 9.786877

H 1.452762 15.750494 10.082916

H 2.532253 20.227117 1.949598

H 1.385820 19.841347 3.281138

H 1.960105 21.524070 3.059289

H 2.216198 19.953169 5.749209

H 2.836546 21.583890 5.515863

H 3.749072 19.105209 3.853065

H 4.336554 20.769678 3.609850

H 0.487054 16.693890 12.181164

H 2.210089 16.312405 12.427879

H 6.184724 20.653509 5.059553

H 6.777524 20.662905 6.756709

H 3.570227 18.732801 16.713815

H 2.155994 17.668099 16.836893

H 4.104975 16.654741 18.034774

H 3.639941 15.615902 16.643451

H 5.088573 16.690088 16.542999

H 4.027082 18.076217 14.392069

H 2.878390 16.700738 14.483706

H 0.337753 16.924754 14.768568

H 0.159240 18.314518 15.890461

H 2.768135 18.806053 11.963690

H 1.032089 19.138082 11.836957

H 6.266381 20.525195 21.097312

H 6.489655 19.892283 19.431209

H 8.200685 25.213527 16.972396

H 7.780914 25.666905 15.292067

H 7.734641 26.914058 16.590277

H 3.421630 25.633192 18.372089

H 1.810266 26.119809 17.861470

H 4.055555 22.968573 22.257771

H 5.828772 22.852273 22.110141

H 9.827938 21.551227 20.026743

H 8.937460 20.508704 21.192875

H 9.034339 20.046366 19.453596

H 7.591144 22.583753 20.516621

H 7.701403 22.071371 18.806876

H 2.749785 29.739879 21.055898

H 2.576477 30.295666 19.357443

H 4.176109 29.753018 19.965309

H 5.205080 27.391758 15.927485

H 5.294115 26.117796 14.665886

H 4.188342 25.488197 21.909587

