Electronic Supplementary Information

for

Cyclometallation of a germylene ligand by concerted metalation-deprotonation of a methyl group†

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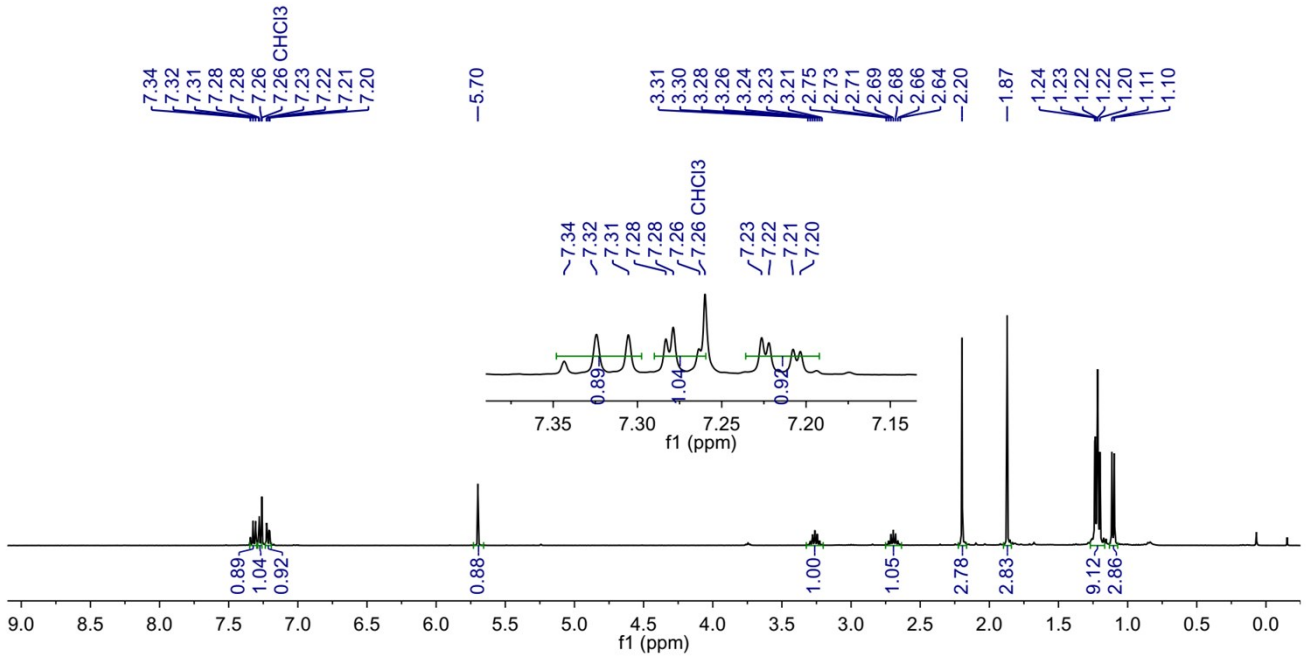
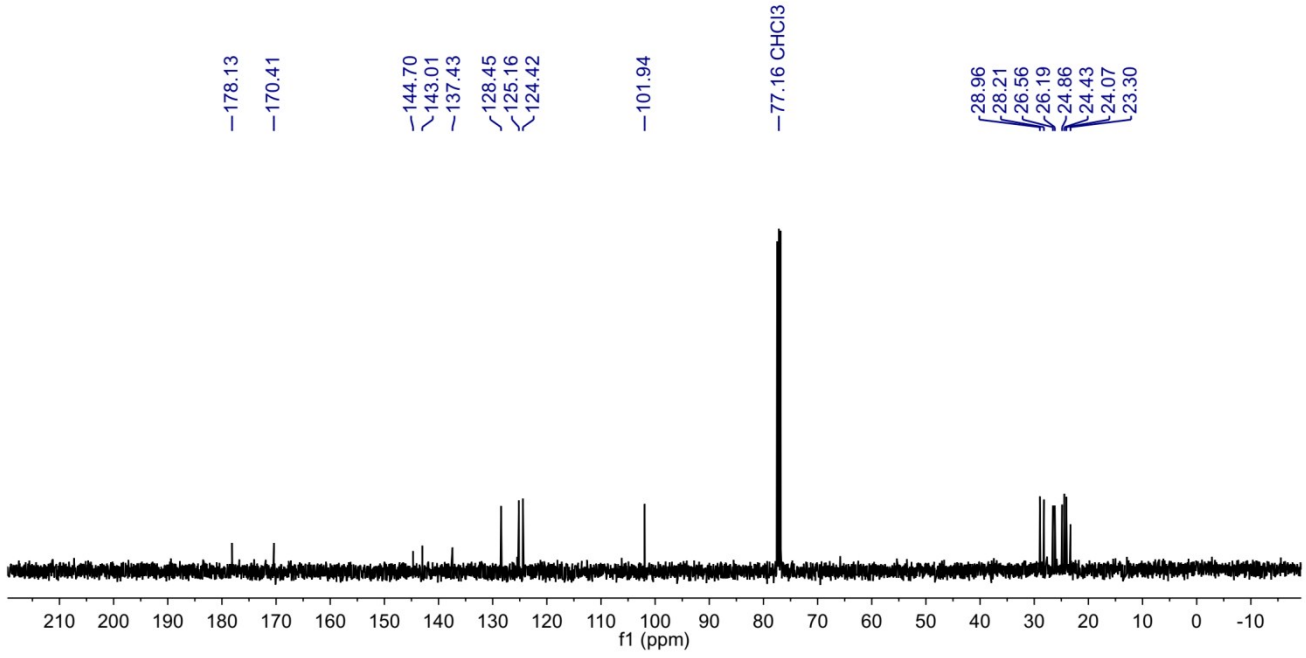
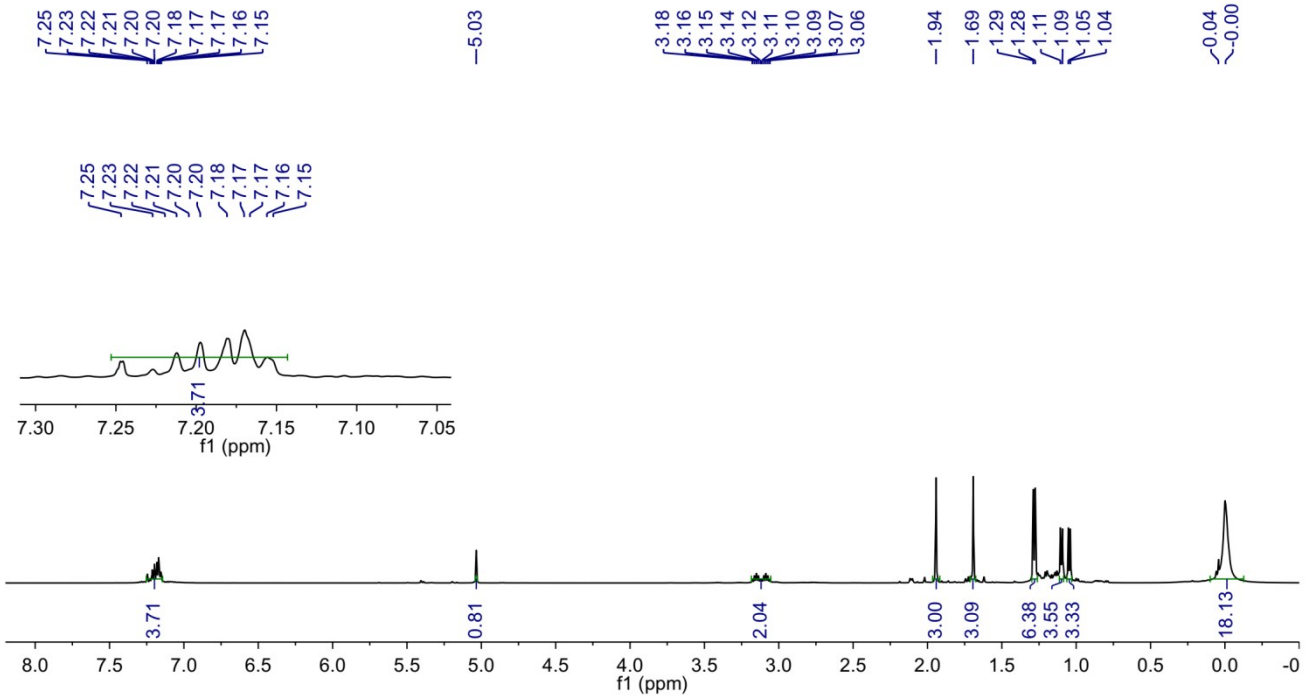


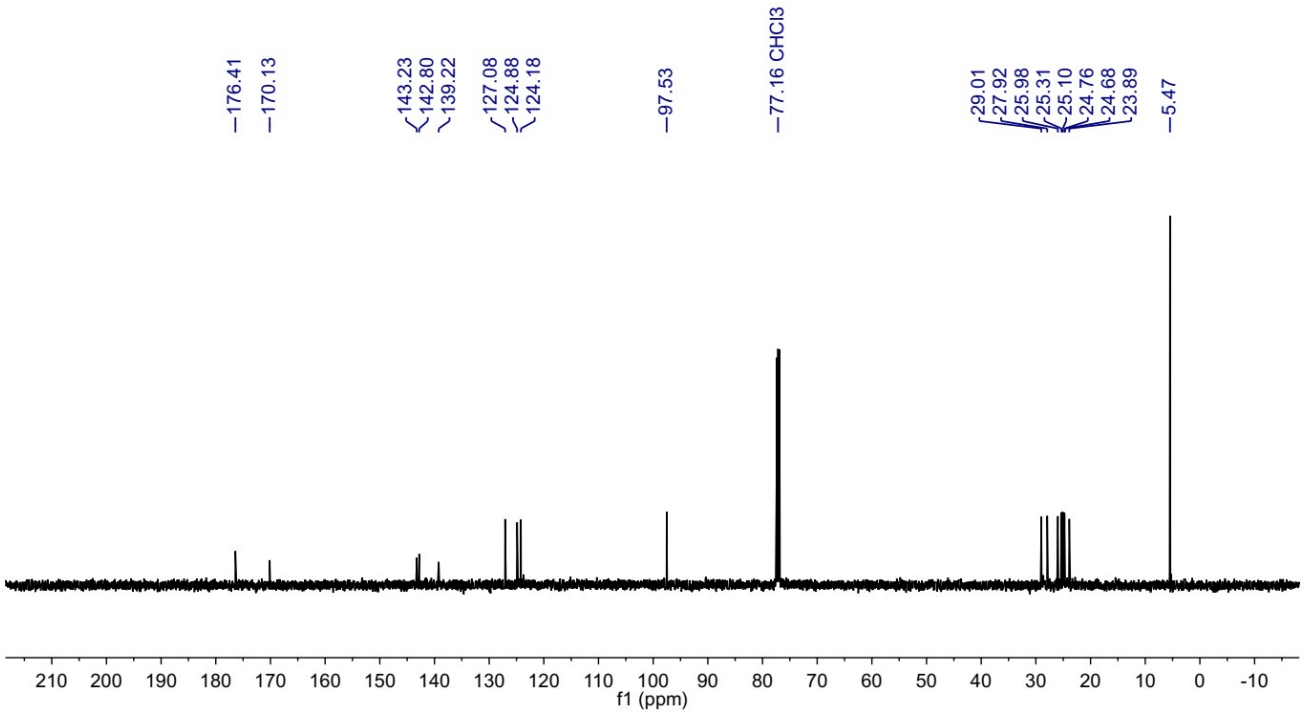
^{1}H NMR spectrum of **1** ($CDCl_3$, 400 MHz).



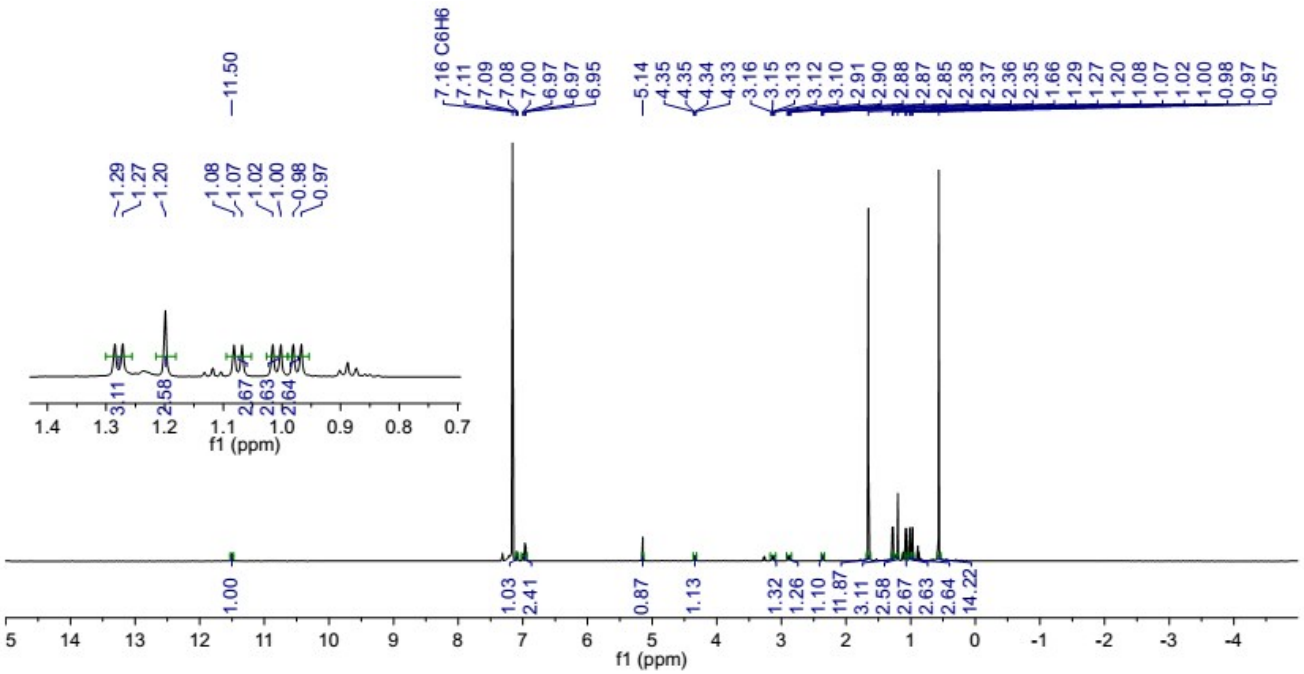
$^{13}C\{^{1}H\}$ NMR spectrum of **1** ($CDCl_3$, 101 MHz).



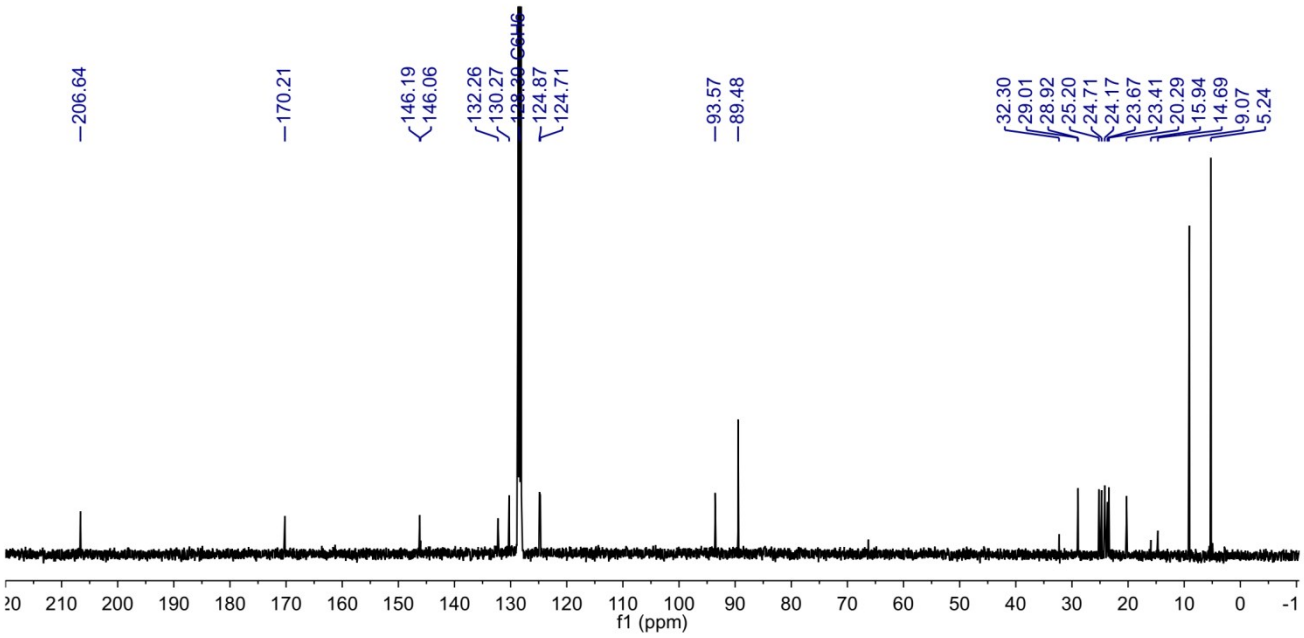
^{1}H NMR spectrum of **2** ($CDCl_3$, 400 MHz).



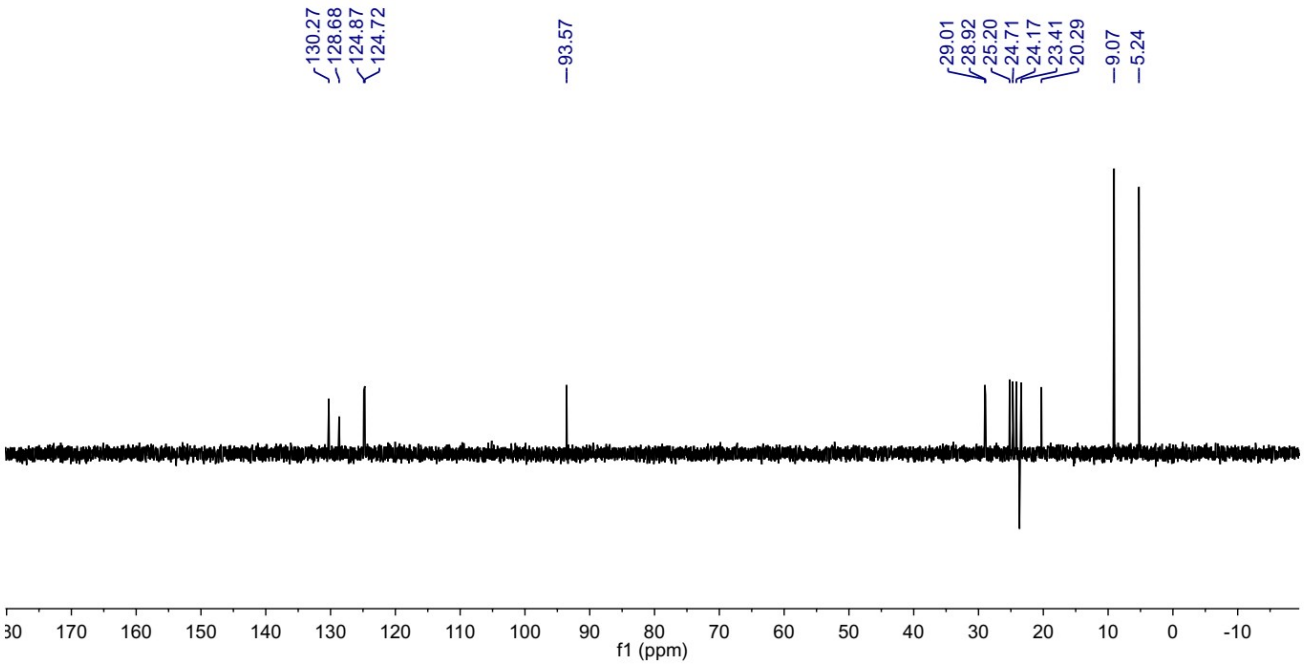
^{13}C{^{1}H} NMR spectrum of **2** ($CDCl_3$, 101 MHz).