H 5.148351 24.953753 23.331881

H 5.977891 25.368678 21.793177

H 1.665740 27.928703 19.670924

H 3.251389 27.391953 20.268629

H 4.290804 28.002567 18.033652

H 2.691409 28.518191 17.441233

H 10.704088 26.036489 15.297074

H 11.684645 24.599230 15.735076

H 12.161627 25.617466 14.331675

H 3.825427 23.773632 19.912110

H 5.603774 23.866544 19.715050

H -0.774675 27.726562 18.464081

H -2.493364 27.789487 18.974960

H -1.972041 28.641339 17.481804

H -3.154994 26.508168 16.873826

H -1.456806 26.436655 16.365005

H -2.637201 25.133781 18.924403

H -0.896852 25.121794 18.520734

H 2.853692 28.117302 15.069555

H 2.684840 26.804472 13.856863

H -0.944939 27.903662 14.190345

H 0.327623 27.479493 13.009880

H 0.484444 28.986809 13.992354

H 0.521398 26.064700 15.065116

H 0.648933 27.521111 16.094597

H 1.976976 29.612017 11.405019

H 2.696072 28.113945 12.059802

H 5.000560 28.895764 11.417314

H 4.314239 30.392540 10.688417

H 4.191499 30.113973 12.458965

H -6.269629 24.909797 15.729398

H -6.510807 23.141298 15.894098

H -7.164932 24.254981 17.146498

H -4.340037 27.673365 8.973217

H -4.942026 28.768614 10.263184

H -4.256100 27.164472 10.698196

H -3.705199 24.515483 15.546658

H -3.923778 22.778507 15.730464

H -5.071675 23.144473 17.993878

H -4.832221 24.902048 17.833275

H 2.742865 28.987876 9.080210

H 3.582808 27.544370 9.741389

H -2.678021 29.556596 9.482858