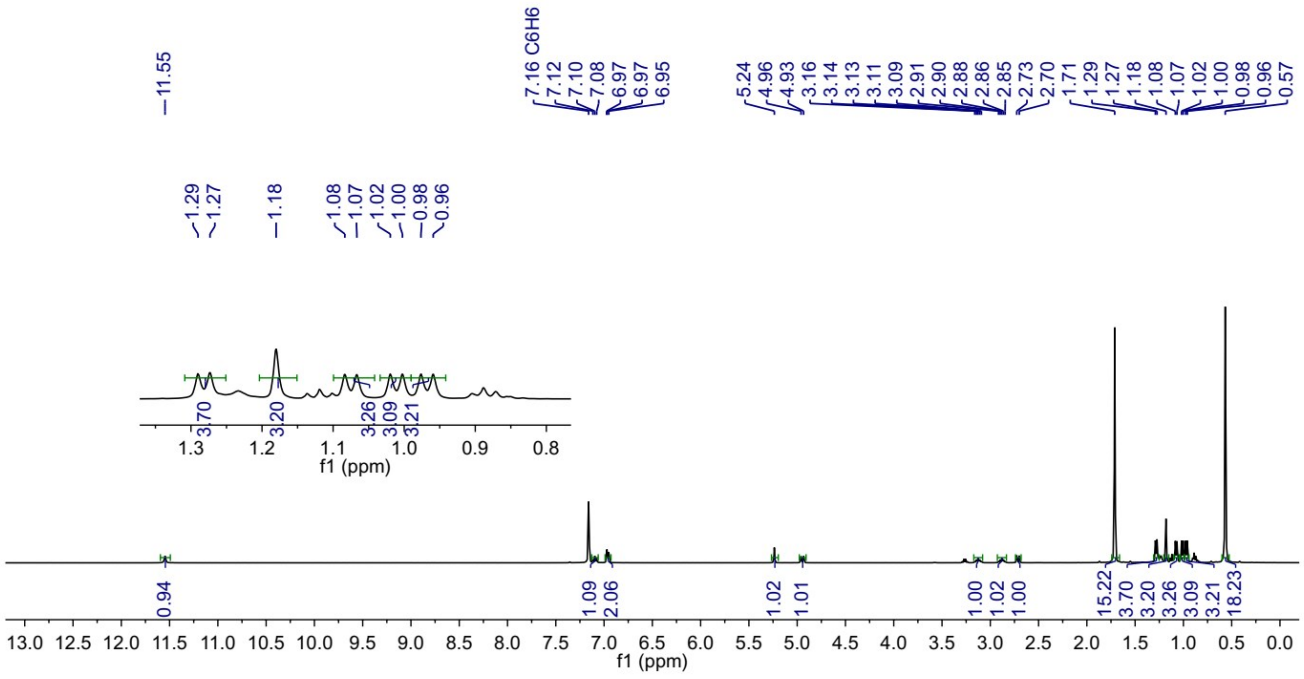
^{1}H NMR spectrum of **3** (C_6D_6, 500 MHz).



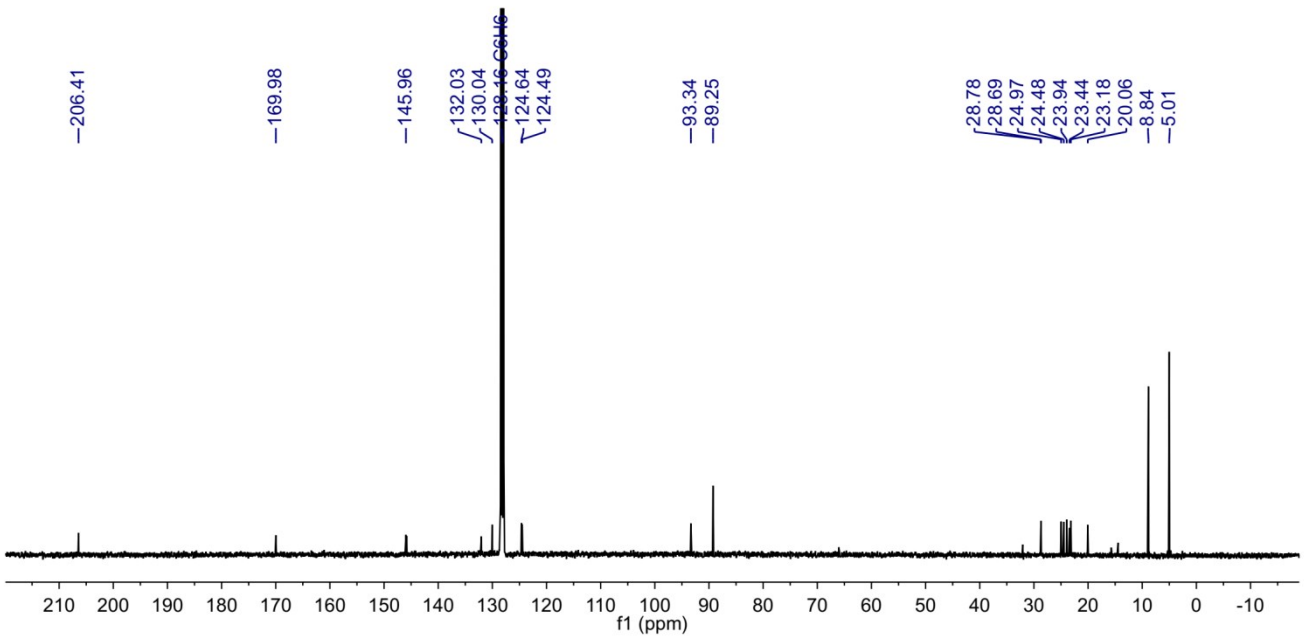
^{13}C{^{1}H} NMR spectrum of **3** (C_6D_6, 126 MHz).



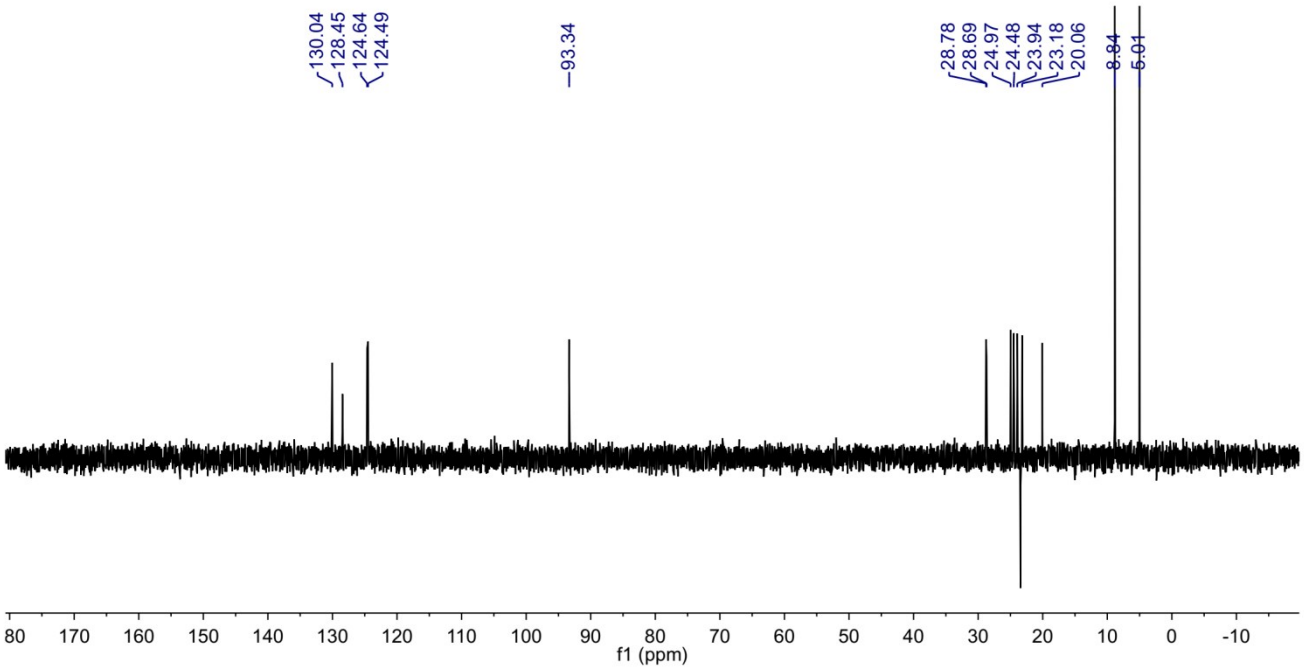
$^{13}C\{^{1}H\}$ DEPT-135 NMR spectrum of compound **3** (C_6D_6, 100 MHz).



^{1}H NMR spectrum of **4** (C_6D_6, 400 MHz).



$^{13}C\{^{1}H\}$ NMR spectrum of **4** (C_6D_6, 101 MHz).



$^{13}C\{^{1}H\}$ DEPT-135 NMR spectrum of compound **4** (C_6D_6, 100 MHz).

2. Details of theoretical calculations

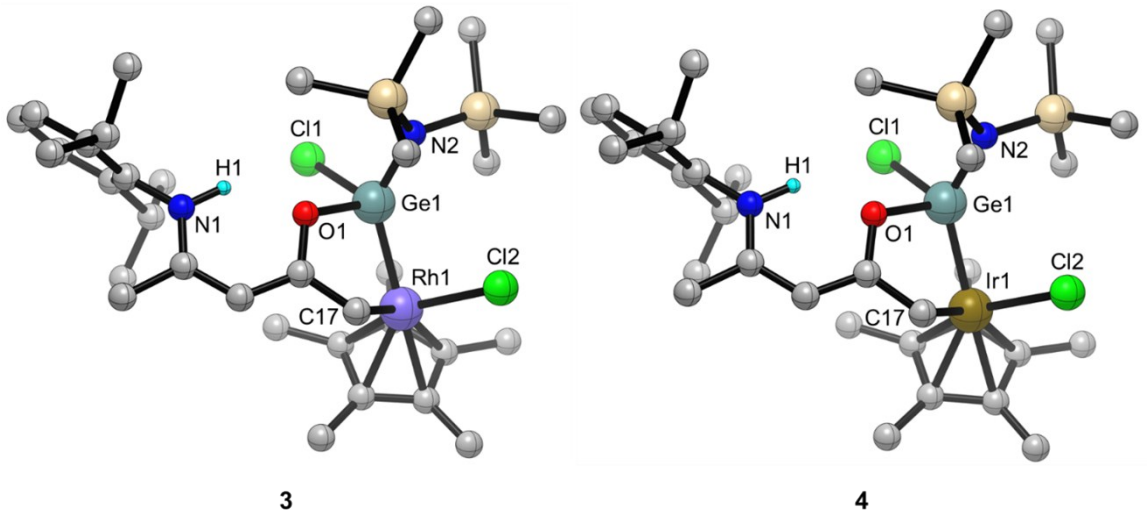


Fig. S1. Optimized geometries of the complexes **3** and **4**with selected geometrical parameters at M06-L/BS1 level of theory. H atoms are omitted for clarity.

Table S1. Selected geometrical parameters of the complexes **3** and **4**optimized at M06-L/BS1 level of theory. Bond distances (d) are in angstroms (Å) and bond angles (A) in degrees (°).

Complex	Geometrical Parameter	Crystal Structure	Calculated
3	Rh1−Ge1	2.380	2.402
	Rh1−Cl2	2.399	2.481
	Rh1−C17	2.147	2.187
	Ge1−O1	1.923	1.956
	Ge1−N2	1.847	1.840
	Ge1−Cl1	2.247	2.304
	N1−H1	0.880	1.022
	Ge1−Rh1−Cl2	92.5	88.4
	C17−Rh1−Ge1	77.4	77.7
	C17−Rh1−Cl2	88.5	87.0
	O1−Ge1−Rh1	98.6	98.1

	O1−Ge1−Cl1	92.7	90.9
	N2−Ge1−Rh1	133.1	134.9
	N2−Ge1−O1	101.1	101.2
	N2−Ge1−Cl1	101.6	101.9
4	Ir1−Ge1	2.370	2.409
	Ir1−Cl2	2.409	2.485
	Ir1−C17	2.151	2.177
	Cl1−Ge1	2.251	2.295
	Ge1−O1	1.923	1.961
	N2−Ge1	1.857	1.840
	N1−H1	0.880	1.022
	Ge1−Ir1−Cl2	88.3	87.8
	C17−Ir1−Ge1	78.3	77.8
	C17−Ir1−Cl2	88.1	85.7
	N2−Ge1−Ir1	132.5	134.9
	N2−Ge1−Cl1	101.1	102.2
	N2−Ge1−O1	101.6	101.0
	Cl1−Ge1−Ir1	120.7	118.1
	O1−Ge1−Ir1	99.1	97.8
	O1−Ge1−Cl1	91.2	91.2

Details of EDA-NOCV calculations: To gain insight into the bonding scenario of the intermediate **2a**, EDA (energy decomposition analysis), which is originally developed by Morokuma[S1] and later modified by Ziegler and Rauk,[S2] calculations were performed in conjunction with the NOCV (natural orbital for chemical valence)[S3] method using ADF 2013.01 program package.[S4] EDA-NOCV calculations were accomplished on the ONIOM{M06-L/BS1:HF/3-21G} optimized geometries at the BP86-D3 level in conjunction with uncontracted Slater-type orbitals (STOs) as basis functions. The basis sets contain a triple-ξ quality augmented by two sets of polarization functions for all atoms without any frozen core approximation. An auxiliary set of s, p, d, f, and g STOs was used to fit the

molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle. This level of theory is denoted as BP86-D3/TZ2P//ONIOM{M06-L/BS1:HF/3-21G}. Scalar relativistic effects were considered using the zeroth-order regular approximation (ZORA).[S5] The instantaneous interaction energy (ΔE_{int}) between two fragments in the molecule is composed of three main components:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp} \quad (1)$$

In [Eq. (1)], ΔE_{elstat} denotes the quasiclassical coulomb interaction energy between the fragments, calculated by means of the frozen electron density distribution of the fragments in the geometry of the adduct. ΔE_{Pauli} corresponds to the repulsive interactions between the fragments, originating by the fact that two electrons with the same spin cannot occupy the same region in space. Therefore, ΔE_{Pauli} accounts for destabilizing interaction between the occupied orbitals. In contrast, the stabilizing orbital interaction term ΔE_{orb} represents the interaction between the occupied and virtual orbitals of the two fragments and also elucidates charge transfer and polarization effects. ΔE_{orb} can be further partitioned into the contributions of the orbitals belonging to different irreducible representations of the interacting system. The EDA-NOCV method merges charge (NOCV) and energy (EDA) partitioning schemes to decompose the deformation density ($\Delta\rho$) into different components of the chemical bond. The EDA-NOCV calculations reveal pairwise energy contributions for each pair of interacting orbitals to the total bond energy. Since the dispersion corrected functional is used, the dispersion correction term, ΔE_{disp}, which represents the dispersion interaction between the two fragments, is added to the ΔE_{int}. The bond dissociation energy (ΔE) between the interacting fragments is given by Eq. (2):

$$\Delta E\ (= -D_e) = \Delta E_{prep} + \Delta E_{int} \quad (2)$$

in which the term ΔE_{prep} (preparation energy) is the energy required to promote the fragmentsfrom their equilibrium geometry and electronic ground state to the geometry and electronic state in the molecule.

Table S2. EDA-NOCV results of the intermediate**2a** at BP86-D3/TZ2P(ZORA)//ONIOM{M06-L/BS1:HF/3-21G} level of theory.

Intermediate	**2a**
Interacting fragments	**2** + **Rh^{M}**
ΔE_{int}	-64.8
ΔE_{Pauli}	124.0
ΔE_{elstat}[a]	-96.9 (60.9%)

ΔE_{orb}[a]	-62.3 (39.1%)
$\Delta E_{orb,1}$[b]	-37.5 (60.2%)
$\Delta E_{orb,2}$[b]	-4.5 (7.2%)
$\Delta E_{orb,rest}$[b]	-20.3 (32.6%)
ΔE_{disp}	-29.6
ΔE_{prep}	35.6
ΔE_{prep} (**2**)	15.2
ΔE_{prep} (**Rh^{M}**)	20.4
ΔE ($-D_e$)	-29.2

Energy values are given in kcal mol^{-1}.[a]The percentage values in parentheses give the contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$. [b]The percentage values in parentheses give the contribution to the total orbital interaction ΔE_{orb}.

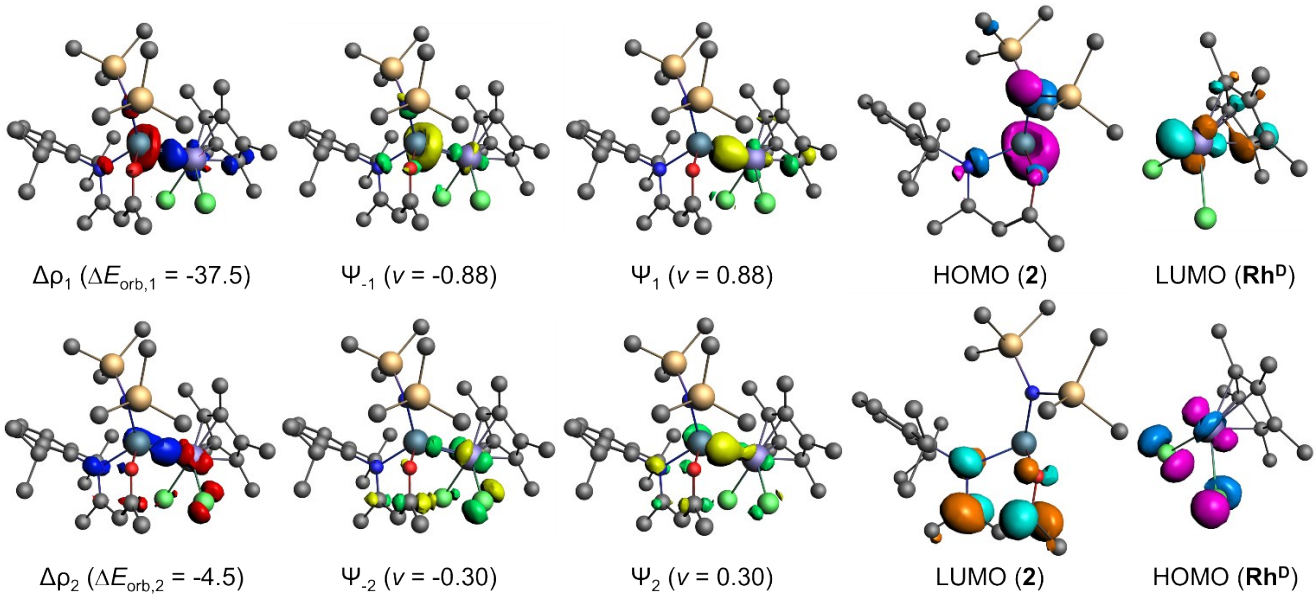


Fig. S2. Plot of deformation densities Δρ of the pairwise orbital interactions in **2a**between fragments **2** and **Rh^{M}**. The associated energies $\Delta E_{orb,n}$ (kcal mol^{-1}) are given in parentheses. The charge flow is color coded red→blue. NOCV pairs (Ψ_n/Ψ_{-n}) withcharge eigenvalues ν (in e) in parentheses are shown. The negative and positive eigenvalues give the amount of donated and accepted electronic charge, respectively. The most important interacting occupied and vacant orbitals of the fragments are also included.