H -2.601704 29.014777 11.180105

H 0.323016 26.332077 7.488232

H 0.959546 28.005957 7.323336

H -1.750441 27.324295 8.731102

H -1.699974 26.770716 10.429790

H -3.941416 20.257664 8.736667

H -2.207836 20.117973 8.281011

H 2.200604 27.333553 5.133978

H 1.572333 25.647989 5.279506

H 3.337111 25.941098 5.169371

H -5.464563 23.249557 8.456804

H -5.668644 21.632164 9.175728

H -1.870135 24.320393 5.424552

H -3.651567 24.338090 5.503945

H -3.972063 23.942342 10.409218

H -4.208980 22.370273 11.176628

H -3.893700 17.811528 9.673488

H -2.618966 17.360773 10.853891

H -2.178324 17.692530 9.143128

H -1.822624 22.382283 7.093217

H -3.615146 22.409135 7.148659

H -1.724465 24.756118 7.897449

H -3.506060 24.833964 7.999401

H -2.801583 26.550214 4.664436

H -1.802230 26.760072 6.138851

H -3.593878 26.780703 6.259985

H -1.572533 19.650217 10.649787

H -3.261134 19.785782 11.183442

H -7.646300 23.096998 9.696920

H -6.780565 22.667364 11.214885

H -6.573614 24.297848 10.498934

H 2.539930 21.179766 20.305334

H 3.777761 20.825883 21.555894

H 4.399985 18.678832 20.324473

H 3.146156 19.042497 19.099672

H 1.457364 16.509463 21.429433

H 3.187821 16.445489 20.951672

H 1.926451 16.783525 19.718479

H 2.597325 18.644812 22.121948

H 1.370268 18.975479 20.868422

H 7.457202 22.914986 4.601891

H 7.154042 24.311933 5.689307

H 8.062373 22.880439 6.292578

H 5.058673 22.921207 5.479827

H 5.664925 22.890076 7.154461

H 8.061430 26.670202 7.279126

H 8.011141 27.734879 8.724743

H 6.810770 27.949895 7.415564

H 7.283097 26.065239 11.345448

H 8.768133 26.193528 10.331258

H 11.569636 22.809410 11.592793

H 9.121723 22.771254 9.692658

H 10.327882 24.102808 9.807983

H 5.756418 26.727414 9.381167

H 5.760763 25.739128 7.903943

H 7.764921 24.474263 8.720755

H 6.337662 24.328328 9.787768

H 3.340027 27.056577 7.408524

H 2.654135 25.408835 7.540743

H -0.105073 29.206052 9.320183

H -0.100134 28.628375 11.015889

H -2.733264 18.088569 18.197398

H -3.492196 17.956932 19.818582

H -4.422222 18.644993 18.443912

H -3.760595 21.003469 17.537235

H -2.054038 20.510385 17.323297

H -3.568948 20.463708 20.026205

H -1.893605 19.915731 19.749530

H -1.309155 22.281762 18.975896

H -3.011497 22.782099 19.211220

H -2.363602 17.942194 15.887431

H -2.125496 16.567969 14.781863

H -1.313660 19.507972 14.213912

H -1.122833 18.162916 13.062563

H -4.504195 17.410105 14.692327

H -3.922890 19.038159 14.183612

H -3.707855 17.627959 13.097898

H 11.031253 23.451022 13.597448

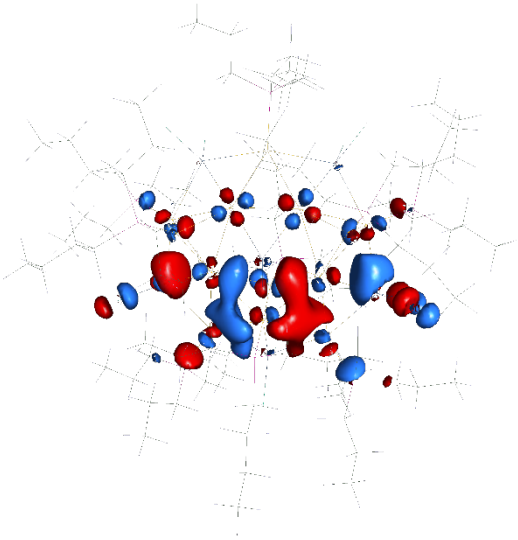
H 9.598529 23.852233 14.558593

H 10.647800 25.539130 12.154789

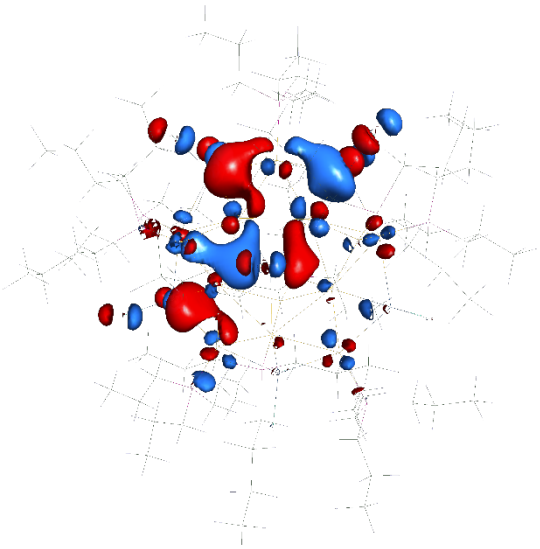
H 9.221755 25.937730 13.158835

H 5.897201 24.401296 16.437140

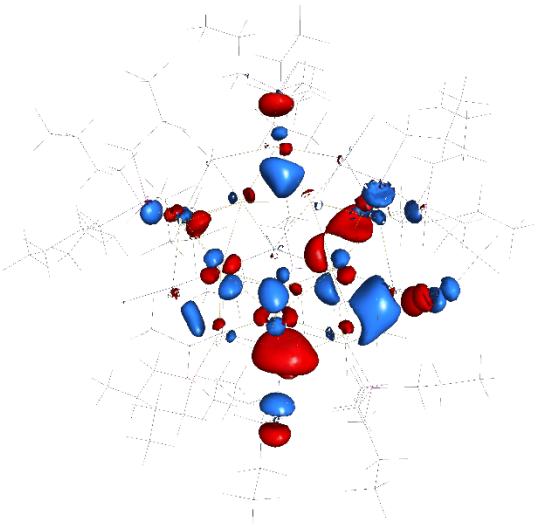