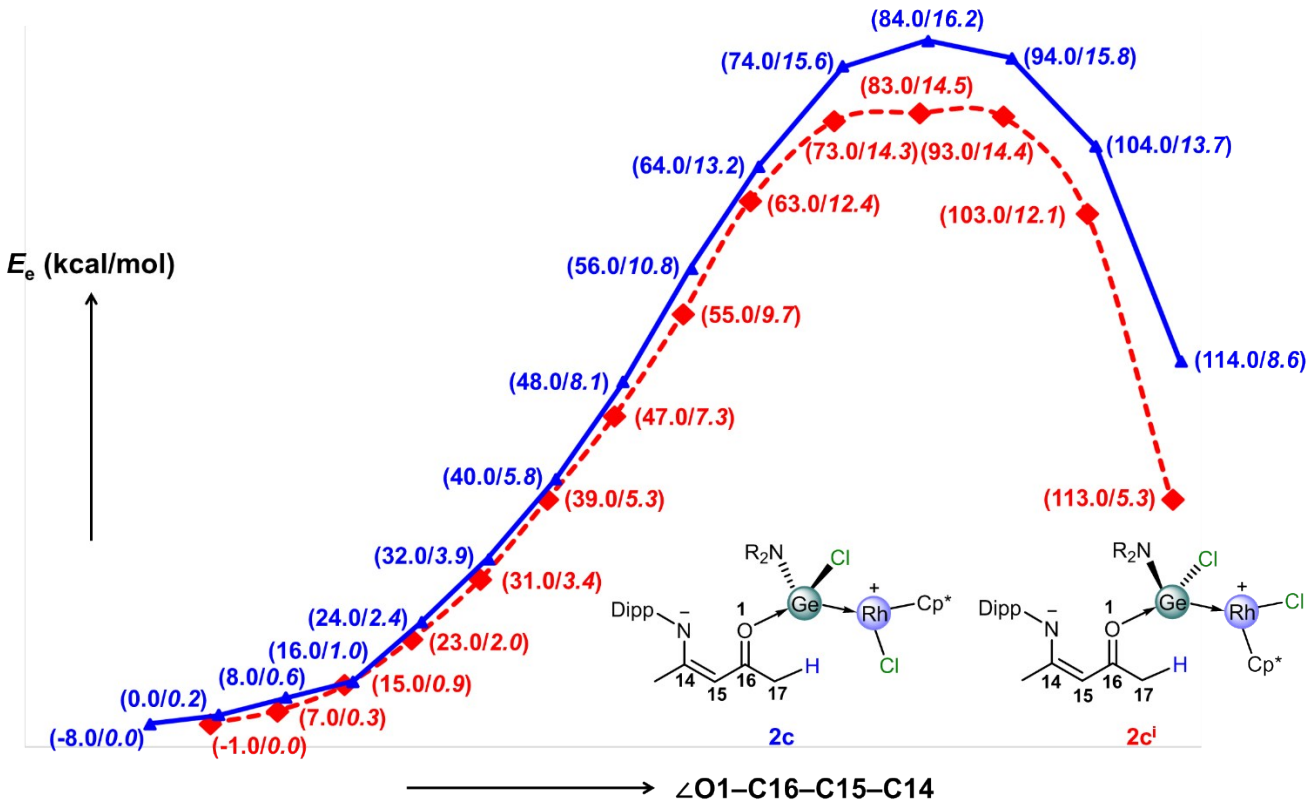
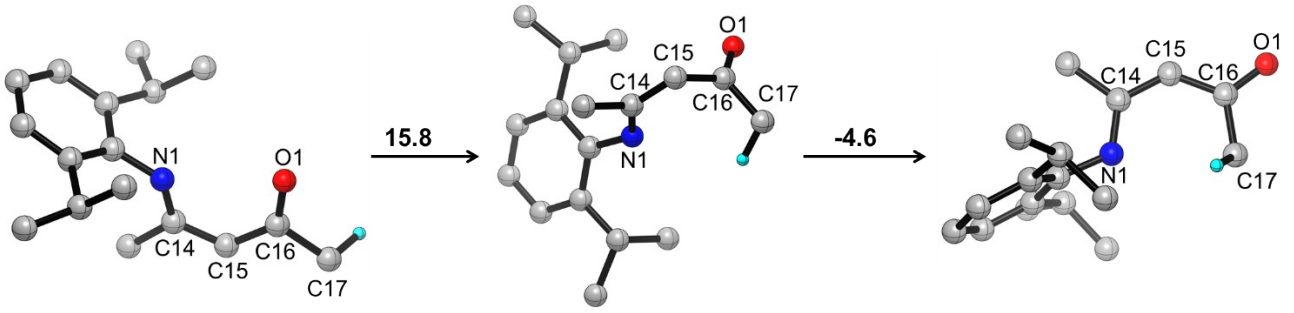


Fig. S3. Potential energy surface profile for the rotation of the C14 atom around the C15–C16 bond in **2c**and **2c^i**(refer to Fig.5 in main text). The values in parentheses (***∠O1–C16–C15–C14/relative energies***) are calculated at ONIOM{M06-L/BS1:HF/3-21G} level. The energy levels are not drawn to the scale.



2cF

C14–N1=1.327
C16–O1=1.246
∠C14–C15–C16–C17=-179.7
∠O1–C16–C15–C14=-1.0

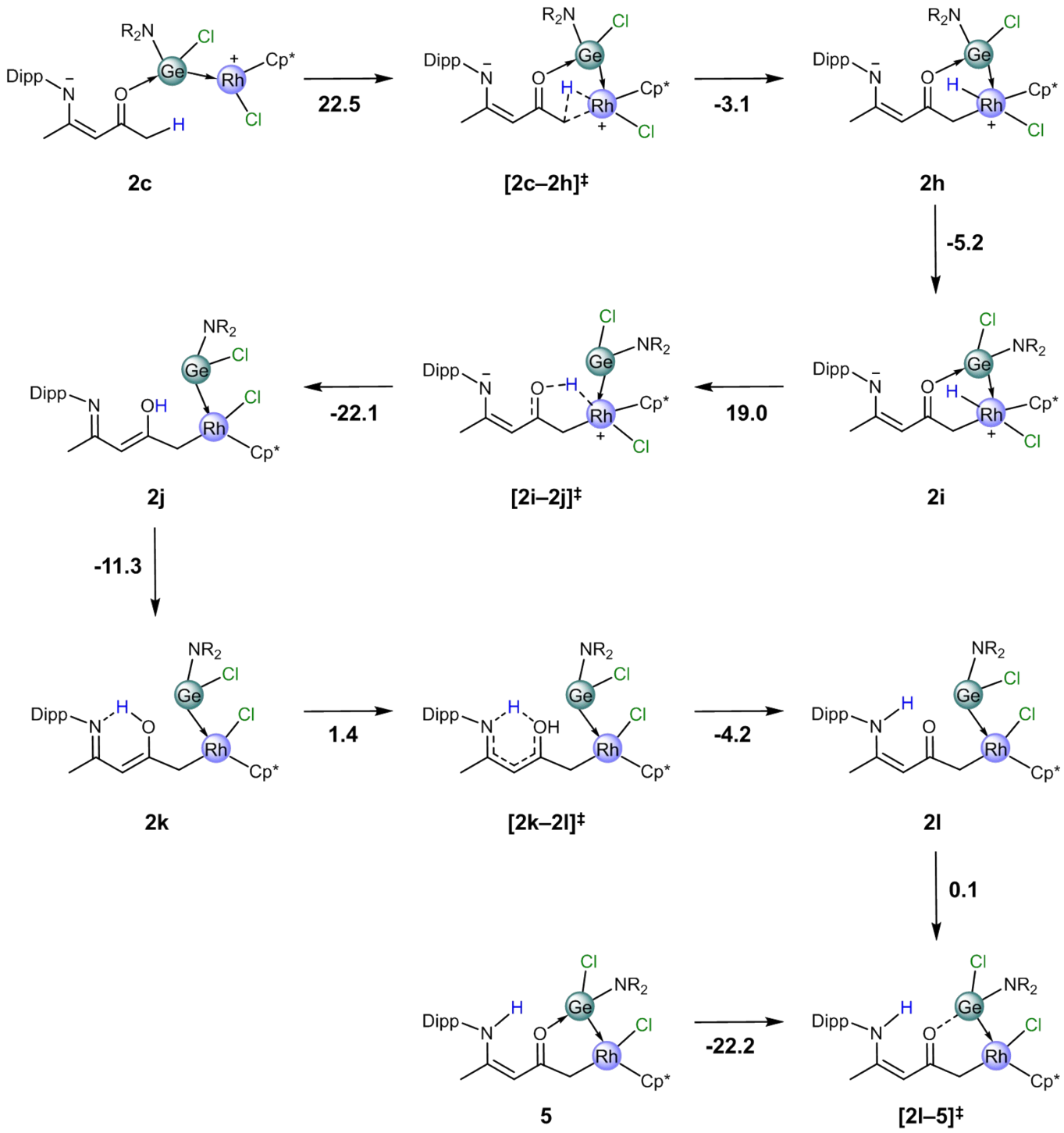
[2cF–2dF]‡

C14–N1=1.371
C16–O1=1.226
∠C14–C15–C16–C17=-88.6
∠O1–C16–C15–C14=92.2

2dF

C14–N1=1.348
C16–O1=1.250
∠C14–C15–C16–C17=-0.0
∠O1–C16–C15–C14=180.0

Fig. S4. Optimized geometries of **2cF**, **2dF** and **[2cF–2dF]‡**with selected geometrical parameters.Bond distances (d) are in angstroms (Å) and bond angles (A) in degrees (°).



Scheme S1. Relative Gibbs free energy (ΔG_L^S in kcal mol^{-1}) for the intermediates and transition states involved in the alternative pathway originating from **2c** (oxidative addition on Rh1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

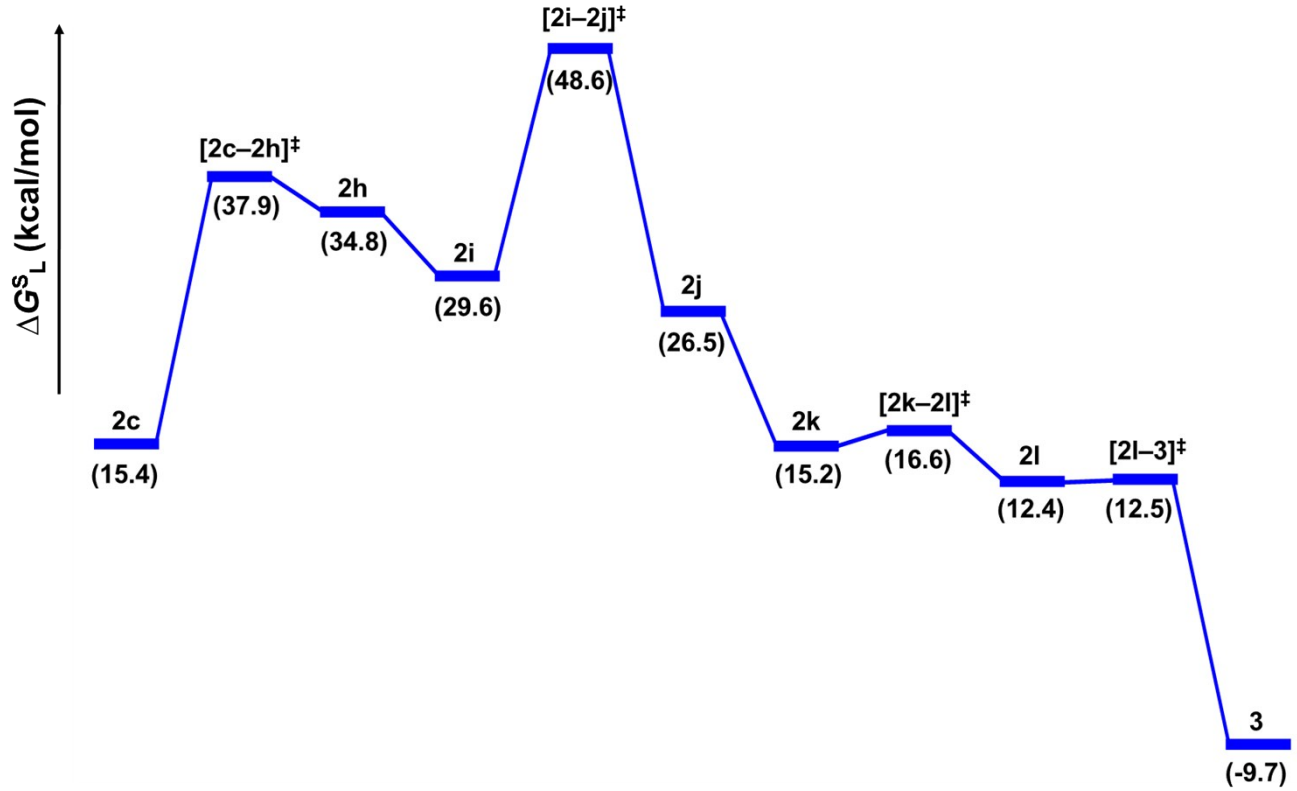
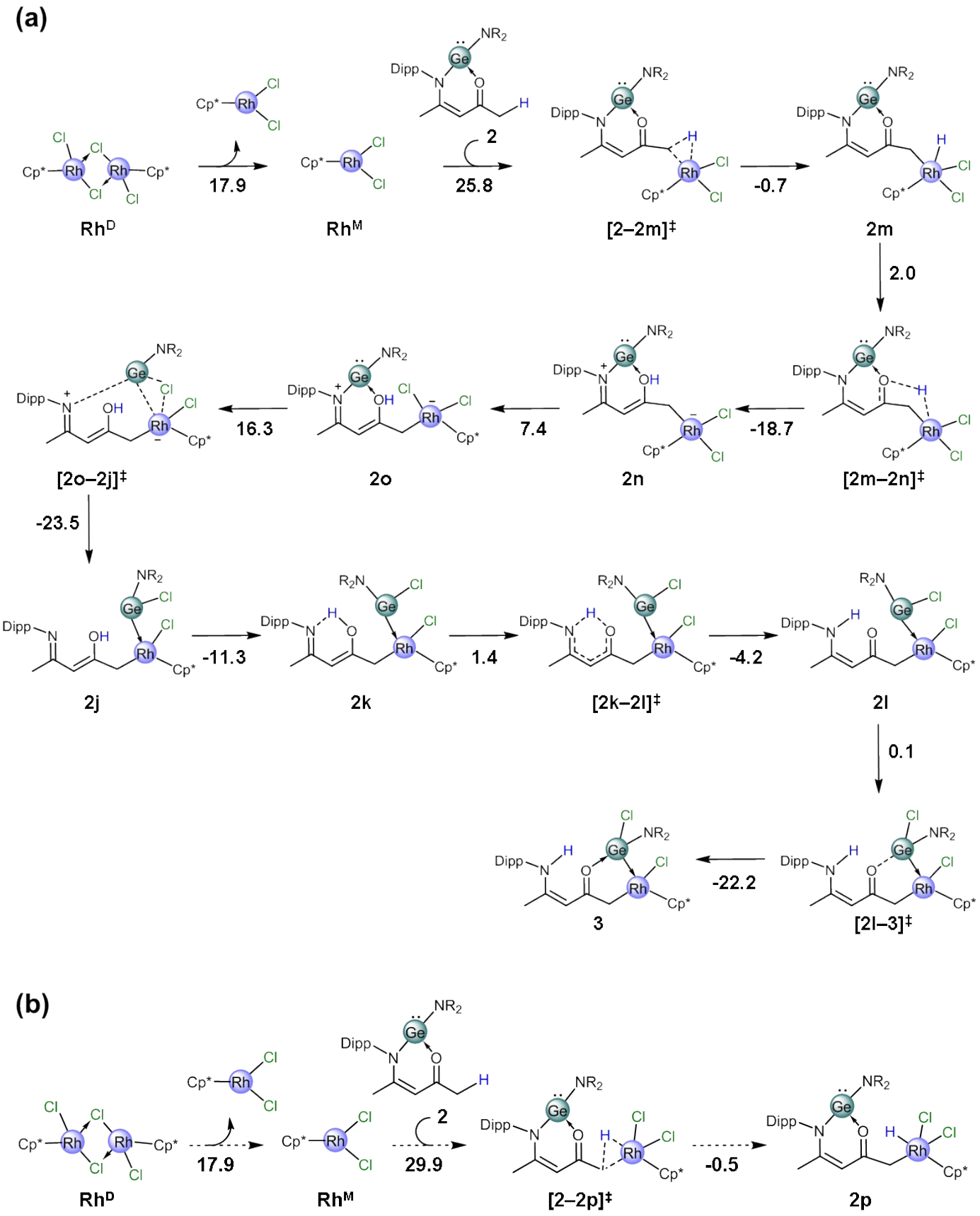


Fig. S5. Energy profile for the alternative pathway originating from **2c** (oxidative addition on Rh1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.



Scheme S2. Relative Gibbs free energy (ΔG_L^S in kcal mol^{-1}) for the intermediates and transition states involved in the unfavorable pathway (a) approach of **Rh^M** toward **2** from the frontside (b) approach of

Rh^{M} toward **2** from the backside (initiated from oxidative addition on Rh1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

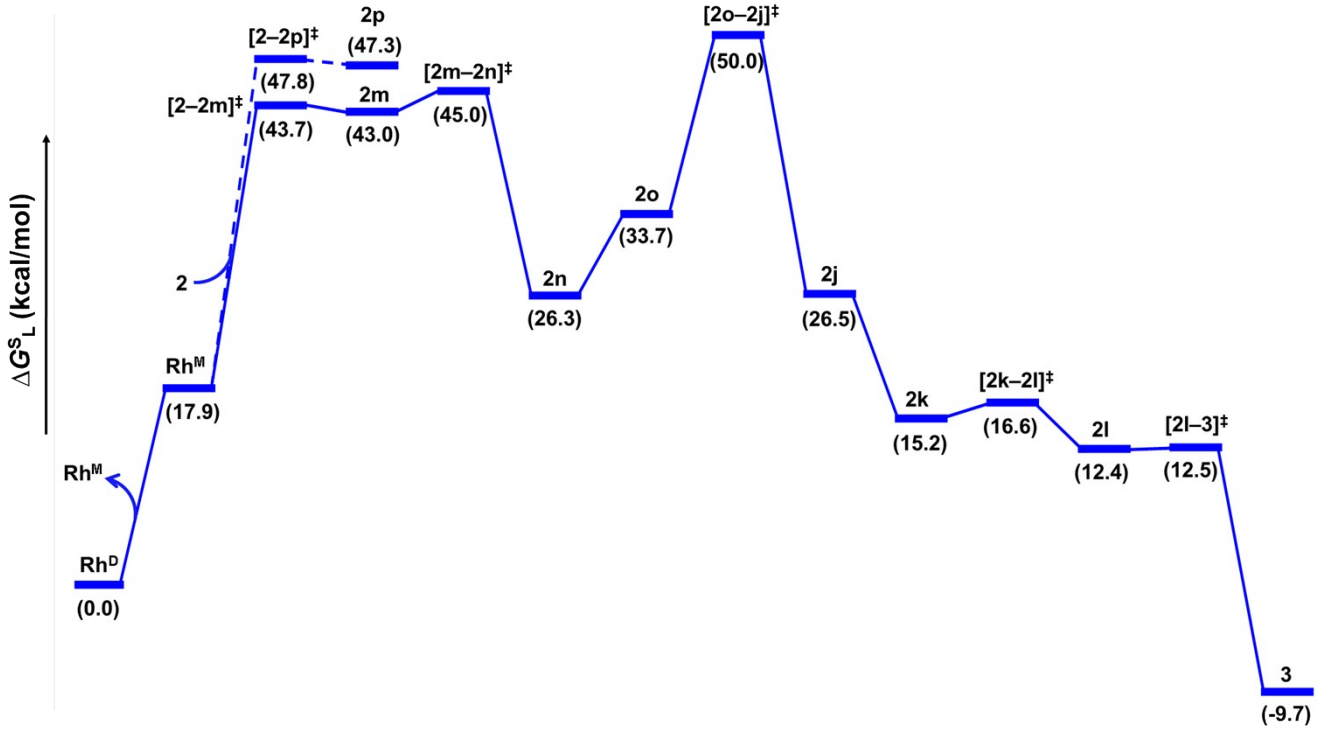
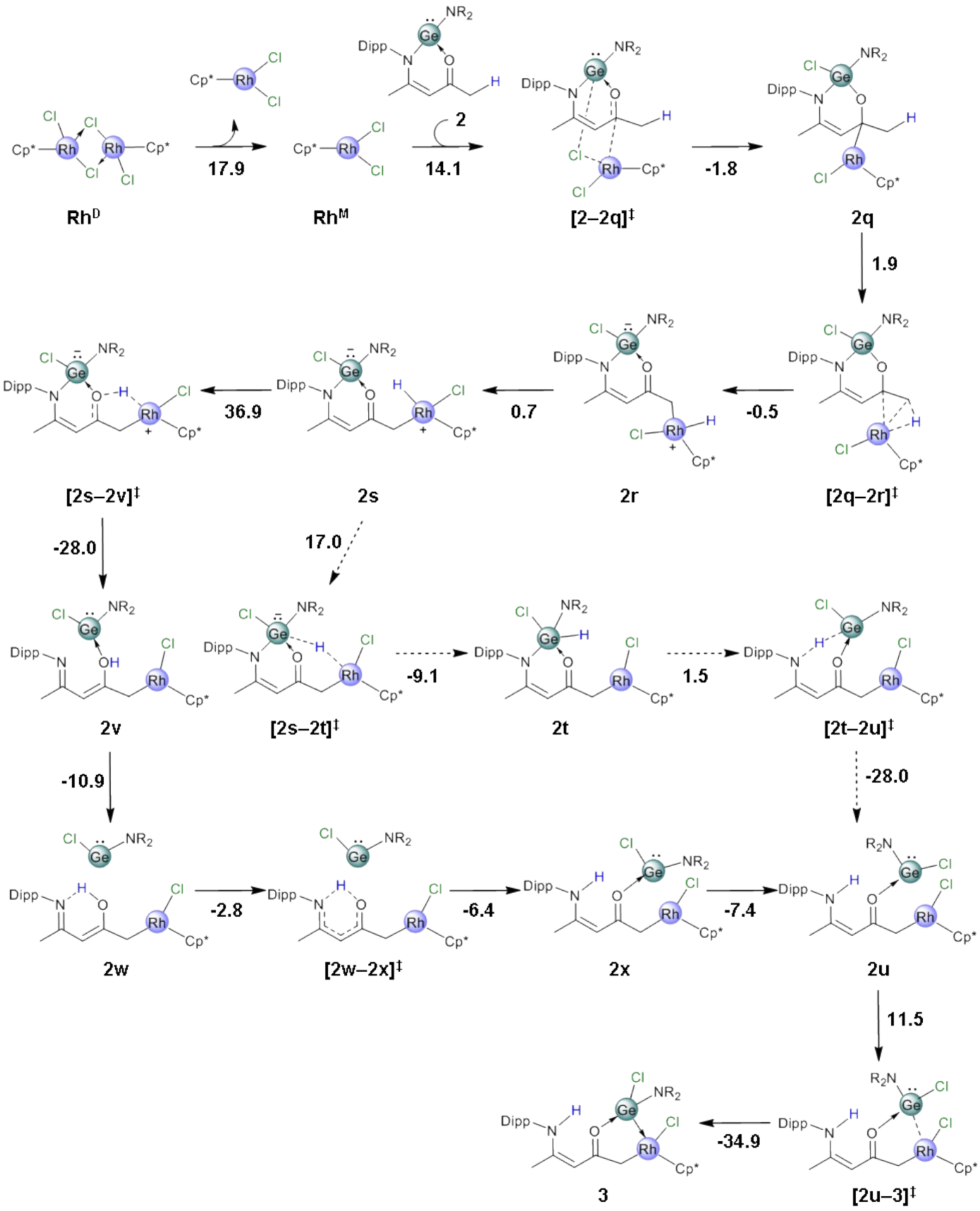


Fig. S6. Energy profile for the unfavorable pathway (initiated from oxidative addition on Rh1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.