H 5.822906 25.657874 17.701625



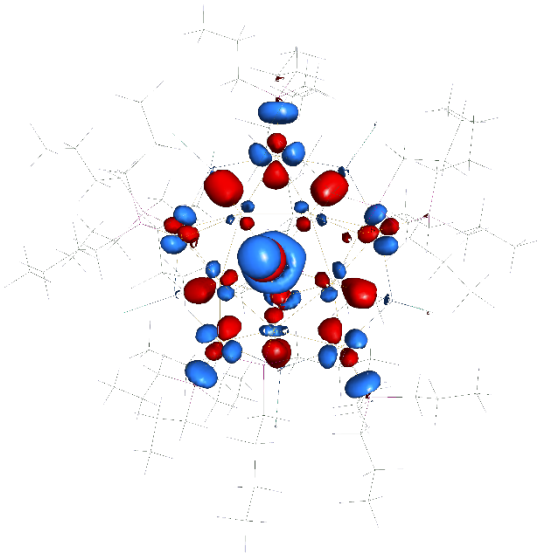
HOMO



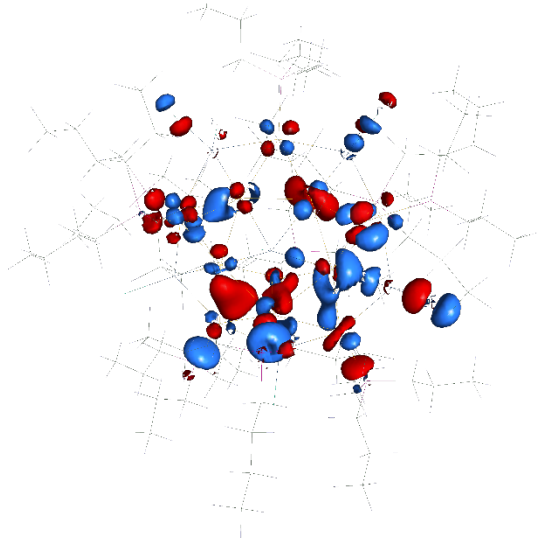
HOMO-2



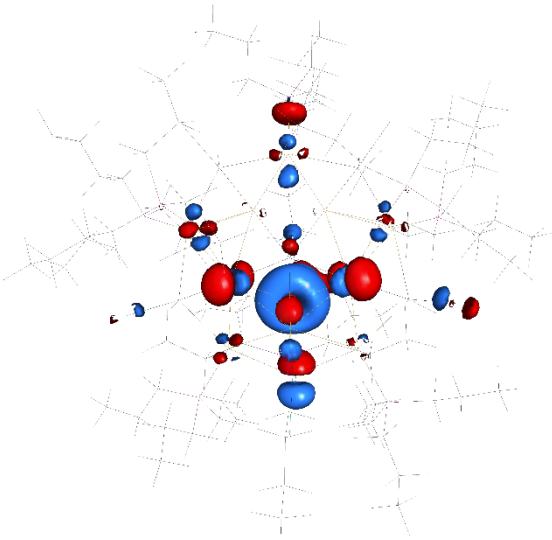
HOMO-3



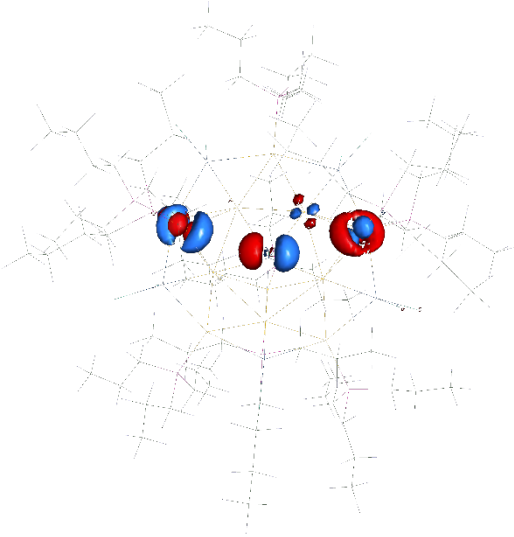
HOMO-4



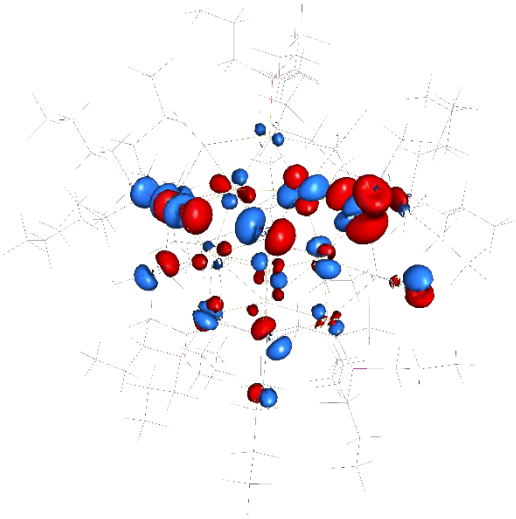
HOMO-6



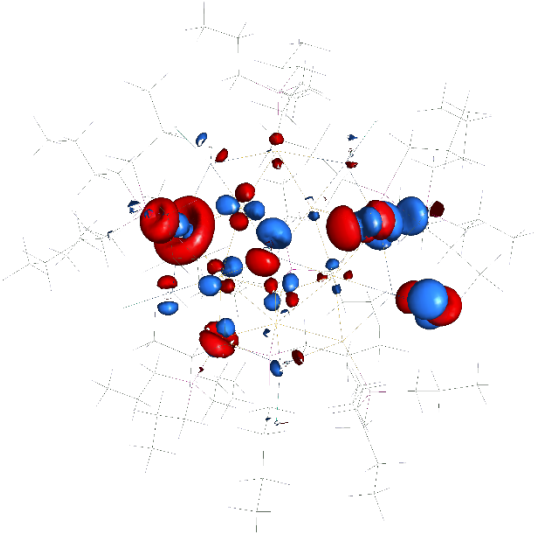
HOMO-7



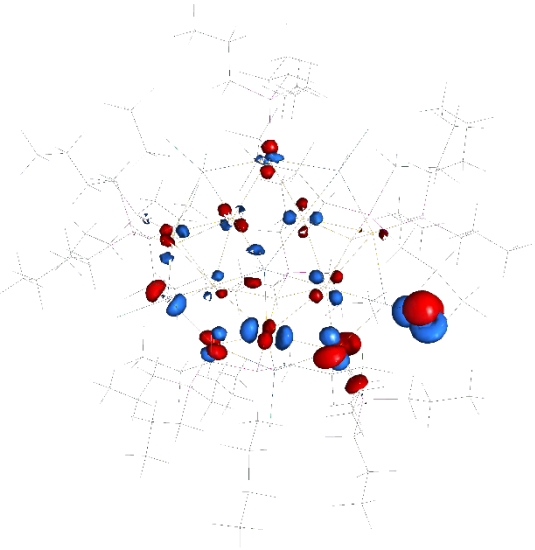
HOMO-9



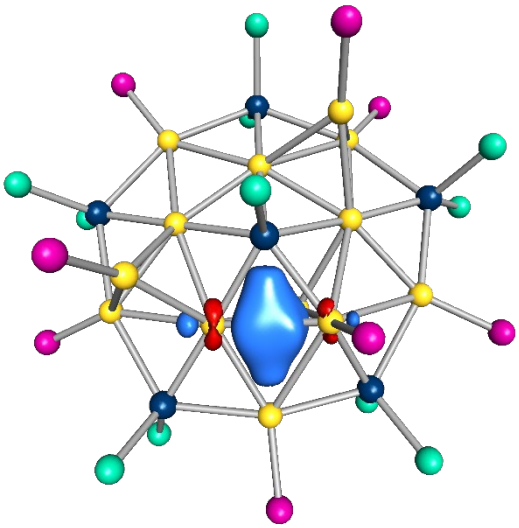
HOMO-10



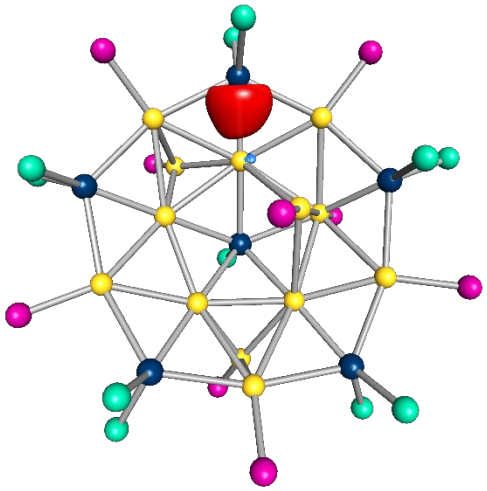
HOMO-11



HOMO-12



LMO750



LMO 748

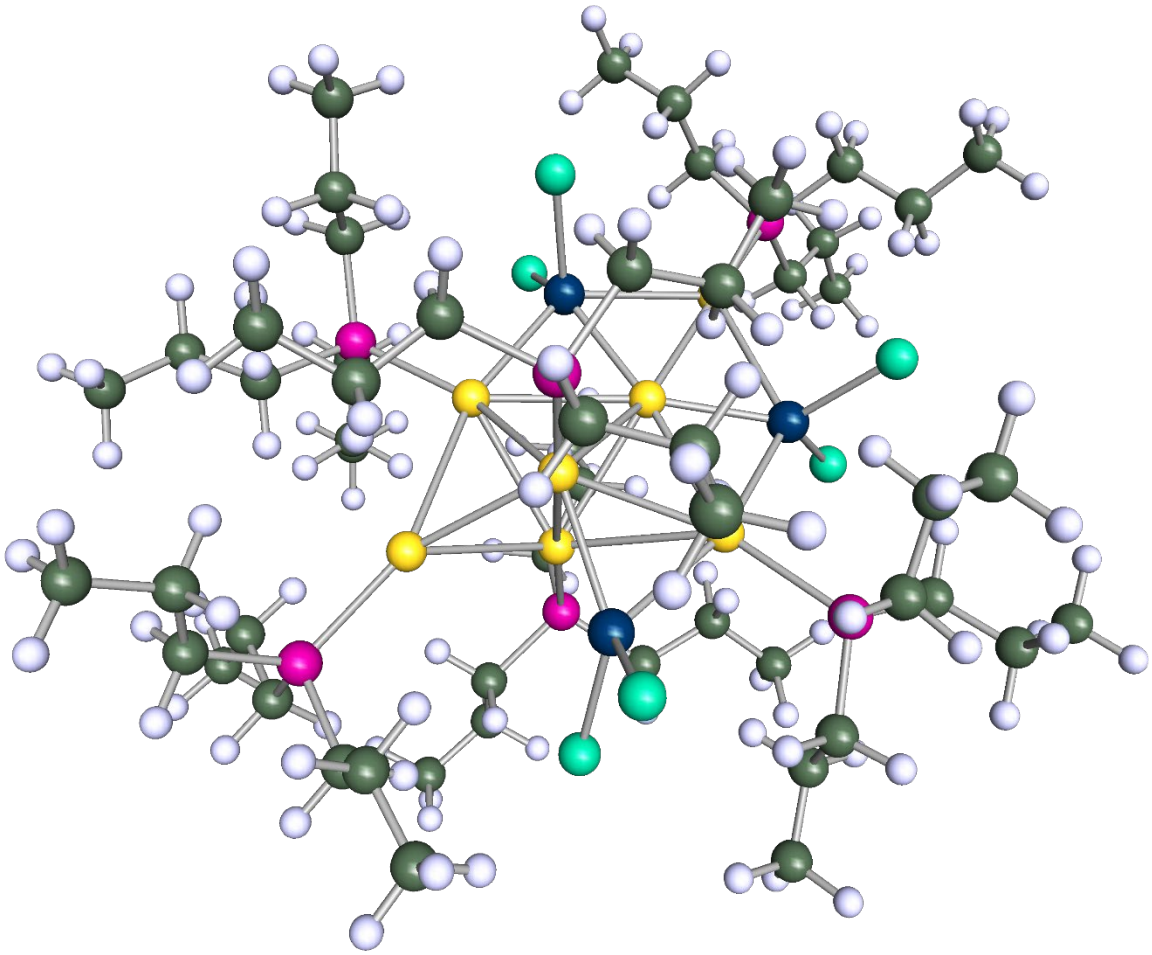


Figure S2: Geometry optimized structure of **4**^{3}

Point group: C_1

Energy: -22261.99453588454 Hartree

HOMO-LUMO-gap: 1.158 eV

Atomic coordinates:

Au 7.670933 8.812156 18.130368	Au 9.702790 7.850164 19.810027	Au 9.602173 3.773619 16.575196
Au 6.951681 7.882274 15.609229	Au 6.926252 6.515631 19.706261	Ga 7.626135 4.250921 18.676763
Au 9.952253 8.672603 16.359283	Au 5.855898 9.202200 20.376102	P 2.780188 7.113433 17.743471
Au 8.714071 6.213012 17.377950	Ga 8.294138 10.893149 16.728515	Ga 4.237752 11.163124 20.323617
Au 4.982530 8.026204 17.738633	P 6.451370 7.333472 13.361071	P 5.082162 13.111029 17.029021
Au 5.903112 11.120848 18.179741	Ga 10.586083 6.145787 15.632359	P 9.133067 12.220252 21.667842
Au 8.556583 10.488736 20.159890	P 11.905052 9.744016 15.347920	P 11.184025 6.687876 21.270886