Scheme S3. Relative Gibbs free energy (ΔG_L^S in kcal mol^{-1}) for the intermediates and transition states involved in the unfavorable pathway (initiated from chloride ion transfer from Rh1 to Ge1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

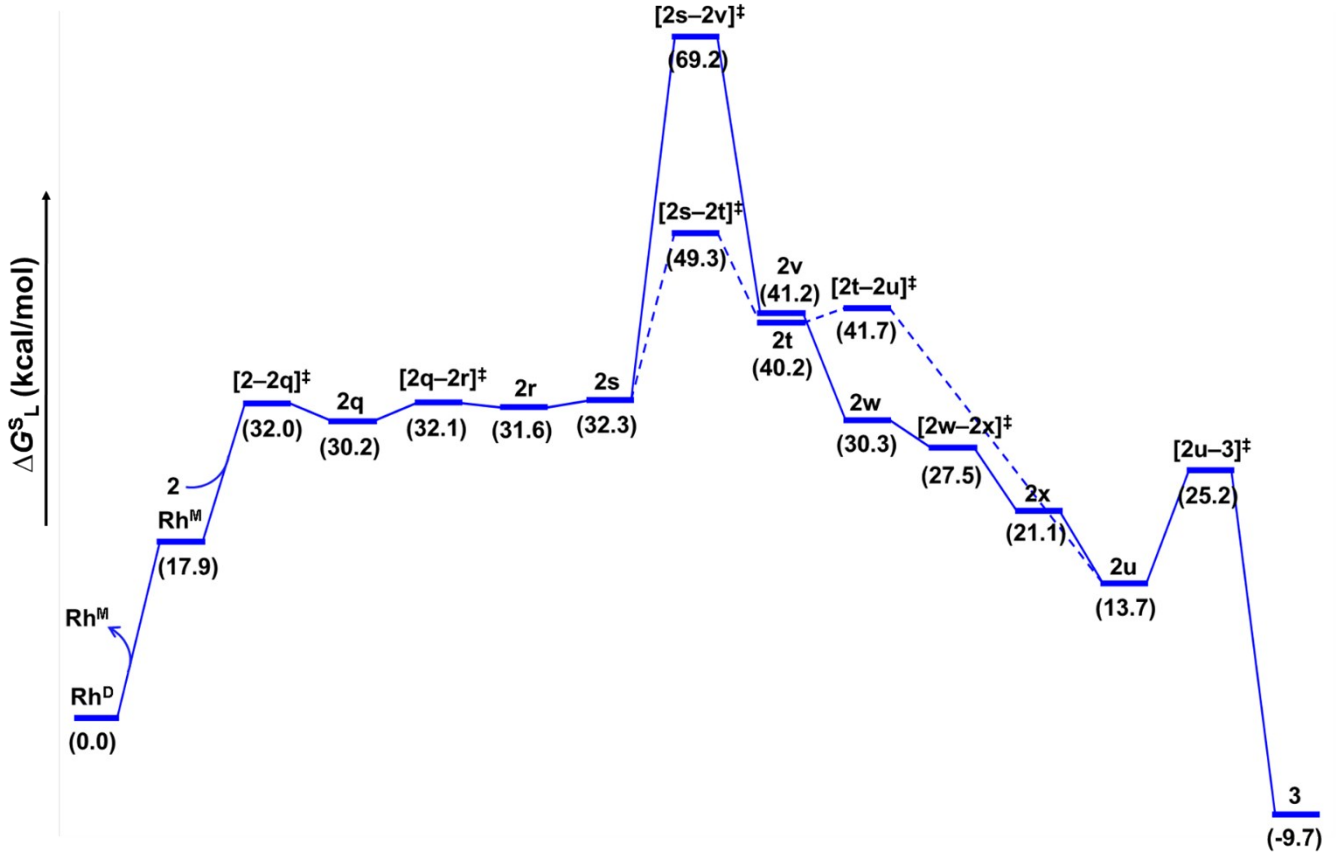
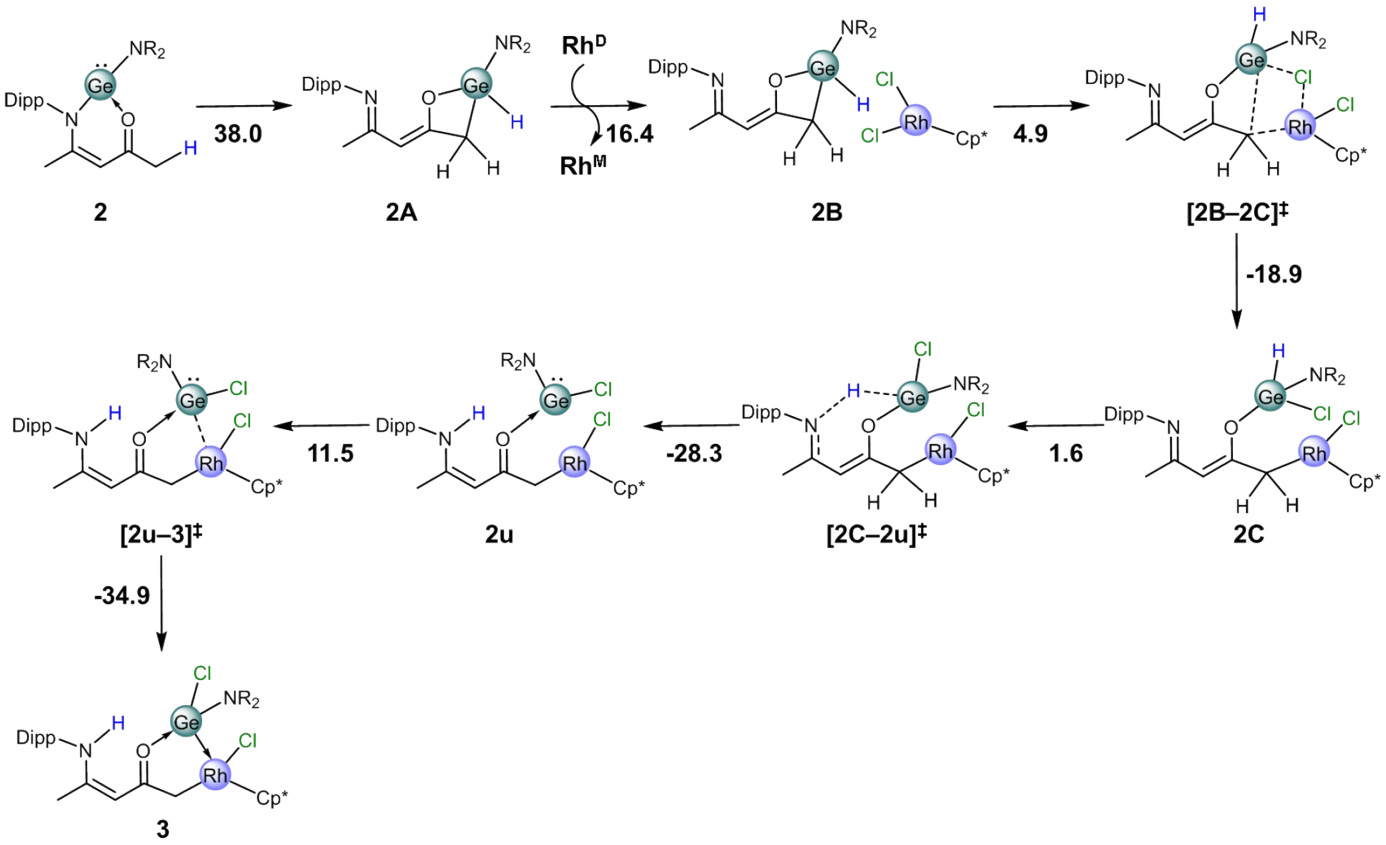


Fig. S7. Energy profile for the unfavorable pathway (initiated from chloride ion transfer from Rh1 to Ge1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.



Scheme S4. Relative Gibbs free energy (ΔG_L^S in kcal mol^{-1}) for the intermediates and transition states involved in the unfavorable pathway (initiated from oxidative addition on Ge1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

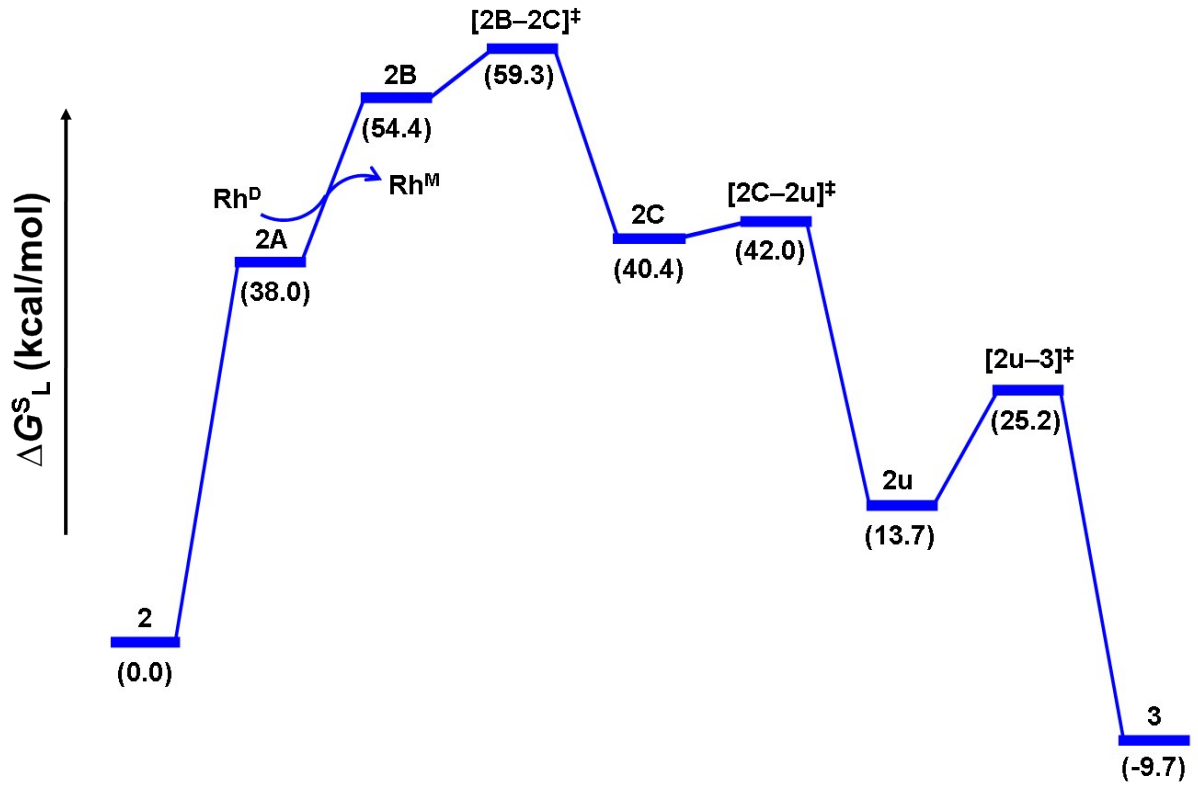
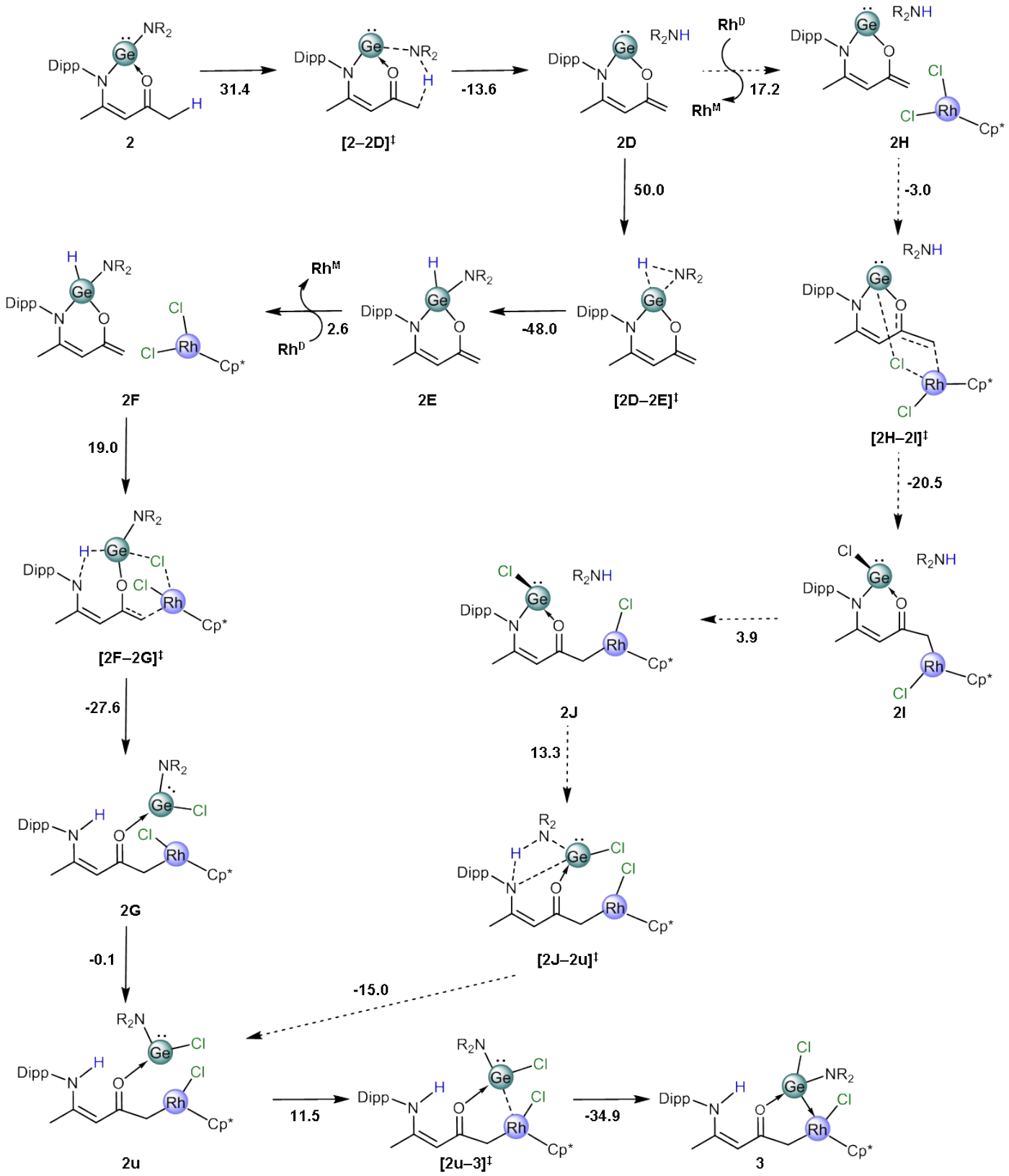


Fig. S8. Energy profile for the unfavorable pathway (initiated from oxidative addition on Ge1 center) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.



Scheme S5. Relative Gibbs free energy (ΔG_L^S in kcal mol^{-1}) for the intermediates and transition states involved in the unfavorable pathway (initiated from Ge1–N2 bond rupture) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

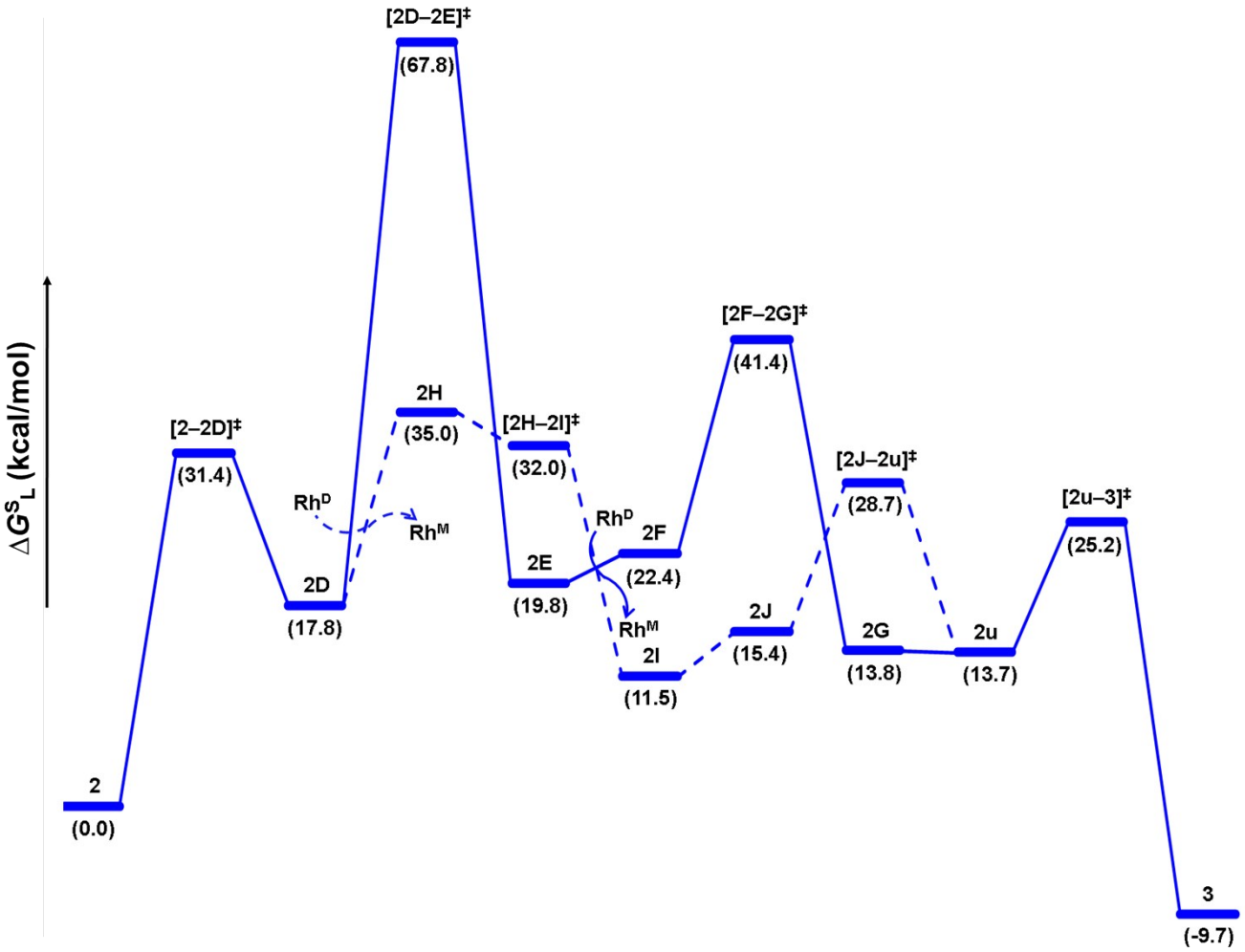


Fig. S9. Energy profile for the unfavorable pathway (initiated from Ge1–N2 bond rupture) for the formation of **3** at BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

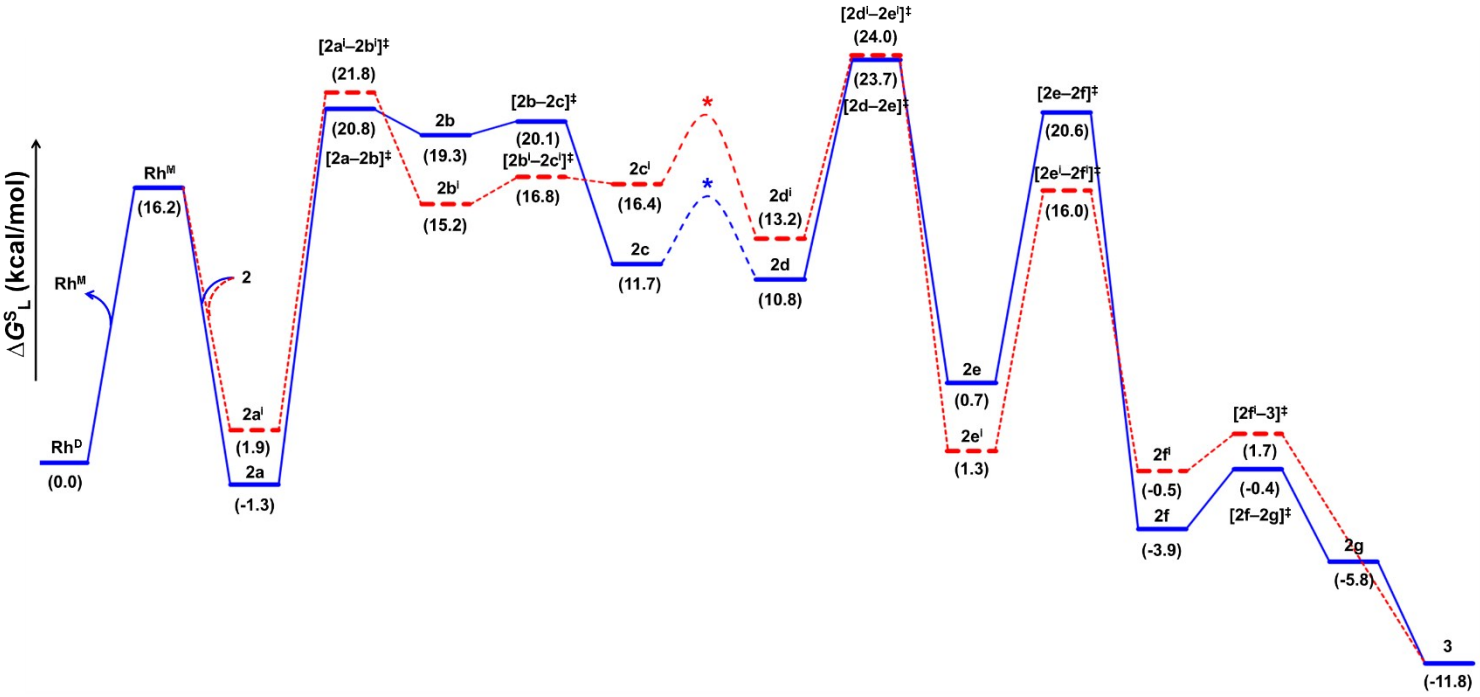


Fig. S10. Energy profile for the formation of **3** at BP86-D3/BS2(CPCM)//M06-L/BS1 level.

Table S3. Energy spans of the unfavorable pathways at BP86-D3/BS2(CPCM)//M06-L/BS1 level and comparison with BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G} level.

Scheme	Figure	Span	Energy span [BP86-D3/BS2(CPCM)//ONIOM{M06-L/BS1:HF/3-21G}]	Energy span [BP86-D3/BS2(CPCM)//M06-L/BS1]
Scheme S1	Fig. S5	**2** + **Rh^{D}** → **[2i–2j]**‡	48.6	47.1
Scheme S2	Fig. S6	**2** + **Rh^{D}** → **[2o–2j]**‡	50.0	48.7
Scheme S3	Fig. S7	**2** + **Rh^{D}** → **[2s–2t]**‡	49.3	47.2
Scheme S4	Fig. S8	**2** + **Rh^{D}** → **[2B–2C]**‡	59.3	59.2
Scheme S5	Fig. S9	**2** + **Rh^{D}** → **[2H–2I]**‡	35.0	33.1

Table S4. Cartesian coordinates (in Å) of the optimized structures of **3** and **4** at M06-L/BS1 level of theory.

3

99
XYZ

Rh	-2.29191	-1.09997	-0.54057
Ge	-0.96935	0.71491	0.31179
Cl	-3.84817	0.57647	-1.50125
O	0.59100	0.48709	-0.84624
N	-1.13695	2.54767	0.32844
C	-0.30492	5.35961	-0.19559
H	-1.34438	5.70549	-0.22118
H	0.09573	5.58151	0.80068
H	0.25485	5.97554	-0.91240
N	3.07885	-0.43138	-0.53807
H	2.32135	0.15256	-0.17828
C	-0.96391	-0.66180	-2.22255
H	-1.05071	-1.45989	-2.96679
H	-1.43713	0.26118	-2.57727
C	2.75392	-1.22098	-1.57475
C	0.37983	-0.46071	-1.73859
C	1.47979	-1.24144	-2.14677
C	3.11449	-2.02785	1.86660
H	2.22970	-1.62243	1.35741
C	5.53297	-1.32607	2.09092
H	5.58016	-1.91088	3.00908
C	4.30569	-0.50210	0.19853
C	5.43441	0.19392	-0.26838
C	-1.64642	-2.88949	0.46253
C	3.83097	-2.09246	-2.13265
H	4.56764	-1.48179	-2.67269
H	4.38434	-2.61404	-1.34316
H	3.42186	-2.82540	-2.83184
C	4.32942	-1.26113	1.38438
C	-2.70835	-2.32332	1.27431
C	2.87573	-1.86919	3.36481
H	3.66161	-2.35265	3.96020
H	2.82633	-0.81378	3.65452
H	1.92189	-2.33351	3.64512
C	-5.21543	-1.73809	0.85874
H	-5.17512	-1.19275	1.80749
H	-5.58417	-1.04354	0.09231
H	-5.95506	-2.54437	0.96561
C	5.39217	1.07691	-1.49818
H	4.43162	0.91208	-2.00634
C	-4.58017	-3.03734	-1.91137
H	-5.11730	-2.09413	-2.07506
H	-4.09899	-3.31019	-2.85678
H	-5.32697	-3.81113	-1.68220
C	-0.27046	-3.20556	0.93223
H	0.45638	-3.16699	0.10970
H	0.06107	-2.49029	1.69542
H	-0.21804	-4.21434	1.37046
C	-3.59260	-2.89270	-0.81042
C	-1.49511	-3.99840	-1.88545
H	-1.95951	-3.83546	-2.86433
H	-0.45288	-3.65878	-1.94674
H	-1.47190	-5.08286	-1.70812
C	3.23246	-3.50666	1.49235
H	3.29152	-3.65298	0.40558
H	4.13168	-3.95447	1.93684
H	2.36368	-4.06986	1.85591
C	-1.98366	4.32351	2.58944
H	-1.13836	3.89455	3.14311
H	-1.67862	5.31165	2.22819
H	-2.79976	4.48116	3.30730
C	6.66715	-0.65887	1.64155
H	7.59550	-0.72159	2.20722
C	6.61351	0.09606	0.47615
H	7.50113	0.63129	0.13868
C	-3.88574	-2.28085	0.47778
C	1.75485	3.16229	-0.33296
H	1.90479	2.68729	0.64646
H	2.16966	2.49169	-1.09490
H	2.35021	4.08524	-0.34220
C	-2.23018	-3.30023	-0.79825
C	-2.58178	-1.91959	2.69971
H	-1.59296	-1.50089	2.92149
H	-3.32861	-1.16790	2.97645
H	-2.72768	-2.78960	3.35682
C	-3.37948	1.69343	2.04662
H	-3.80002	0.99433	1.31072
H	-2.69968	1.14070	2.71112
H	-4.20910	2.05275	2.67073
C	-3.76187	4.00242	0.07735
H	-3.32987	4.84638	-0.47407
H	-4.13427	3.27914	-0.65879

H	-4.62379	4.38884	0.63737
C	5.44793	2.55001	-1.08991
H	4.64740	2.80332	-0.38570
H	6.40582	2.78375	-0.60616
H	5.34724	3.20250	-1.96634
C	-0.46859	3.31302	-2.46806
H	-0.22486	2.29661	-2.80343
H	-1.53907	3.46515	-2.65676
H	0.08919	4.00926	-3.10843
Cl	0.32081	0.33798	2.18291
C	6.51169	0.75143	-2.48501
H	7.49870	0.97972	-2.06253
H	6.51766	-0.30851	-2.76963
H	6.40521	1.34729	-3.39941
Si	-2.53730	3.16011	1.21832
Si	-0.06768	3.54794	-0.64906
H	1.32347	-1.93015	-2.97309

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99
XYZ

Ge	-0.77762	0.82354	0.36680
Cl	-3.63103	0.77745	-1.47084
O	0.77180	0.50426	-0.79193
N	-0.86500	2.66080	0.33652
C	0.10182	5.42181	-0.23722
H	-0.91949	5.81735	-0.27228
H	0.51116	5.64455	0.75537
H	0.69195	5.99526	-0.96489
N	3.23787	-0.47155	-0.53402
H	2.50018	0.13275	-0.16672
C	-0.84640	-0.59886	-2.14366
H	-0.93560	-1.39986	-2.88684
H	-1.24332	0.33590	-2.56331
C	2.87701	-1.25146	-1.56528
C	0.52260	-0.42982	-1.68262
C	1.59369	-1.23317	-2.11779
C	3.20665	-2.03283	1.88611
H	2.33585	-1.57560	1.39596
C	5.65121	-1.42024	2.11093
H	5.67342	-1.98844	3.04023
C	4.46282	-0.58251	0.20026
C	5.61924	0.05796	-0.27710
C	-1.61234	-2.75060	0.57651
C	3.91868	-2.15616	-2.13698
H	4.65426	-1.57080	-2.70562
H	4.47975	-2.67937	-1.35408
H	3.47452	-2.88898	-2.81462
C	4.45290	-1.32022	1.39990
C	-2.66093	-2.11778	1.36644
C	2.99275	-1.89307	3.38959
H	3.75397	-2.43478	3.96651
H	3.00786	-0.84328	3.70282
H	2.01623	-2.30731	3.66982
C	-5.13897	-1.42461	0.92063
H	-5.06885	-0.83835	1.84298
H	-5.49227	-0.75150	0.12899
H	-5.90282	-2.20018	1.07272
C	5.61522	0.91980	-1.52252
H	4.64812	0.78821	-2.02800
C	-4.53561	-2.80285	-1.83355
H	-5.05782	-1.85267	-2.00153
H	-4.05031	-3.07958	-2.77580
H	-5.29254	-3.56825	-1.61027
C	-0.26358	-3.13842	1.07230
H	0.46842	-3.17127	0.25464
H	0.10769	-2.41631	1.81066
H	-0.27775	-4.13173	1.54660
C	-3.55236	-2.67235	-0.72621
C	-1.49411	-3.89052	-1.76236
H	-1.93542	-3.70685	-2.74813
H	-0.43457	-3.60841	-1.81154
H	-1.53654	-4.97250	-1.57635
C	3.24816	-3.50818	1.48196
H	3.27890	-3.63536	0.39154
H	4.13460	-4.00476	1.89947
H	2.36158	-4.03784	1.85264
C	-1.63451	4.52623	2.55428
H	-0.81694	4.06681	3.12496
H	-1.27574	5.48880	2.17406
H	-2.44686	4.74190	3.26123
C	6.81261	-0.80850	1.65150
H	7.73648	-0.89821	2.22086
C	6.79236	-0.07484	0.47174
H	7.70185	0.41688	0.12637
C	-3.83050	-2.02779	0.55392
C	2.05580	3.12884	-0.32856
H	2.18218	2.64653	0.65058
H	2.44568	2.44333	-1.09059
H	2.68917	4.02613	-0.33364

C	-2.20397	-3.14488	-0.68985	H	6.70213	2.59699	-0.66084
C	-2.53002	-1.69354	2.78555	H	5.66307	3.03633	-2.02945
H	-1.52102	-1.32926	3.01154	C	-0.15457	3.34363	-2.47023
H	-3.23393	-0.89265	3.03543	H	0.03927	2.31039	-2.78619
H	-2.73662	-2.54074	3.45552	H	-1.21572	3.54472	-2.66553
C	-3.15777	1.95978	2.06098	H	0.43857	3.99968	-3.12125
H	-3.60780	1.26487	1.33931	Cl	0.48396	0.43008	2.24306
H	-2.51151	1.38868	2.74306	C	6.71956	0.52765	-2.50223
H	-3.97094	2.37732	2.67028	H	7.71531	0.72142	-2.08309
C	-3.41265	4.23651	0.03783	H	6.68029	-0.53687	-2.76630
H	-2.94191	5.05436	-0.52109	H	6.63906	1.11002	-3.42793
H	-3.80682	3.51800	-0.69156	Si	-2.23656	3.36103	1.20543
H	-4.26413	4.66530	0.58278	Si	0.25255	3.59208	-0.65417
C	5.73513	2.39620	-1.14118	H	1.40195	-1.91841	-2.93943
H	4.94634	2.69643	-0.44220	Ir	-2.17281	-0.95979	-0.45521

Table S5. Cartesian coordinates (in Å) of the optimized structures of catalyst, reactant, intermediates, transition states and product in the favorable pathway for formation of **3** at ONIOM{M06-L/BS1:HF/3-21G} level of theory.

Rh^{D}

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XYZ

Rh	1.85011	-0.20854	0.00001
C	3.49947	0.35843	1.16609
C	3.95817	-0.35354	0.00000
C	3.70608	-0.05450	-2.61290
H	3.81351	-1.12676	-2.68852
H	2.85355	0.23587	-3.20939
H	4.59803	0.42054	-3.00702
C	2.17596	2.63470	-1.57220
H	2.09783	2.31231	-2.59865
H	1.18098	2.86411	-1.21663
H	2.79320	3.52614	-1.52695
C	3.70606	-0.05440	2.61290
H	2.85354	0.23604	3.20937
H	3.81344	-1.12666	2.68856
H	4.59804	0.42061	3.00699
C	2.81404	1.55595	-0.71324
C	2.17596	2.63477	1.57207
H	1.18098	2.86417	1.21650
H	2.09783	2.31243	2.59854
H	2.79320	3.52621	1.52679
C	3.49948	0.35838	-1.16611
C	2.81404	1.55599	0.71317
C	4.77076	-1.63565	0.00003
H	4.54833	-2.23232	0.87057
H	4.54826	-2.23241	-0.87043
H	5.82446	-1.37582	-0.00002
Rh	-1.85011	0.20854	-0.00001
C	-3.49950	-0.35834	1.16610
C	-3.95817	0.35354	-0.00005
C	-3.70602	0.05430	-2.61293
H	-3.81354	1.12655	-2.68862
H	-2.85343	-0.23603	-3.20935
H	-4.59791	-0.42084	-3.00706
C	-2.17593	-2.63482	-1.57200
H	-2.09783	-2.31252	-2.59849
H	-1.18093	-2.86416	-1.21644
H	-2.79314	-3.52628	-1.52666
C	-3.70612	0.05459	2.61286
H	-2.85366	-0.23588	3.20940
H	-3.81341	1.12687	2.68845
H	-4.59816	-0.42032	3.00695
C	-2.81403	-1.55601	-0.71313
C	-2.17598	-2.63466	1.57227
H	-1.18102	-2.86412	1.21670
H	-2.09782	-2.31222	2.59871
H	-2.79326	-3.52608	1.52708
C	-3.49945	-0.35847	-1.16611
C	-2.81405	-1.55594	0.71327
C	-4.77076	1.63565	-0.00014
H	-4.54842	2.23235	0.87040
H	-4.54818	2.23238	-0.87060
H	-5.82446	1.37582	-0.00029
Cl	0.00003	0.00003	1.75181
Cl	-0.00003	-0.00002	-1.75182
Cl	1.46795	-2.63904	0.00003
Cl	-1.46795	2.63904	-0.00000

Rh^{M}

28
XYZ

Rh	0.00217	-0.44803	0.01937
C	-0.73342	1.28056	0.96693
C	0.72625	1.28731	0.96529
C	2.62373	1.31397	-0.84313
H	3.13737	0.43277	-0.48291
H	2.68375	1.32664	-1.92150
H	3.11369	2.20307	-0.46464
C	-0.00843	1.07912	-2.73473
H	0.86629	0.53382	-3.05987
H	-0.88237	0.53126	-3.05759
H	-0.01030	2.05718	-3.20353
C	-1.61532	1.24264	2.20039
H	-2.58697	0.83946	1.95616
H	-1.17694	0.61879	2.96721
H	-1.73279	2.24748	2.59194
C	-0.00682	1.23292	-1.22524
C	-2.63649	1.29458	-0.83632
H	-2.69938	1.33230	-1.91398

H	-3.13567	0.39737	-0.49557
H	-3.13890	2.16685	-0.43586
C	1.17248	1.30650	-0.38869
C	-1.18384	1.29851	-0.38591
C	1.61102	1.25921	2.19697
H	1.17893	0.63425	2.96643
H	2.58518	0.86267	1.95201
H	1.72169	2.26602	2.58541
Cl	-1.70771	-2.07920	0.07641
Cl	1.72543	-2.06375	0.09921