Au 6.144698 4.340820 21.107538

Ga 5.809525 7.145006 21.939846

Au 4.455803 9.587616 22.663748

Cl 7.991618 11.454300 14.492298

Cl 9.452945 12.781393 17.479778

C 4.708701 7.813351 12.873823

C 7.598525 8.187523 12.171705

C 6.603991 5.520829 12.985674

Cl 10.406879 5.723509 13.371258

Cl 12.846091 5.875928 15.955736

C 12.591016 8.992964 13.786888

C 11.732789 11.556303 14.973109

C 13.365967 9.581659 16.487474

P 10.484949 1.785775 15.614269

Cl 5.950533 3.020739 17.704025

Cl 8.947504 2.625462 19.685224

C 2.807383 5.466754 16.867860

C 2.179702 6.885934 19.487289

C 1.420212 8.111446 16.958340

Cl 2.061279 10.793151 19.667446

Cl 4.042719 13.164925 21.438899

C 6.236338 14.569757 17.022409

C 3.481125 13.738990 17.743586

C 4.768790 12.901662 15.210122

C 9.676724 11.621424 23.343086

C 10.501769 13.328380 21.069393

C 7.744801 13.413738 21.996338

C 10.272293 5.329417 22.149250

C 11.887696 7.713786 22.660884

C 12.701608 5.885598 20.543194

P 5.451846 2.341032 22.195739

Cl 7.204598 7.082871 23.752725

Cl 3.884679 6.160096 22.805920

P 3.183487 10.143367 24.591678

C 4.046390 7.075368 11.694552

C 7.272559 8.158623 10.668043

C 5.803738 4.625295 13.946535

C 11.736676 9.183547 12.525869

C 12.970774 12.293809 14.435567

C 13.170747 10.166139 17.893944

C 9.823180 0.215270 16.357303

C 10.147912 1.710748 13.786225

C 12.287702 1.615552 15.809955

C 1.485412 4.744475 16.552309

C 0.822992 6.202418 19.747002

C 1.635708 8.473178 15.482601

C 6.616323 15.108335 18.408119

C 2.822180 14.954332 17.069420

C 3.816414 11.759530 14.831936

C 8.622218 10.757911 24.056442

C 11.837616 12.628623 20.778599

C 7.946516 14.455672 23.111608

C 11.068520 4.457031 23.135807

C 12.781085 8.882268 22.217174

C 12.422108 4.702407 19.602894

C 6.177674 2.082770 23.889892

C 5.925592 0.823088 21.231986

C 3.614313 2.235233 22.466162

C 4.043206 11.177896 25.878213

C 2.584978 8.657317 25.536198

C 1.648834 11.108999 24.181651

C 2.656713 7.637009 11.357199

C 8.354617 8.850246 9.824675

C 5.926474 3.133512 13.612006

C 12.341525 8.461309 11.313331

C 12.672612 13.774562 14.149696

C 14.422999 9.991669 18.765023

C 8.310202 0.017917 16.167210

C 10.672976 0.478273 13.033081

C 13.199510 2.341934 15.122793

C 1.718222 3.432910 15.785789

C 0.345210 6.405238 21.193323

C 0.491616 9.328193 14.918018

C 7.601624 16.282480 18.322836

C 1.534597 15.381476 17.792292

C 3.612328 11.671736 13.312630

C 9.105131 10.222053 25.410881

C 12.859112 13.580352 20.139236

C 6.828040 15.509516 23.130101

C 10.199898 3.338217 23.730916

C 13.404357 9.634462 23.402297

C 13.715345 4.056057 19.090140

C 5.953774 3.250383 24.867279

C 5.501107 -0.543198 21.796657

C 2.790335 2.231463 21.167627

C 4.504885 12.563271 25.397101

C 3.694130 7.876166 26.264194

C 0.636032 10.351371 23.305212

C 7.792351 -1.235089 16.887071

C 10.394847 0.554143 11.523919

C 14.684967 2.279498 15.320295

C 6.579963 2.987031 26.244157

C 5.952689 -1.709188 20.903755

C 1.277887 2.240221 21.431727

C 5.262714 13.336946 26.485434

C 3.184115 6.545868 26.835313

C -0.547956 11.235505 22.889292

H 11.477898 5.081626 23.962562

H 11.945999 4.000348 22.623324

H 13.069523 14.455157 20.795810

H 13.825302 13.063936 19.946515

H 12.480655 13.967909 19.167518

H 4.111620 8.497787 27.089186

H 4.531888 7.673146 25.559195

H 10.061681 0.286130 17.443303