2

71
XYZ

Ge	0.37314	0.47616	-1.31757
O	1.11597	2.28082	-0.94145
N	1.71375	-0.49468	-0.29064
C	4.11944	-0.88485	1.55240
H	3.58010	-1.43668	2.31567
H	4.61919	-1.59933	0.90809
H	4.89159	-0.30415	2.05293
N	-1.14963	0.90666	0.14187
C	1.33245	4.56380	-0.45683
H	0.80655	5.41374	-0.01315
H	1.57667	4.79451	-1.49988
C	-1.47118	2.12305	0.55256
C	0.54219	3.29635	-0.38100
C	-0.67463	3.26622	0.27815
C	-2.69717	2.38265	1.37983
H	-3.39288	1.54425	1.38840
H	-2.40526	2.59122	2.41631
H	-3.21306	3.27736	1.01362
C	3.60602	-2.14100	-2.00337
H	3.54143	-1.43165	-2.82479
H	4.49233	-1.89822	-1.42681
H	3.74973	-3.13065	-2.43009
C	4.11096	1.36664	-0.51436
H	3.53282	2.08665	-1.07781
H	4.85450	1.89909	0.07513
H	4.64224	0.72932	-1.21577
C	0.59123	-2.65473	-2.13212
H	-0.38473	-2.59304	-1.65909
H	0.55454	-2.09397	-3.05910
H	0.76475	-3.69929	-2.38402
C	2.09003	-3.49180	0.34222
H	2.81686	-3.31658	1.12478
H	1.11976	-3.63728	0.80704
H	2.35772	-4.42129	-0.15626
C	2.27508	1.45016	2.01415
H	1.42355	2.04321	1.71213
H	1.97808	0.84352	2.86390
H	3.05265	2.13038	2.35631
Si	2.00086	-2.09778	-0.96226
Si	2.97042	0.33365	0.62315
H	-1.03479	4.20780	0.68455
C	-2.01621	-0.23928	0.40677
C	-1.88431	-0.96056	1.59854
C	-2.93249	-0.63760	-0.57701
C	-2.64850	-2.10647	1.76741
C	-3.67613	-1.78932	-0.36134
C	-3.52987	-2.52654	0.79441
H	-2.55406	-2.67204	2.67208
H	-4.38062	-2.10707	-1.10261
H	-4.10869	-3.41693	0.94102
H	2.28805	4.42855	0.06519
C	-3.19393	0.18194	-1.84097
C	-4.59539	0.83171	-1.77012
C	-3.06748	-0.66737	-3.12308
H	-2.46066	0.96952	-1.89886
H	-4.69444	1.45513	-0.88946
H	-4.76480	1.44866	-2.64647
H	-5.36669	0.07116	-1.73548
H	-2.08983	-1.12603	-3.18318
H	-3.82062	-1.44559	-3.15548
H	-3.20265	-0.03522	-3.99437
C	-0.96663	-0.51268	2.73271
C	0.13249	-1.55783	3.00908
C	-1.77821	-0.24047	4.02037
H	-0.48025	0.40145	2.43498
H	0.75323	-1.67903	2.13490
H	0.75662	-1.23239	3.83536
H	-0.29885	-2.51679	3.27157
H	-2.57705	0.46927	3.84208
H	-2.21807	-1.15503	4.40004
H	-1.12630	0.16189	4.78877

3

99
XYZ

Rh	-2.31206	-1.17343	-

0.53895

Ge	-1.05022	0.70379	0.33779
Cl	-3.81880	0.52582	-1.57694
O	0.60816	0.43171	-0.71412
N	-1.30660	2.54457	0.27231
C	-0.89930	5.38515	-0.72637
H	-1.81770	5.48002	-1.29532
H	-1.06146	5.80708	0.25790
H	-0.14509	5.99382	-1.22055
N	3.16571	-0.47488	-0.48542
H	2.43670	0.13247	-0.11324
C	-0.90946	-0.68321	-2.16078
H	-0.97501	-1.45869	-2.92773
H	-1.37200	0.24879	-2.50031
C	2.79178	-1.29778	-1.48615
C	0.41255	-0.50086	-1.62223
C	1.50578	-1.30842	-2.01663
C	3.62653	-2.14041	1.87051
H	2.73768	-2.05819	1.26455
C	5.97615	-1.23925	1.82939
H	6.17794	-1.84657	2.68799
C	4.47939	-0.46103	0.13653
C	5.47091	0.37638	-0.38081
C	-1.69168	-2.96247	0.45600
C	3.81758	-2.23638	-2.03000
H	4.68302	-1.69603	-2.42470
H	4.20428	-2.89906	-1.24950
H	3.39563	-2.84750	-2.83091
C	4.71441	-1.26641	1.25347
C	-2.77551	-2.40922	1.24030
C	3.27296	-1.63803	3.28819
H	4.13640	-1.69104	3.94105
H	2.91816	-0.61673	3.25521
H	2.48605	-2.25211	3.71301
C	-5.30862	-1.83159	0.76814
H	-5.29115	-1.30315	1.71035
H	-5.66153	-1.15124	0.00539
H	-5.99938	-2.66419	0.85281
C	5.21333	1.31564	-1.55576
H	4.20816	1.14926	-1.91224
C	-4.57289	-3.08363	-2.02717
H	-5.05263	-2.13423	-2.22340
H	-4.06713	-3.40007	-2.92872
H	-5.32985	-3.82168	-1.78256
C	-0.31165	-3.32885	0.98743
H	0.42444	-3.29914	0.19576
H	-0.00364	-2.63579	1.75741
H	-0.33064	-4.33035	1.40621
C	-3.59195	-2.94420	-0.87384
C	-1.46719	-4.08816	-1.91381
H	-1.88319	-3.88445	-2.89041
H	-0.42656	-3.79698	-1.91565
H	-1.52454	-5.15655	-1.73220
C	4.04985	-3.62530	1.91382
H	4.30760	-3.99091	0.92625
H	4.90672	-3.76701	2.56128
H	3.23559	-4.22958	2.29933
C	-1.84077	4.21038	2.72735
H	-1.12394	3.62497	3.29643
H	-1.32960	5.09098	2.35437
H	-2.62005	4.54407	3.40845
C	6.97184	-0.43413	1.31709
H	7.94135	-0.42532	1.77468
C	6.71868	0.36967	0.22526
H	7.49386	1.00368	-0.15413
C	-3.92415	-2.34997	0.40960
C	1.49864	3.57916	-0.00777
H	1.49637	3.87741	1.03652
H	1.93273	2.58902	-0.07244
H	2.13354	4.26853	-0.55877
C	-2.23451	-3.35223	-0.82615
C	-2.69723	-2.05870	2.71976
H	-1.73890	-1.63105	2.97374
H	-3.46605	-1.35154	2.99261
H	-2.83991	-2.96429	3.30180
C	-3.42664	1.65160	2.21005
H	-3.85656	0.95251	1.50196
H	-2.75641	1.12365	2.88011
H	-4.24192	2.04414	2.81437
C	-3.95630	4.06250	0.39674
H	-3.64452	5.03666	0.04009
H	-4.28057	3.46766	-0.45129
H	-4.81266	4.20958	1.05103
C	5.31561	2.78683	-1.09388
H	4.62460	2.98546	-0.28498
H	6.31912	3.01226	-0.75256
H	5.07908	3.45205	-1.91759
C	-0.24997	3.03045	-2.53887
H	0.38487	2.16795	-2.69718
H	-1.25332	2.78860	-2.87798

H	0.12656	3.84018	-3.15924
Cl	0.13329	0.43464	2.26631
C	6.19241	1.05487	-2.72163
H	7.21348	1.26309	-2.42574
H	6.14070	0.02583	-3.05755
H	5.94774	1.69859	-3.55953
Si	-2.58740	3.13150	1.33837
Si	-0.27757	3.57905	-0.70908
H	1.32436	-2.00337	-2.83197

2a

99

XYZ

Rh	2.28333	-0.39664	0.09366
Ge	-0.14687	0.36778	0.25410
Cl	1.64806	-2.64362	0.95065
O	-0.48882	1.17986	1.95789
N	-0.90172	1.88121	-0.64145
C	-0.60397	2.82217	-3.60283
H	-0.56287	3.89134	-3.44577
H	0.41225	2.46156	-3.71048
H	-1.10752	2.65223	-4.55269
N	-1.50036	-1.05734	0.80995
C	0.00837	1.19036	4.27065
H	0.29213	0.51646	5.08301
H	-0.87583	1.76244	4.58250
C	-1.22744	-1.59762	2.01042
C	-0.29285	0.44111	3.02087
C	-0.49481	-0.92509	3.00793
C	2.79493	-0.23300	-2.00488
C	-1.74060	-2.95199	2.38519
H	-1.92419	-3.01777	3.46109
H	-2.64347	-3.23489	1.84610
H	-0.95594	-3.68085	2.14315
C	3.15737	0.98612	-1.32373
C	4.86893	1.64699	0.55396
H	4.20794	2.42806	0.89693
H	5.27381	1.15524	1.42307
H	5.67750	2.08492	-0.02370
C	5.29715	-1.53518	0.55297
H	5.14713	-1.21778	1.57561
H	5.08658	-2.59290	0.50217
H	6.33033	-1.36686	0.26760
C	1.97344	-0.31478	-3.27998
H	1.48256	-1.27182	-3.37079
H	1.22531	0.46017	-3.30712
H	2.63285	-0.18448	-4.13288
C	4.36627	-0.76591	-0.36957
C	3.52385	-2.75643	-1.86722
H	3.61447	-3.41734	-1.02011
H	2.59699	-2.98866	-2.36918
H	4.34865	-2.92291	-2.55287
C	0.93543	3.59768	1.16647
H	1.55921	2.71580	1.11915
H	1.49759	4.43886	0.76950
H	0.74881	3.78564	2.21826
C	4.13475	0.65381	-0.33124
C	-1.82537	0.13751	-2.95152
H	-2.58825	-0.42037	-2.42760
H	-2.13167	0.21662	-3.99243
H	-0.91326	-0.44433	-2.93242
C	3.54642	-1.30512	-1.41907
C	2.73397	2.39020	-1.73077
H	1.66066	2.49203	-1.73429
H	3.14054	3.12010	-1.04695
H	3.11193	2.60430	-2.72518
C	-2.17963	3.75528	1.44095
H	-3.13631	3.75665	0.92798
H	-2.20532	3.00422	2.21827
H	-2.05323	4.73008	1.90753
C	-0.75211	4.92547	-0.95685
H	0.13001	4.95599	-1.58781
H	-1.62784	4.99781	-1.59009
H	-0.73079	5.81675	-0.33248
C	-3.34492	2.69368	-2.26342
H	-3.43731	3.51629	-1.56397
H	-3.57982	3.07250	-3.25507
H	-4.09474	1.95320	-2.00763
Cl	2.62984	0.26850	2.47016
Si	-0.73427	3.42629	0.23858
Si	-1.60863	1.89195	-2.25679
H	-0.23875	-1.48698	3.90070
C	-2.64695	-1.53584	0.03197
C	-2.54948	-2.62473	-0.83834
C	-3.86372	-0.85035	0.19696
C	-3.66663	-2.96940	-1.59167
C	-4.94833	-1.23160	-0.57576
C	-4.84852	-2.27580	-1.47559
H	-3.60431	-3.79571	-2.27012
H	-5.88096	-0.71880	-0.47195

H	-5.69691	-2.55424	-2.06923
H	0.82169	1.89963	4.09232
C	-4.02067	0.23815	1.26040
C	-4.36573	-0.41801	2.62028
C	-5.11798	1.27240	0.93758
H	-3.07986	0.75589	1.35217
H	-3.58987	-1.09366	2.94679
H	-4.48893	0.34536	3.38168
H	-5.29349	-0.97290	2.53582
H	-4.98959	1.70101	-0.04560
H	-6.10647	0.83191	1.00006
H	-5.07100	2.07448	1.66498
C	-1.29465	-3.48492	-0.96204
C	-0.70074	-3.45094	-2.38558
C	-1.59841	-4.95632	-0.58886
H	-0.54394	-3.11287	-0.28769
H	-0.40466	-2.44944	-2.65762
H	0.17587	-4.08885	-2.42400
H	-1.41420	-3.80675	-3.11991
H	-2.08573	-5.03290	0.37373
H	-2.24013	-5.41947	-1.32989
H	-0.67042	-5.51586	-0.54611

[2a–2b]‡

99
XYZ

Rh	2.31992	-0.73582	0.14996
Ge	0.11131	0.67849	0.37122
Cl	1.34689	-2.22864	1.85408
O	-0.66188	1.16555	1.99591
N	-0.28274	2.30606	-0.50839
C	0.22408	2.96841	-3.44506
H	0.44116	4.01187	-3.24301
H	1.17172	2.44214	-3.49840
H	-0.24103	2.91351	-4.42663
N	-2.12669	-0.91256	0.78239
C	-0.04483	0.92160	4.27707
H	-0.22659	0.29816	5.15730
H	-0.40166	1.93931	4.47438
C	-2.10648	-1.40727	2.00127
C	-0.69459	0.36531	3.05852
C	-1.32236	-0.84282	3.05961
C	2.88640	-1.13601	-1.89744
C	-2.91842	-2.59877	2.44080
H	-3.35661	-2.43051	3.43058
H	-3.70693	-2.87453	1.74269
H	-2.23388	-3.45093	2.54702
C	3.68337	-0.06805	-1.36617
C	5.42988	0.17242	0.60405
H	5.25730	1.23406	0.53047
H	5.33407	-0.10452	1.64374
H	6.43542	-0.05113	0.26315
C	4.63747	-2.93240	0.95769
H	5.31428	-2.42691	1.63081
H	3.82759	-3.35488	1.53553
H	5.17878	-3.72665	0.45472
C	2.09177	-1.09849	-3.19016
H	1.25232	-1.77543	-3.15639
H	1.72741	-0.10564	-3.40277
H	2.74920	-1.40455	-3.99808
C	4.09154	-1.96721	-0.07910
C	2.49948	-3.68164	-1.25228
H	2.22762	-4.09975	-0.29395
H	1.61606	-3.64701	-1.86902
H	3.23457	-4.31999	-1.73185
C	2.00843	4.32521	-0.31900
H	2.70533	3.67236	0.19045
H	2.18459	4.25888	-1.38862
H	2.21882	5.34731	-0.01162
C	4.43766	-0.59815	-0.25016
C	-1.24780	0.38377	-2.59135
H	-2.07342	-0.02695	-2.02333
H	-1.51727	0.32111	-3.64367
H	-0.38952	-0.25504	-2.43462
C	3.08562	-2.29383	-1.06588
C	3.85108	1.32386	-1.95104
H	2.98386	1.60888	-2.52532
H	3.98238	2.05488	-1.16806
H	4.71952	1.34099	-2.60151
C	0.00294	4.06317	2.02691
H	-0.99168	3.76677	2.33445
H	0.71335	3.45277	2.56460
H	0.16115	5.10443	2.29999
C	-0.87248	5.28296	-0.61426
H	-0.78781	5.37775	-1.69084
H	-1.92080	5.15740	-0.36616
H	-0.54297	6.22477	-0.18075
C	-2.63855	3.07479	-2.31732
H	-3.15175	3.11227	-1.36404
H	-2.55079	4.08807	-2.69134

H	-3.26268	2.51514	-3.00979
Cl	2.36422	1.29134	1.66409
Si	0.20388	3.89101	0.14208
Si	-0.94694	2.20609	-2.13727
H	-1.28510	-1.41179	3.98560
C	-3.20544	-1.32520	-0.10450
C	-3.10411	-2.43755	-0.94393
C	-4.37204	-0.54062	-0.10242
C	-4.19560	-2.78013	-1.73368
C	-5.43276	-0.91693	-0.90951
C	-5.35367	-2.03654	-1.71458
H	-4.13657	-3.64204	-2.36725
H	-6.33072	-0.33476	-0.91010
H	-6.18731	-2.31979	-2.32665
H	1.03786	0.99110	4.10702
C	-4.48372	0.69505	0.79178
C	-5.06867	0.31404	2.17200
C	-5.36456	1.80355	0.17539
H	-3.48662	1.08456	0.94125
H	-4.42790	-0.38278	2.69050
H	-5.17301	1.19905	2.79157
H	-6.04688	-0.13793	2.04813
H	-5.08916	2.00809	-0.85045
H	-6.41415	1.53310	0.20254
H	-5.24789	2.71552	0.75129
C	-1.83945	-3.28888	-1.02712
C	-1.35892	-3.41221	-2.49150
C	-2.07376	-4.70690	-0.45857
H	-1.06542	-2.80784	-0.44628
H	-1.20552	-2.43743	-2.93415
H	-0.42936	-3.96942	-2.53022
H	-2.08259	-3.94736	-3.09389
H	-2.40945	-4.66972	0.56744
H	-2.82145	-5.23088	-1.04363
H	-1.15207	-5.27910	-0.49209

2b

99

XYZ

Rh	2.54612	-1.10082	0.11939
Ge	0.94768	0.75715	0.35596
Cl	1.07769	-2.24896	1.69818
O	-0.54775	0.86347	1.44154
N	0.79258	2.41807	-0.48058
C	0.29638	2.91898	-3.43016
H	0.69671	3.92645	-3.39388
H	1.09736	2.25691	-3.74481
H	-0.47221	2.89736	-4.19894
N	-3.18272	-0.38426	0.71654
C	0.12387	0.48040	3.72513
H	-0.31220	0.19517	4.68680
H	0.46785	1.51935	3.78245
C	-3.13697	-0.70543	1.97687
C	-0.85757	0.30450	2.61334
C	-2.05126	-0.31633	2.85038
C	3.10198	-1.28107	-1.94064
C	-4.18581	-1.53229	2.68755
H	-4.52141	-1.01921	3.59754
H	-5.05096	-1.74938	2.06197
H	-3.74611	-2.48278	3.01643
C	4.19717	-0.75316	-1.19391
C	5.74039	-1.55293	0.77322
H	5.58958	-0.62944	1.31738
H	5.77657	-2.36252	1.48638
H	6.69109	-1.50231	0.25394
C	3.78010	-4.16435	0.45928
H	4.60249	-4.16972	1.15927
H	2.85667	-4.26131	1.01425
H	3.89107	-5.01168	-0.20785
C	2.47010	-0.65592	-3.17224
H	1.45647	-1.00022	-3.31005
H	2.46085	0.42151	-3.10459
H	3.05095	-0.94370	-4.04279
C	3.76882	-2.88015	-0.35207
C	1.66223	-3.50331	-1.80929
H	1.27537	-4.05451	-0.96467
H	0.84281	-2.95557	-2.25107
H	2.05659	-4.19916	-2.54280
C	3.38796	3.95394	-0.14697
H	3.91563	3.13605	0.32625
H	3.58098	3.92068	-1.21661
H	3.80098	4.88441	0.23519
C	4.61979	-1.76350	-0.23100
C	-1.08538	0.58585	-1.88173
H	-1.63415	0.29906	-0.98672
H	-1.79456	0.54004	-2.70604
H	-0.32195	-0.15953	-2.08394
C	2.76134	-2.55865	-1.35623
C	4.91717	0.56141	-1.44437
H	4.24933	1.29035	-1.87974

H	5.30039	0.97039	-0.52073
H	5.74630	0.39664	-2.12484
C	1.15707	4.02798	2.06259
H	0.12054	3.77424	2.26466
H	1.78906	3.37953	2.65593
H	1.32413	5.05063	2.39167
C	0.77339	5.45422	-0.61381
H	0.77272	5.43163	-1.69751
H	-0.23861	5.64220	-0.27452
H	1.38175	6.30284	-0.30868
C	-1.95688	3.44517	-1.34144
H	-2.26654	3.26335	-0.31671
H	-1.78805	4.50674	-1.47212
H	-2.78167	3.15832	-1.98814
Cl	2.87571	0.92320	1.81205
Si	1.51041	3.88579	0.19260
Si	-0.43718	2.37483	-1.75152
H	-2.18159	-0.63036	3.88490
C	-4.28324	-0.81582	-0.10921
C	-4.26723	-2.07338	-0.72142
C	-5.33483	0.07673	-0.35703
C	-5.33336	-2.43693	-1.53263
C	-6.38273	-0.32755	-1.16776
C	-6.39170	-1.58051	-1.74889
H	-5.33421	-3.40266	-1.99826
H	-7.19970	0.34127	-1.34916
H	-7.21168	-1.88093	-2.37129
H	1.00746	-0.14545	3.55333
C	-5.32956	1.46769	0.26939
C	-6.22716	1.49836	1.52671
C	-5.78339	2.56173	-0.71988
H	-4.31322	1.67952	0.56691
H	-5.89046	0.77731	2.26008
H	-6.20911	2.48321	1.98332
H	-7.25177	1.26180	1.26033
H	-5.21773	2.50893	-1.64186
H	-6.83705	2.46974	-0.95692
H	-5.62817	3.54067	-0.27842
C	-3.09879	-3.03847	-0.54050
C	-2.42200	-3.33057	-1.89777
C	-3.54994	-4.36024	0.11867
H	-2.36589	-2.56989	0.09790
H	-2.08054	-2.40981	-2.35544
H	-1.56923	-3.98643	-1.75260
H	-3.10983	-3.81769	-2.57932
H	-4.03268	-4.17419	1.06978
H	-4.24877	-4.89061	-0.51867
H	-2.69269	-5.00302	0.29148