H 10.398337 -0.645323 15.943145

H 7.030860 0.890508 21.109201

H 5.521463 0.981402 20.206076

H 1.735588 7.544657 14.873451

H 2.600716 9.018904 15.380262

H 1.150961 9.984352 22.388716

H 0.261528 9.453606 23.848243

H 9.330458 3.762201 24.280796

H 10.782519 2.708507 24.440155

H 9.803334 2.680146 22.926397

H 3.628840 13.160965 25.060425

H 5.147620 12.442475 24.496246

H 7.982229 13.940646 24.098804

H 8.929008 14.968856 22.995732

H 7.678111 9.235999 12.540590

H 8.588412 7.714452 12.369804

H 2.000890 12.018737 23.643878

H 1.181884 11.440279 25.140067

H 1.355766 9.035148 17.578649

H 0.458251 7.562973 17.084636

H 4.726316 4.913892 13.931146

H 6.153464 4.800430 14.988815

H 12.849770 3.073065 14.368144

H -0.614410 5.871825 21.376953

H 1.101474 6.031683 21.917317

H 0.184386 7.484764 21.411200

H 10.876989 11.634908 14.264692

H 11.360688 12.034145 15.907356

H 8.296894 -2.159086 16.522954

H 7.963190 -1.163166 17.984144

H 6.699077 -1.360172 16.725959

H 15.064214 3.283367 15.620538

H 15.206320 2.016483 14.370439

H 14.976536 1.542197 16.098914

H 3.532069 15.813018 17.049023

H 2.585180 14.722556 16.005759

H 3.072922 3.120374 20.558941

H 3.053338 1.340542 20.552789

H 2.167007 7.928446 19.883061

H 2.992477 6.368801 20.043360

H 10.710641 8.797327 12.714540

H 11.627925 10.269122 12.299977

H 5.763977 1.135658 24.309134

H 7.268587 1.920172 23.729883

H 12.317278 14.296441 15.065772

H 13.578958 14.304747 13.780897

H 11.877072 13.882640 13.379085

H 4.863288 3.438428 24.988755

H 6.373008 4.186169 24.434324

H 7.680302 2.836142 26.166614

H 6.149527 2.079422 26.725984

H 6.407491 3.847211 26.927718

H 2.101020 7.998013 24.781359

H 1.794154 8.990558 26.249990

H 14.336386 3.662930 19.928168

H 14.327810 4.785314 18.515805

H 13.483856 3.210538 18.406542

H 9.332237 11.045545 26.126081

H 10.029868 9.612357 25.295319

H 8.334497 9.564774 25.868436

H 14.246251 10.047622 15.985419

H 13.563125 8.486228 16.543178

H 3.486438 4.818527 17.469211

H 3.368930 5.657243 15.924381

H 1.740088 15.655051 18.850977

H 0.787014 14.557318 17.803708

H 1.066930 16.260665 17.295626

H 5.374767 2.518789 14.355205

H 6.991368 2.810853 13.638883

H 5.525970 2.902272 12.598389

H 3.690054 13.951472 18.816975

H 2.785955 12.869248 17.760725

H 8.074272 -0.058631 15.080603

H 7.766516 0.912689 16.547533

H 12.623909 10.048258 24.079960

H 14.051189 8.964010 24.012195

H 14.034223 10.483152 23.054540

H 9.413190 5.825782 22.658195

H 9.823042 4.696138 21.350713

H 13.378786 8.810837 11.106028

H 11.737742 8.641369 10.396376

H 12.375296 7.363866 11.489323

H 7.863209 16.661249 19.336210

H 8.543740 15.969005 17.821285

H 7.173669 17.134549 17.747032

H 5.636778 -2.687887 21.328566

H 7.060107 -1.727542 20.795226

H 5.519702 -1.626264 19.882058

H 0.821109 5.408011 15.952129

H 0.933742 4.527506 17.492375

H 7.689255 11.349248 24.204629

H 8.336130 9.903479 23.402528

H 4.393309 -0.579996 21.912414

H 5.923460 -0.681589 22.818137

H 5.827775 15.032460 23.218333

H 6.957200 16.216817 23.979498

H 6.823490 16.105410 22.190065

H 2.332722 6.697079 27.537713

H 2.842816 5.874690 26.016803

H 3.990945 6.017321 27.389231

H 7.151313 14.224273 16.490010

H 5.770243 15.368269 16.398422

H 13.339503 11.808002 13.503021

H 13.804796 12.224875 15.171375

H 13.352227 5.567226 21.392529