[2b–2c]‡

99
XYZ

Rh	2.22502	-1.39530	0.03044
Ge	1.17233	0.78712	0.49560
Cl	0.78926	-2.30119	1.68744
O	-0.43723	0.99144	1.42298
N	1.14402	2.36410	-0.51176
C	0.20642	3.07232	-3.33438
H	0.30656	4.15013	-3.36313
H	1.13951	2.63839	-3.68323
H	-0.57285	2.79528	-4.04048
N	-3.16140	-0.13623	0.71749
C	0.11696	0.72326	3.76169
H	-0.38433	0.56806	4.72113
H	0.59694	1.70839	3.76251
C	-3.19589	-0.26789	2.01153
C	-0.84364	0.58842	2.62475
C	-2.10989	0.13445	2.87687
C	3.20031	-1.10076	-1.85176
C	-4.34321	-0.89421	2.77471
H	-4.67686	-0.21899	3.57308
H	-5.19270	-1.13818	2.13760
H	-4.00549	-1.81336	3.27087
C	4.16461	-1.15363	-0.80810
C	4.95609	-2.87638	1.00924
H	4.82722	-2.14941	1.80219
H	4.66116	-3.84275	1.38872
H	6.00487	-2.90928	0.73639
C	2.64716	-4.64477	-0.52251
H	3.27199	-5.09816	0.23242
H	1.63167	-4.62559	-0.14870
H	2.68959	-5.25622	-1.41618
C	3.00423	0.03072	-2.84864
H	2.01879	-0.00930	-3.28844
H	3.11618	0.99321	-2.37186
H	3.73882	-0.06349	-3.64140
C	3.12496	-3.23743	-0.83947
C	1.35093	-2.78613	-2.72340
H	0.66953	-3.44026	-2.20017
H	0.79286	-1.93582	-3.08432

H	1.76541	-3.31783	-3.57434
C	3.84645	3.70587	-0.06301
H	4.25350	2.97484	0.62153
H	4.14595	3.44666	-1.07646
H	4.29152	4.67017	0.17138
C	4.12001	-2.48816	-0.19694
C	-0.94219	0.64548	-1.81314
H	-1.43718	0.30233	-0.90928
H	-1.70013	0.66373	-2.59388
H	-0.19103	-0.07868	-2.11223
C	2.48231	-2.35505	-1.80986
C	5.19648	-0.09372	-0.46658
H	4.87492	0.88100	-0.79909
H	5.36606	-0.04347	0.59875
H	6.12913	-0.34327	-0.96298
C	1.39185	4.30642	1.81027
H	0.31144	4.23804	1.89992
H	1.83557	3.65971	2.55705
H	1.68442	5.32883	2.03594
C	1.53424	5.32162	-1.09690
H	1.96450	5.19020	-2.08415
H	0.47681	5.52517	-1.20992
H	1.98996	6.20769	-0.66012
C	-1.65975	3.43853	-0.82017
H	-2.01116	2.90021	0.05422
H	-1.34792	4.42908	-0.50831
H	-2.49211	3.55081	-1.50869
Cl	2.87263	1.06092	2.02971
Si	1.94357	3.84108	0.04289
Si	-0.25800	2.41277	-1.60046
H	-2.30312	-0.04428	3.93353
C	-4.22833	-0.66526	-0.09648
C	-4.20968	-2.00951	-0.48857
C	-5.23962	0.18710	-0.55503
C	-5.22588	-2.48462	-1.30429
C	-6.24145	-0.32941	-1.36200
C	-6.24354	-1.65848	-1.73398
H	-5.22131	-3.51407	-1.60402
H	-7.02832	0.31344	-1.70278
H	-7.02664	-2.04410	-2.35696
H	0.91761	-0.02143	3.67257
C	-5.25295	1.66105	-0.16542
C	-6.34059	1.93513	0.89691
C	-5.46693	2.57877	-1.38780
H	-4.28938	1.89021	0.26196
H	-6.17678	1.33244	1.78164
H	-6.33117	2.98066	1.18922
H	-7.32257	1.69917	0.50123
H	-4.74220	2.35990	-2.16292
H	-6.46034	2.45782	-1.80400
H	-5.35366	3.61702	-1.09322
C	-3.08537	-2.94954	-0.06330
C	-2.28678	-3.42530	-1.29540
C	-3.62098	-4.16400	0.72519
H	-2.40427	-2.40521	0.57033
H	-1.88994	-2.57304	-1.83369
H	-1.46007	-4.05297	-0.97580
H	-2.91249	-3.99954	-1.96944
H	-4.19415	-3.84345	1.58653
H	-4.25989	-4.78125	0.10325
H	-2.79388	-4.77395	1.07379

2c

99
XYZ

Rh	-2.74483	-1.14407	-0.19579
Ge	-1.40013	0.88640	-0.67736
O	0.36504	0.24238	-1.15168
N	-1.05965	2.19205	0.62601
C	0.55557	4.39062	2.01175
H	-0.11380	5.19257	1.72634
H	0.32461	4.09466	3.02964
H	1.56445	4.79796	2.01553
N	3.21765	-0.59656	-0.51516
C	-0.53104	-0.90717	-3.08949
H	-0.83208	-0.00779	-3.63800
C	3.04984	-1.23385	-1.63809
C	0.57792	-0.62043	-2.12893
C	1.77923	-1.27529	-2.32438
C	3.92439	-2.71545	1.38217
H	3.03269	-2.59648	0.78717
C	6.11302	-1.50597	1.65251
H	6.39918	-2.27308	2.34467
C	4.51134	-0.57235	0.12670
C	5.37357	0.50554	-0.11208
C	-1.41537	-2.06545	1.22098
C	4.12881	-2.02629	-2.34322
H	3.85078	-3.08802	-2.37565
H	4.22200	-1.70064	-3.38668
H	5.09981	-1.93906	-1.85725

C	4.87345	-1.57395	1.03328
C	-2.56554	-1.56070	1.88683
C	3.51970	-2.63851	2.87116
H	4.38501	-2.76392	3.51123
H	3.07070	-1.67729	3.09131
H	2.80723	-3.42241	3.11278
C	-5.17500	-1.97706	1.75536
H	-5.36567	-0.91221	1.76759
H	-5.85729	-2.42935	1.05111
H	-5.36850	-2.37692	2.74508
C	4.97476	1.63592	-1.05579
H	3.91980	1.53462	-1.25820
C	-4.20609	-4.12678	-0.41964
H	-4.83071	-3.54689	-1.08740
H	-3.60981	-4.80711	-1.01046
H	-4.83312	-4.71406	0.23990
C	0.03972	-1.75963	1.54091
H	0.60157	-1.45363	0.67129
H	0.10276	-0.96280	2.26571
H	0.49519	-2.64573	1.96782
C	-3.30946	-3.21226	0.40148
C	-1.00064	-3.77377	-0.73894
H	-1.52301	-3.94689	-1.66977
H	-0.09957	-3.21534	-0.94795
H	-0.72544	-4.73185	-0.30916
C	4.54216	-4.09420	1.06374
H	4.82785	-4.15825	0.02060
H	5.42417	-4.27172	1.66780
H	3.82792	-4.88477	1.27367
C	-2.62588	3.47415	2.90182
H	-2.33432	2.60737	3.48720
H	-2.00344	4.30591	3.20748
H	-3.65295	3.72104	3.16077
C	6.98366	-0.46906	1.39309
H	7.94188	-0.43465	1.87295
C	6.60643	0.53153	0.52021
H	7.27899	1.34360	0.32992
C	-3.73809	-2.26330	1.35877
C	1.71914	1.61006	1.63781
H	1.26751	1.21117	2.54390
H	1.95005	0.80005	0.95747
H	2.65835	2.07811	1.92336
C	-1.88457	-3.02632	0.24287
C	-2.57017	-0.53820	3.00948
H	-1.85435	0.24610	2.81132
H	-3.54680	-0.09032	3.12274
H	-2.30845	-1.03169	3.93982
C	-4.09628	2.16901	0.55321
H	-4.24827	2.07168	-0.51579
H	-4.14551	1.17550	0.98532
H	-4.94243	2.73066	0.94422
C	-2.60222	4.77722	0.06842
H	-1.72749	5.40131	0.21081
H	-2.70264	4.58442	-0.99431
H	-3.47126	5.34514	0.39284
C	5.20640	3.02334	-0.42018
H	4.69431	3.09872	0.53138
H	6.26077	3.21501	-0.25914
H	4.82506	3.79642	-1.07895
C	1.24870	3.44760	-0.85621
H	1.42010	2.58873	-1.49368
H	0.55606	4.11180	-1.36375
H	2.19122	3.97224	-0.72806
C	5.74736	1.53187	-2.38959
H	6.81407	1.62530	-2.21658
H	5.56381	0.57920	-2.87093
H	5.43994	2.32154	-3.06776
Si	-2.50861	3.12847	1.02379
Si	0.56572	2.88503	0.83095
H	1.78440	-1.90221	-3.21470
Cl	-1.85086	2.11865	-2.48817
H	-0.25454	-1.68436	-3.80684
Cl	-4.25772	-0.75326	-1.96726
H	-1.43789	-1.23617	-2.55595

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XYZ

Rh	1.22398	1.79655	-0.37164
Ge	2.00965	-0.56791	-0.61985
O	0.55373	-1.69528	-0.11370
N	3.36264	-1.38188	0.40169
C	4.66547	-3.58202	2.05787
H	5.50931	-3.70969	1.39032
H	4.97209	-2.94268	2.87915
H	4.43444	-4.55950	2.47588
N	-3.58879	-0.75085	0.06111
C	-0.99788	-0.49862	-1.51141
H	-0.36441	-0.73086	-2.37694
C	-3.10416	-1.93945	0.28987

C	-0.71746	-1.44838	-0.40440
C	-1.67199	-2.14662	0.29787
C	-5.13623	-1.20980	-2.39036
H	-4.14461	-1.56801	-2.16546
C	-7.12473	-0.40690	-1.07136
H	-7.71352	-0.55276	-1.95451
C	-5.01270	-0.51203	0.06328
C	-5.61230	0.00539	1.21779
C	0.32394	1.83120	1.57942
C	-3.93346	-3.15598	0.60968
H	-3.97803	-3.81114	-0.27045
H	-3.46657	-3.74587	1.40753
H	-4.95642	-2.90663	0.89463
C	-5.77289	-0.71508	-1.09493
C	1.67031	2.28312	1.65576
C	-5.00049	-0.03807	-3.38831
H	-5.97766	0.35691	-3.64235
H	-4.41148	0.76229	-2.95576
H	-4.51550	-0.36896	-4.30102
C	3.03462	4.27246	0.53717
H	3.92084	3.66432	0.64027
H	3.01266	4.67353	-0.46619
H	3.09239	5.09197	1.24650
C	-4.80107	0.25757	2.48482
H	-3.76382	0.07845	2.24933
C	0.16676	4.93781	-0.65159
H	0.58595	4.75794	-1.63380
H	-0.90257	5.05900	-0.74925
H	0.57565	5.85648	-0.24931
C	-0.30611	0.71357	2.39385
H	-1.05611	0.18001	1.82945
H	0.43956	0.00310	2.71646
H	-0.77385	1.14926	3.27153
C	0.48282	3.77999	0.28332
C	-1.86002	2.60629	0.29881
H	-2.00797	2.96839	-0.70943
H	-2.20950	1.58428	0.34657
H	-2.46036	3.20716	0.97462
C	-5.92229	-2.37481	-3.02801
H	-6.05176	-3.18678	-2.32177
H	-6.90150	-2.05438	-3.36301
H	-5.38397	-2.75263	-3.89087
C	6.08751	-0.49838	1.45131
H	5.55103	0.06455	2.20981
H	6.46133	-1.40453	1.91153
H	6.94745	0.09253	1.14446
C	-7.72692	0.08406	0.06866
H	-8.77502	0.30972	0.07091
C	-6.96944	0.28790	1.20325
H	-7.43812	0.67170	2.08758
C	1.77837	3.46606	0.80872
C	1.81599	-2.72563	2.62820
H	2.16162	-1.98540	3.34702
H	0.85502	-2.42007	2.23918
H	1.68908	-3.66503	3.16111
C	-0.40027	2.74046	0.70072
C	2.77122	1.68640	2.51713
H	2.75633	0.60760	2.46967
H	3.74309	2.02235	2.18644
H	2.62981	2.00350	3.54499
C	4.88110	0.79611	-1.04269
H	4.42853	0.69649	-2.02315
H	4.34460	1.57545	-0.51247
H	5.89795	1.15154	-1.19620
C	5.83976	-2.10676	-1.21336
H	5.93130	-3.08989	-0.76450
H	5.27468	-2.21251	-2.13387
H	6.83990	-1.76450	-1.46846
C	-4.93969	1.71917	2.96334
H	-4.67147	2.40880	2.17173
H	-5.95590	1.93579	3.27030
H	-4.28942	1.89698	3.81460
C	2.48346	-4.26271	-0.01603
H	1.53549	-3.97582	-0.45142
H	3.19722	-4.39837	-0.82337
H	2.36034	-5.21777	0.48923
C	-5.21839	-0.71339	3.61145
H	-6.25896	-0.56476	3.87655
H	-5.09183	-1.74312	3.29969
H	-4.61481	-0.54776	4.49853
Si	4.98007	-0.84684	-0.06861
Si	3.07912	-2.93154	1.20991
H	-1.30379	-2.95770	0.92626
Cl	2.32377	-1.40427	-2.66589
H	-2.04930	-0.48338	-1.79720
Cl	1.52163	2.22068	-2.67599
H	-0.73164	0.53079	-1.21696

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XYZ

Rh	0.98604	1.72290	-0.38566
Ge	1.79206	-0.60379	-0.32790
O	0.48114	-1.31166	0.90459
N	3.35336	-1.37486	0.36855
C	4.99547	-3.25150	2.11086
H	5.53718	-3.69173	1.28209
H	5.61457	-2.47681	2.55124
H	4.86386	-4.02898	2.86025
N	-3.54735	-0.60268	0.43368
C	-1.16281	0.03737	-0.29453
H	-0.67748	-0.07567	-1.26733
C	-3.07011	-1.22067	1.50628
C	-0.73664	-0.82095	0.80928
C	-1.67702	-1.24741	1.75472
C	-4.22954	-2.84319	-1.28385
H	-3.40497	-2.81453	-0.58790
C	-6.55457	-1.85594	-1.35114
H	-6.84325	-2.66465	-1.99061
C	-4.90248	-0.72473	-0.03619
C	-5.82745	0.27418	0.27847
C	1.01709	2.50022	1.61873
C	-3.98659	-1.95368	2.43624
H	-4.39685	-2.84537	1.94844
H	-3.46142	-2.27069	3.34185
H	-4.84560	-1.33738	2.71946
C	-5.25880	-1.79768	-0.86242
C	2.31312	2.62046	1.02138
C	-3.67627	-2.48522	-2.68234
H	-4.47691	-2.49097	-3.41362
H	-3.22341	-1.50163	-2.67494
H	-2.92150	-3.20240	-2.98624
C	3.26744	3.91132	-1.10385
H	4.15841	3.31224	-0.99264
H	2.92833	3.83234	-2.12718
H	3.51829	4.94480	-0.88791
C	-5.42903	1.48346	1.11708
H	-4.43962	1.30160	1.50701
C	0.26578	4.85956	-1.28432
H	0.40331	4.41440	-2.26084
H	-0.78885	5.04281	-1.13651
H	0.78652	5.80994	-1.24523
C	0.68263	1.80106	2.92891
H	-0.27678	1.30559	2.87774
H	1.42683	1.05628	3.16699
H	0.65695	2.53291	3.72986
C	0.80761	3.93414	-0.20754
C	-1.37132	3.53344	1.18233
H	-1.95486	3.65177	0.28032
H	-1.76244	2.69281	1.73704
H	-1.48592	4.42565	1.78931
C	-4.79503	-4.27881	-1.28110
H	-5.24243	-4.52248	-0.32371
H	-5.54323	-4.41255	-2.05305
H	-3.99347	-4.98329	-1.47430
C	6.32382	-0.72642	0.13844
H	6.14300	0.10839	0.80953
H	6.77018	-1.52701	0.71546
H	7.05541	-0.40647	-0.59990
C	-7.48045	-0.88232	-1.03265
H	-8.47847	-0.94410	-1.41963
C	-7.11571	0.17511	-0.22627
H	-7.83569	0.93411	0.00581
C	2.17443	3.45571	-0.15215
C	2.57120	-1.82060	3.25619
H	3.18915	-0.98862	3.58685
H	1.55827	-1.47373	3.10393
H	2.56331	-2.55987	4.05362
C	0.10278	3.34046	0.86194
C	3.61639	2.06215	1.57218
H	3.46929	1.09904	2.03511
H	4.34625	1.94247	0.78602
H	4.01077	2.75569	2.30790
C	4.36507	0.05458	-2.08503
H	3.57870	-0.22360	-2.77801
H	4.10532	1.02393	-1.67494
H	5.27251	0.18559	-2.67100
C	5.01497	-2.91353	-1.66183
H	5.20791	-3.74079	-0.98716
H	4.14419	-3.16566	-2.25864
H	5.86794	-2.82578	-2.33052
C	-5.36565	2.74310	0.22474
H	-4.66816	2.59389	-0.59150
H	-6.33970	2.96028	-0.19798
H	-5.04694	3.60461	0.80453
C	2.17482	-4.06551	1.12931
H	1.15652	-3.73904	0.96071
H	2.53947	-4.51744	0.21163
H	2.17103	-4.82886	1.90379
C	-6.38539	1.71105	2.30679

H	-7.38443	1.95548	1.96653
H	-6.44625	0.82595	2.92974
H	-6.03061	2.53530	2.91734
Si	4.71849	-1.26527	-0.74988
Si	3.26207	-2.59023	1.64993
H	-1.32455	-1.84262	2.59344
Cl	1.25843	-1.94449	-2.02605
H	-2.48498	-0.27909	-0.28734
Cl	0.75539	1.64561	-2.80225
H	-1.44299	1.06336	-0.04170

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XYZ

Rh	0.76563	1.43515	0.34423
Ge	2.01600	-0.42201	-0.59651
O	0.66194	-1.81773	-0.42307
N	3.58487	-1.27649	0.02097
C	5.08652	-3.46043	1.52793
H	5.86694	-3.58224	0.78567
H	5.45491	-2.79925	2.30552
H	4.91446	-4.43511	1.97936
N	-3.60263	-0.96567	-0.05454
C	-0.59717	-0.22287	0.77139
H	-1.56473	0.27233	0.86027
C	-2.92673	-1.69997	-0.96594
C	-0.52336	-1.30703	-0.19724
C	-1.55321	-1.88991	-0.97102
C	-4.45150	1.38453	-1.55198
H	-3.46934	0.94094	-1.52911
C	-6.79167	0.78002	-0.82711
H	-7.13859	1.63403	-1.37191
C	-5.01829	-0.64256	-0.10036
C	-5.91847	-1.43887	0.61079
C	1.22892	2.03697	2.34133
C	-3.74595	-2.35242	-2.03003
H	-4.21975	-1.60092	-2.67033
H	-3.12239	-2.99043	-2.65878
H	-4.55808	-2.95252	-1.60703
C	-5.43695	0.47747	-0.82110
C	2.30430	2.47834	1.48682
C	-4.35644	2.74714	-0.83038
H	-5.30733	3.26733	-0.85816
H	-4.07247	2.61151	0.20749
H	-3.60462	3.36097	-1.31159
C	2.49590	4.17401	-0.55289
H	3.48090	3.76513	-0.72543
H	1.94311	4.11732	-1.48182
H	2.60350	5.21645	-0.27099
C	-5.45112	-2.62982	1.44155
H	-4.42143	-2.83427	1.19068
C	-0.55024	4.52784	0.10053
H	-0.55899	4.27363	-0.95020
H	-1.56133	4.46207	0.47507
H	-0.20392	5.54890	0.22214
C	1.39325	1.15871	3.57364
H	0.48245	0.61899	3.79541
H	2.18337	0.43598	3.42738
H	1.64288	1.77262	4.43328
C	0.37349	3.59028	0.86146
C	-1.31840	2.68347	2.64863
H	-2.11682	2.77768	1.92529
H	-1.43216	1.73580	3.15758
H	-1.42255	3.47591	3.38231
C	-4.83963	1.58961	-3.03171
H	-4.94119	0.63985	-3.54409
H	-5.77480	2.12952	-3.12515
H	-4.06456	2.16029	-3.52949
C	6.47532	-0.45518	0.54563
H	6.14281	0.21278	1.33419
H	6.83387	-1.36543	1.00906
H	7.32175	0.01503	0.04968
C	-7.69509	0.00044	-0.13553
H	-8.73760	0.25062	-0.14981
C	-7.26194	-1.09742	0.58062
H	-7.97267	-1.68883	1.12064
C	1.76826	3.40623	0.54173
C	2.23799	-2.73127	2.29700
H	2.59304	-1.99837	3.01624
H	1.23758	-2.46057	1.98802
H	2.18248	-3.69194	2.80319
C	0.04071	2.77290	1.97008
C	3.76522	2.10527	1.69941
H	3.88406	1.03856	1.81920
H	4.37404	2.42408	0.86766
H	4.12545	2.60179	2.59473
C	4.87893	0.87818	-1.70144
H	4.57824	0.69487	-2.72484
H	4.14792	1.55229	-1.26894
H	5.83263	1.40049	-1.71633