H 13.253710 6.681727 19.994084

H 13.597704 8.505678 21.560814

H 12.182219 9.581219 21.589848

H 0.705128 2.226850 20.478161

H 0.961865 1.352423 22.025418

H 0.973639 3.149712 21.995970

H 6.297513 8.664587 10.485253

H 7.152856 7.107196 10.319542

H 12.618361 0.914975 16.601802

H 3.354598 11.270397 26.752213

H 4.920552 10.582724 26.218608

H 10.878205 1.447489 11.069085

H 9.303632 0.621486 11.314217

H 10.784374 -0.346173 10.999072

H 3.352575 3.131209 23.072988

H 3.391476 1.333550 23.083938

H 10.563696 2.656541 13.368864

H 9.042958 1.807984 13.681322

H 8.487281 9.911446 10.132638

H 9.338091 8.342710 9.937194

H 8.088706 8.840464 8.744182

H 11.814867 5.051010 18.737582

H 11.803301 3.936214 20.119823

H 3.168198 12.609242 12.907157

H 2.931201 10.834459 13.043279

H 4.582350 11.508224 12.792470

H 5.705421 15.418513 18.968964

H 7.075969 14.279509 18.990895

H 3.952173 5.993700 11.940023

H 4.691384 7.129108 10.790854

H 10.206482 -0.444870 13.447610

H 11.768094 0.379319 13.207425

H 4.747617 8.910706 12.683834

H 4.090725 7.693237 13.791037

H 11.651959 11.767599 20.097085

H 12.260258 12.207028 21.719467

H 0.664604 9.580313 13.848312

H -0.484280 8.795961 14.985102

H 0.390695 10.283355 15.479957

H 1.969803 7.571537 12.230677

H 2.189625 7.075122 10.518115

H 2.713502 8.707166 11.056124

H 6.826034 12.814860 22.179759

H 7.565399 13.914677 21.018544

H 10.107292 13.772289 20.126850

H 10.643362 14.155865 21.802973

H 5.771499 12.719168 14.759737

H 4.395205 13.876206 14.816747

H 12.296395 9.672942 18.378823

H 12.912608 11.247372 17.826819

H 0.757747 2.910348 15.578760

H 2.219674 3.618716 14.809296

H 2.369562 2.740422 16.363738

H -0.202215 12.093858 22.272317

H -1.276883 10.658280 22.279001

H -1.091207 11.640646 23.773502

H 2.829740 11.892706 15.332729

H 4.235709 10.800951 15.215391

H 14.268255 10.413645 19.782241

H 15.304944 10.504242 18.317662

H 14.686112 8.915952 18.880472

H 6.173074 12.787400 26.815620

H 4.627777 13.503763 27.385016

H 5.585529 14.333720 26.112482

H 9.965646 12.502895 23.962383

H 10.602605 11.026663 23.174738

H 7.693245 5.297890 13.063197

H 6.303882 5.342329 11.927154

H 0.908337 5.111609 19.541407

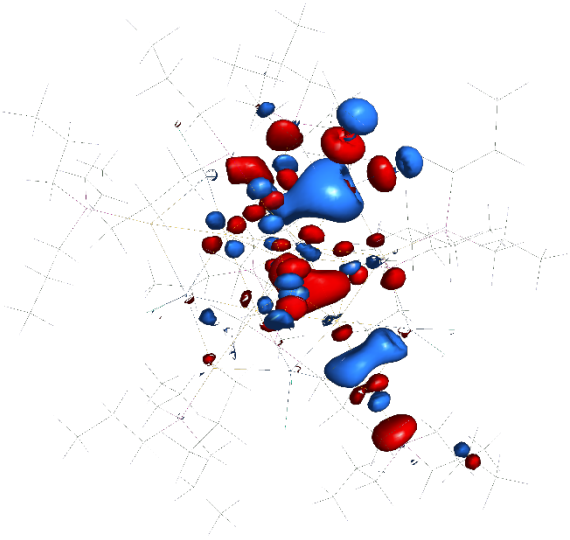
H 0.046552 6.591825 19.049792

H 13.608760 9.424127 13.635435

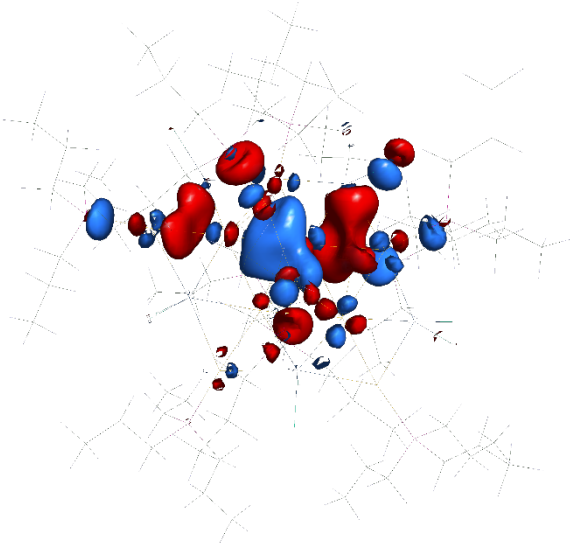
H 12.732977 7.910989 14.006900

H 11.013035 8.086155 23.242094

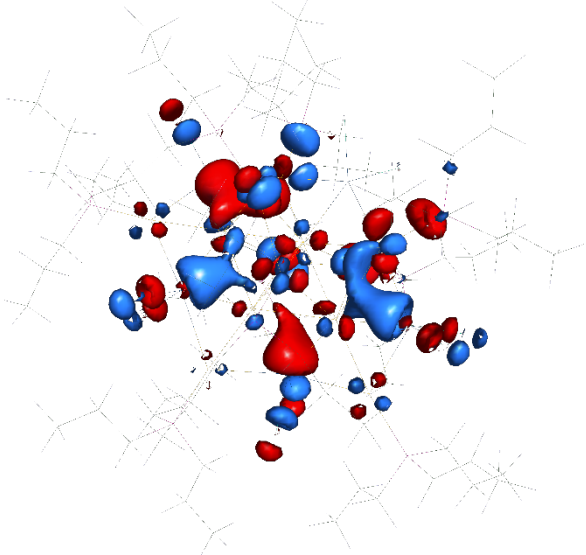
H 12.457694 7.030146 23.332029



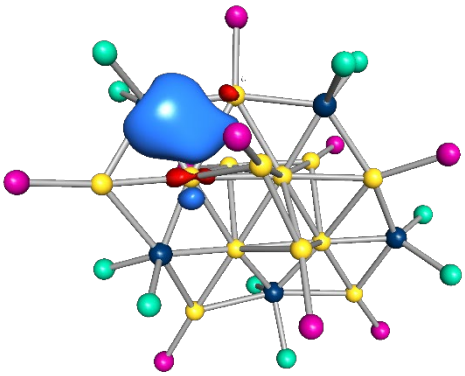
HOMO-2



HOMO-3



HOMO-4



LMO687

5. References

[1] (a) G. M. Sheldrick, Acta Crystallogr. 2008, A64, 112−122. (b) G. M. Sheldrick, Acta Crystallogr., Sect. C: Struct. Chem. 2015, C71, 3−8.

[2] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, J. Appl. Crystallogr. 2009, 42, 339−341.

[3] Turbomole: O. Treutler, R. Ahlrichs, J. Chem. Phys. 1995, 102, 346 – 354; BP86 functional: J. P. Perdew, Phys. Rev. B 1986, 33, 8822 – 88824; A. D. Becke, Phys. Rev. A 1988, 38, 3098 – 3100; RI-DFT: K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, Chem. Phys. Lett. 1995, 240, 283 – 290; SVP: A. Schäfer, H. Horn, R. Ahlrichs, J. Chem. Phys. 1992, 97, 2751 – 2577, TmoleX client: C. Steffen, K. Thomas, U. Huniar, A. Hellweg, O.Rubner, A. Schroer, J. Comput. Chem. 2010, 31, 2967 – 2970.