C	5.72093	-2.06779	-1.99170
H	5.91664	-3.03131	-1.53213
H	4.98513	-2.21191	-2.77629
H	6.64516	-1.72811	-2.45327
C	-5.51607	-2.27644	2.94478
H	-4.91154	-1.40309	3.16186
H	-6.53698	-2.06383	3.23984
H	-5.15080	-3.10425	3.54332
C	2.79729	-4.17811	-0.40921
H	1.83293	-3.89190	-0.80826
H	3.48411	-4.30491	-1.24091
H	2.69737	-5.13770	0.09306
C	-6.27311	-3.90368	1.15218
H	-7.30410	-3.78728	1.46281
H	-6.26020	-4.14371	0.09532
H	-5.85364	-4.74195	1.69774
Si	5.09514	-0.76690	-0.74352
Si	3.42635	-2.84917	0.80463
H	-1.18313	-2.56964	-1.73397
Cl	2.13927	-0.76631	-2.79666
H	-3.06052	-0.52530	0.67758
Cl	-0.49904	1.55175	-1.78786
H	-0.23286	-0.55702	1.74899

[2e–2f]‡

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XYZ

Rh	-2.07054	-1.54515	-0.17876
Ge	-1.59417	0.85476	-0.59581
O	0.34134	0.63489	-0.86264
N	-1.71856	2.34842	0.56138
C	-0.60176	4.45263	2.46252
H	-1.17500	5.26855	2.03994
H	-1.11959	4.09355	3.34616
H	0.35249	4.86198	2.78662
N	3.58564	-0.15419	-0.44248
C	0.15727	-1.39501	0.32778
H	0.55744	-2.40423	0.42023
C	3.06089	-0.92483	-1.47974
C	0.71820	-0.60025	-0.69187
C	1.73206	-1.11505	-1.62513
C	4.30772	-2.42851	1.22260
H	3.52345	-2.43768	0.48113
C	6.62549	-1.41743	1.30944
H	6.93613	-2.24029	1.91941
C	4.94715	-0.26901	0.04293
C	5.85303	0.74611	-0.26343
C	-2.63635	-2.29163	1.73464
C	4.04497	-1.46313	-2.46528
H	4.74837	-2.16341	-2.00071
H	3.52402	-1.98498	-3.27198
H	4.64842	-0.66110	-2.90669
C	5.32524	-1.35910	0.83483
C	-3.72394	-1.51434	1.21210
C	3.67738	-2.06129	2.58611
H	4.44205	-2.03027	3.35366
H	3.19950	-1.08944	2.54339
H	2.93113	-2.79666	2.87073
C	-5.29717	-1.71246	-0.93016
H	-5.58451	-0.68703	-0.75117
H	-4.99283	-1.79760	-1.96500
H	-6.16188	-2.34637	-0.76315
C	5.43699	1.95696	-1.08997
H	4.44320	1.77064	-1.46432
C	-3.56763	-4.30916	-1.34458
H	-2.86671	-5.12772	-1.26892
H	-4.57428	-4.71233	-1.32448
H	-3.39903	-3.80268	-2.28467
C	-1.94484	-2.04255	3.06703
H	-0.93590	-2.43044	3.06407
H	-1.89978	-0.98373	3.28366
H	-2.49801	-2.53263	3.86144
C	-3.39198	-3.34267	-0.18519
C	-1.43992	-4.56460	1.05309
H	-0.95224	-4.79264	0.11463
H	-0.68109	-4.28368	1.76944
H	-1.93497	-5.45827	1.41727
C	4.90927	-3.84749	1.28120
H	5.41957	-4.09260	0.35706
H	5.61083	-3.94943	2.10028
H	4.11616	-4.57133	1.43559
C	-3.97050	3.69504	2.10076
H	-4.14238	2.77913	2.65881
H	-3.36758	4.35100	2.71548
H	-4.93413	4.17740	1.95272
C	7.53140	-0.41833	1.00794
H	8.53426	-0.47631	1.38337
C	7.14786	0.65300	0.23096
H	7.85634	1.42500	0.00870
C	-4.15717	-2.13183	-0.01339

C	0.70684	1.74256	2.29250
H	0.04218	1.25134	2.99896
H	1.18571	0.98338	1.68970
H	1.48085	2.24679	2.86583
C	-2.45442	-3.44457	0.87207
C	-4.36706	-0.34263	1.94206
H	-3.62793	0.37793	2.26186
H	-5.08471	0.16068	1.31392
H	-4.88714	-0.72090	2.81595
C	-4.52738	2.41639	-0.62110
H	-4.42913	2.63801	-1.67599
H	-4.51192	1.33791	-0.51714
H	-5.50504	2.76029	-0.29172
C	-2.84014	4.96707	-0.51368
H	-2.11324	5.59512	-0.01052
H	-2.47019	4.75916	-1.51281
H	-3.76098	5.53787	-0.60812
C	5.38578	3.21595	-0.19586
H	4.70068	3.06924	0.63117
H	6.36656	3.44059	0.20829
H	5.04791	4.07125	-0.77153
C	0.91351	3.69544	-0.12652
H	1.18708	2.90510	-0.81441
H	0.42738	4.48203	-0.69629
H	1.82108	4.10847	0.30792
C	6.37883	2.18672	-2.29085
H	7.38153	2.43698	-1.96455
H	6.43415	1.30202	-2.91468
H	6.00916	3.00770	-2.89585
Si	-3.18267	3.32584	0.39730
Si	-0.23894	3.03020	1.23796
H	1.33102	-1.61138	-2.50812
Cl	-1.84820	1.79380	-2.58532
H	2.91850	0.15924	0.25202
Cl	-1.49747	-1.78914	-2.56148
H	-0.03835	-0.88816	1.27191

2f

99
XYZ

Rh	2.16953	-1.32678	-0.31955
Ge	0.90276	0.66962	0.33051
O	-0.55715	0.45464	-0.95426
N	1.32683	2.50859	0.18286
C	1.33467	5.24369	-1.15089
H	1.22985	5.79490	-0.22429
H	2.38530	5.23053	-1.42272
H	0.80444	5.80018	-1.92055
N	-3.09389	-0.52372	-0.57932
C	0.98598	-0.91828	-2.12180
H	1.04553	-1.80632	-2.75797
C	-2.76665	-1.27594	-1.64537
C	-0.37062	-0.57466	-1.75290
C	-1.48760	-1.30148	-2.19711
C	-5.13366	1.41892	-1.32324
H	-4.14837	1.27457	-1.73912
C	-6.59365	0.28464	0.38530
H	-7.36928	0.97416	0.12025
C	-4.37884	-0.56730	0.10108
C	-4.58278	-1.50098	1.11979
C	4.00992	-1.42513	-1.40986
C	-3.82663	-2.15194	-2.22583
H	-4.71803	-1.57693	-2.49363
H	-3.45772	-2.66391	-3.11724
H	-4.15450	-2.90502	-1.50270
C	-5.37078	0.34481	-0.26606
C	4.25905	-0.78519	-0.14344
C	-5.17309	2.82070	-0.67434
H	-6.15413	3.02398	-0.26107
H	-4.44283	2.89449	0.12159
H	-4.94967	3.58140	-1.41484
C	4.22594	-1.58715	2.40055
H	4.54728	-0.58492	2.64215
H	3.31770	-1.79488	2.95180
H	4.99753	-2.27513	2.72871
C	-3.48754	-2.45738	1.58333
H	-2.61784	-2.33492	0.95902
C	3.18637	-4.22316	1.00454
H	2.71020	-3.99319	1.94585
H	2.49302	-4.80798	0.41973
H	4.08087	-4.81052	1.18957
C	4.28725	-0.80998	-2.77411
H	3.65415	-1.24468	-3.53455
H	4.11321	0.25733	-2.76073
H	5.32260	-0.98490	-3.04719
C	3.57206	-2.94872	0.27214
C	3.22185	-3.84875	-2.16624
H	2.27200	-4.30271	-1.91368
H	3.14198	-3.42571	-3.15801
H	3.98358	-4.62053	-2.18854

C	-6.16303	1.32967	-2.47088
H	-6.14814	0.35039	-2.93533
H	-7.16673	1.51756	-2.10895
H	-5.93553	2.07018	-3.23036
C	3.60307	4.23312	1.24976
H	4.29087	3.64000	0.65430
H	3.41675	5.15864	0.71954
H	4.10253	4.48421	2.18275
C	-6.81972	-0.64541	1.37896
H	-7.77009	-0.67819	1.87459
C	-5.82152	-1.52316	1.74579
H	-6.00044	-2.22860	2.53124
C	4.00070	-1.74237	0.90105
C	0.95952	2.75040	-2.83056
H	2.00098	2.45407	-2.92786
H	0.33316	1.89596	-3.05013
H	0.76242	3.50722	-3.58599
C	3.58553	-2.77672	-1.14957
C	4.88385	0.59441	0.01839
H	4.49989	1.28494	-0.71930
H	4.68058	1.00425	0.99530
H	5.95936	0.51653	-0.10519
C	2.48330	1.93637	2.93090
H	1.61813	1.57976	3.47501
H	2.98920	1.07408	2.51328
H	3.16241	2.39370	3.64702
C	0.74379	4.41115	2.48138
H	0.40198	5.21646	1.84004
H	-0.12426	3.83798	2.79196
H	1.18632	4.85952	3.36779
C	-3.05933	-2.11648	3.02816
H	-2.69672	-1.09940	3.08589
H	-3.88797	-2.23909	3.71732
H	-2.25352	-2.77522	3.33109
C	-1.28409	3.62634	-0.87260
H	-1.74222	2.64740	-0.93487
H	-1.53172	4.05506	0.09390
H	-1.71462	4.26033	-1.64417
C	-3.94243	-3.93047	1.49265
H	-4.76070	-4.13239	2.17443
H	-4.26652	-4.18353	0.48924
H	-3.11438	-4.57936	1.75420
Si	2.00326	3.25586	1.63129
Si	0.60412	3.47743	-1.09793
H	-1.31359	-2.03617	-2.97785
Cl	-0.61170	0.72733	2.00280
H	-2.33954	0.01318	-0.15146
Cl	0.20425	-2.56935	0.54470
H	1.52263	-0.07550	-2.56506

[2f–2g]‡

99

XYZ

Rh	-2.72209	-1.08752	-0.13437
Ge	-0.99272	0.52805	-0.36470
O	0.58452	-0.55946	0.26891
N	-0.75589	2.21107	0.46036
C	0.44802	4.20747	2.41357
H	0.47148	5.04495	1.72539
H	-0.45766	4.28024	3.00691
H	1.29443	4.31819	3.08799
N	3.24672	-1.11228	0.02622
C	-1.01987	-2.34224	-0.05137
H	-1.09065	-3.02593	-0.90866
C	2.80539	-2.36986	-0.15433
C	0.36782	-1.81809	0.04171
C	1.45420	-2.70253	-0.10626
C	4.95564	-1.10335	2.38781
H	3.95262	-1.48783	2.28261
C	6.77239	-0.26937	0.85497
H	7.42958	-0.26487	1.70056
C	4.62697	-0.67901	-0.11356
C	5.07995	-0.23927	-1.35951
C	-3.53346	-1.15324	1.85791
C	3.81771	-3.43255	-0.42233
H	4.56420	-3.48511	0.37582
H	3.33686	-4.40826	-0.51840
H	4.37039	-3.22515	-1.34367
C	5.45953	-0.68815	1.00834
C	-4.21132	-0.06631	1.17406
C	4.89599	0.12624	3.32170
H	5.88537	0.54366	3.46720
H	4.26007	0.89493	2.90122
H	4.49794	-0.15723	4.29041
C	-5.77035	0.10517	-0.96099
H	-5.71443	1.17774	-0.83938
H	-5.43408	-0.14300	-1.95950
H	-6.80748	-0.19464	-0.85249
C	4.16949	-0.16985	-2.58344
H	3.18200	-0.50392	-2.30557

C	-5.35431	-3.00819	-0.89850
H	-5.08417	-2.71842	-1.90444
H	-5.00702	-4.01824	-0.72995
H	-6.43480	-2.99548	-0.79702
C	-2.79575	-1.03686	3.18600
H	-1.97988	-1.74583	3.24223
H	-2.38127	-0.04605	3.30583
H	-3.47460	-1.22611	4.01167
C	-4.73358	-2.04999	0.10529
C	-3.58907	-3.79366	1.68177
H	-3.28340	-4.41024	0.84642
H	-2.78740	-3.77704	2.40708
H	-4.45368	-4.25221	2.14960
C	5.83296	-2.20858	3.01506
H	5.89940	-3.07305	2.36472
H	6.83716	-1.85018	3.20525
H	5.40627	-2.52531	3.96065
C	-2.51937	4.69935	0.69613
H	-3.14827	4.15474	1.39200
H	-1.87757	5.35665	1.27022
H	-3.16568	5.32553	0.08505
C	7.24204	0.14938	-0.37328
H	8.26025	0.46928	-0.47525
C	6.40247	0.16801	-1.46693
H	6.77350	0.50796	-2.41209
C	-4.91329	-0.60941	0.07383
C	0.62302	1.21077	2.94571
H	-0.28201	1.27857	3.54315
H	0.70425	0.20373	2.55951
H	1.46693	1.39146	3.60722
C	-3.94154	-2.38395	1.22712
C	-4.20597	1.38024	1.64850
H	-3.20710	1.70515	1.90079
H	-4.59185	2.03856	0.88426
H	-4.83717	1.47089	2.52685
C	-2.75851	2.81115	-1.72431
H	-2.26209	2.37686	-2.58415
H	-3.42701	2.05853	-1.32190
H	-3.37712	3.62944	-2.08699
C	-0.24527	4.56729	-1.39259
H	0.46326	5.05768	-0.73200
H	0.31117	3.94211	-2.08287
H	-0.74767	5.34122	-1.96793
C	4.03987	1.28615	-3.08400
H	3.68331	1.93378	-2.29378
H	4.99385	1.66150	-3.43634
H	3.32896	1.32876	-3.90067
C	2.25254	2.50284	0.60242
H	2.26411	1.73779	-0.16404
H	2.41181	3.45405	0.10280
H	3.09172	2.33712	1.27222
C	4.68740	-1.07921	-3.71979
H	5.65807	-0.74771	-4.06965
H	4.77852	-2.10816	-3.39157
H	3.99718	-1.05015	-4.55525
Si	-1.53152	3.52388	-0.44462
Si	0.59065	2.51178	1.54869
H	1.20602	-3.74744	-0.26769
Cl	0.12461	0.82181	-2.29227
H	2.52457	-0.41122	0.17815
Cl	-2.68592	-1.42219	-2.58332
H	-1.17762	-2.95252	0.85139

2g

99

XYZ

Rh	-2.63070	-1.17017	-0.17170
Ge	-1.18599	0.71163	-0.61377
O	0.55617	-0.27980	-0.39206
N	-0.88457	2.31817	0.32353
C	0.69391	4.34046	1.97222
H	0.44925	5.18079	1.33273
H	0.01886	4.35070	2.82136
H	1.70070	4.50366	2.35091
N	3.19484	-0.94739	0.06956
C	-0.90392	-1.98351	-1.20658
H	-1.06230	-1.53832	-2.19982
C	2.72430	-2.20587	-0.09840
C	0.35813	-1.54961	-0.63532
C	1.39163	-2.48214	-0.36828
C	4.76709	-0.55462	2.50976
H	3.72021	-0.79481	2.40499
C	6.70966	-0.10284	0.97573
H	7.31561	0.02243	1.84988
C	4.60271	-0.58776	-0.04281
C	5.15391	-0.39716	-1.31455
C	-2.48738	-1.78402	1.87819
C	3.70472	-3.32776	-0.01244
H	4.27707	-3.28601	0.91845
H	3.19349	-4.29142	-0.06802

H	4.43779	-3.27882	-0.82369
C	5.36679	-0.42472	1.11365
C	-3.47834	-0.72882	1.81605
C	4.87926	0.78817	3.26638
H	5.91667	1.04534	3.44391
H	4.42333	1.58888	2.69753
H	4.37857	0.71820	4.22621
C	-5.80222	-0.42668	0.58117
H	-5.77607	0.59827	0.92313
H	-5.91395	-0.42388	-0.49494
H	-6.66348	-0.91248	1.02784
C	4.32413	-0.50386	-2.59305
H	3.31568	-0.78810	-2.33421
C	-5.14025	-3.35491	-0.34138
H	-5.35297	-2.81152	-1.25169
H	-4.66882	-4.29099	-0.60606
H	-6.07008	-3.57348	0.17366
C	-1.28115	-1.82240	2.80817
H	-0.44932	-2.34114	2.35014
H	-0.95553	-0.82310	3.05572
H	-1.54259	-2.33434	3.72908
C	-4.23689	-2.52799	0.55937
C	-2.33185	-4.27197	1.02544
H	-2.56479	-4.74056	0.07924
H	-1.25783	-4.17412	1.10219
H	-2.67410	-4.92115	1.82490
C	5.45166	-1.67625	3.32165
H	5.37967	-2.63001	2.81294
H	6.50075	-1.45564	3.47823
H	4.97889	-1.77267	4.29321
C	-2.72819	4.46771	1.45139
H	-2.99829	3.75700	2.22672
H	-2.01961	5.17089	1.87194
H	-3.62401	5.02397	1.18529
C	7.27303	0.06678	-0.27120
H	8.31189	0.31629	-0.36002
C	6.49884	-0.07106	-1.40472
H	6.94170	0.08072	-2.36779
C	-4.53222	-1.16707	0.97342
C	1.03041	1.34725	2.40813
H	0.23715	1.35511	3.15136
H	1.09846	0.35134	1.99053
H	1.96142	1.56782	2.92142
C	-3.00707	-2.91374	1.14278
C	-3.40248	0.58487	2.58360
H	-2.40923	1.00749	2.54066
H	-4.09073	1.30943	2.17329
H	-3.66667	0.41145	3.62199
C	-3.56151	2.79297	-0.97610
H	-3.34329	2.38780	-1.95773
H	-4.02637	2.00136	-0.39873
H	-4.30870	3.57219	-1.11349
C	-1.28729	4.85753	-1.28408
H	-0.41555	5.34651	-0.86032
H	-0.98491	4.37406	-2.20745
H	-2.01268	5.62952	-1.52896
C	4.25433	0.86512	-3.30707
H	3.84931	1.62332	-2.64957
H	5.23946	1.18025	-3.63058
H	3.61396	0.79439	-4.17905
C	2.05973	2.69848	-0.23785
H	1.98256	1.86237	-0.92180
H	1.98879	3.60527	-0.83220
H	3.04214	2.68057	0.22848
C	4.89141	-1.57590	-3.54976
H	5.88491	-1.30726	-3.88797
H	4.94732	-2.54504	-3.06791
H	4.25187	-1.66580	-4.42068
Si	-2.05771	3.57489	-0.10061
Si	0.66656	2.65918	1.06866
H	1.14222	-3.52689	-0.53250
Cl	-0.68634	1.27312	-2.71238
H	2.50473	-0.20982	-0.05687
Cl	-3.64956	-0.85362	-2.40733
H	-0.98339	-3.07209	-1.28277

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