

## Low-valent oligogermanium amidophenolate complex comprising a unique Ge<sub>4</sub> chain

Kseniya V. Tsys, Maxim G. Chegerev, Georgy K. Fukin, Andrey G. Starikov and Alexandr V. Piskunov

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## Materials and methods

All reagents were purchased from Sigma Aldrich. All manipulations on complexes were performed under Schlenk line conditions, wherein oxygen and moisture were excluded. Solvents were purified according to the standard methods.<sup>S1</sup> Starting 4,6-di-*tert*-butyl-*N*-(*tert*-butyl)-*o*-aminophenol was prepared according to the method described previously.<sup>S2</sup> NMR spectra were recorded using a Bruker Avance III 400 MHz instrument with TMS as an internal standard. Elemental analyses were performed with an Elemental Analyzer Euro EA 3000 instrument. The density functional theory (DFT) calculations were performed in the Gaussian 09 program package.<sup>S3</sup>

The X-ray data for compounds **1** and **2** were collected on Bruker D8 Quest (**1**) and Agilent Xcalibur E(**2**) diffractometers (MoK $\alpha$ -radiation,  $\omega$ -scans technique,  $\lambda = 0.71073 \text{ \AA}$ ,  $T = 100 \text{ K}$ ) using APEX3<sup>S4</sup> and CrysAlisPro<sup>S5</sup> software packages. The structures were solved by dual methods and were refined by full-matrix least squares on  $F^2$  for all data using SHELXL 2017/1.<sup>S6</sup> SADABS 2016/2<sup>S7</sup> and SCALE3 ABSPACK54 were used to perform area-detector scaling and absorption corrections. All non-hydrogen atoms were found from Fourier syntheses of electron density and were refined anisotropically. Hydrogen atoms were placed in calculated positions and were refined in the 'riding' model with  $U(H)_{iso} = 1.2U_{eq}$  of their parent atoms ( $U(H)_{iso} = 1.5U_{eq}$  for methyl groups). CCDC 1914424 (**1**) and 1914425 (**2**) contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre: [ccdc.cam.ac.uk/structures](http://ccdc.cam.ac.uk/structures). The crystallographic data and structure refinement details for **1** and **2** are given in Table S1.

## Experimental details

**Synthesis of Bu<sup>t</sup>ApGe (1).** Hexane solution of Li[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub> (0.635 g; 3.8 ml) was added to the solution of 4,6-di-*tert*-butyl-(*N*-*tert*-butyl)-*o*-aminophenol (0.53 g, 1.91 mmol) in THF (5 ml). Mixture was heated for 1 h. Resulting solution was added to the GeCl<sub>2</sub>•dioxane (0.44 g, 1.91 mmol) in THF (10 ml). The reaction mixture was stirred for 1h under heating on a water bath (60 °C) and color of solution turned to orange. All volatiles were evaporated under reduced pressure. The residue was dissolved in 15 ml of hexane and filtered. Complex **1** was isolated as a yellow solid from concentrated hexane solution. Single crystals of **1** suitable for X-ray analysis were growth by storing its concentrated pentane solution overnight at -35 °C.

Yield 0.49 g (74 %). C<sub>18</sub>H<sub>29</sub>GeNO. Calculated C, 61.11; H, 8.40. Found C, 61.23; H, 8.52.

$^1\text{H}$  (benzene- $d_6$ , 20°C,  $\delta$ /ppm.,  $J$ /Hz): 7.28 (d, 1H,  $H_{\text{AP}}$ ,  $J_{\text{H,H}} = 2.1$ ); 7.23 (d, 1H,  $H_{\text{AP}}$ ,  $J_{\text{H,H}} = 1.99$ ); 1.78 (s, 9H, N-(Bu $^t$ )); 1.45 (s, 9H, Bu $^t$ ); 1.42 (s, 9H, Bu $^t$ ).

$^{13}\text{C}$  (benzene- $d_6$ , 20°C,  $\delta$ /ppm.,  $J$ /Hz): 154.7 (C-O); 141.1 (C-(Bu $^t$ )); 135.0 (C-N); 138.5 (C-(Bu $^t$ )); 113.1, 109.7 ( $C_{\text{aryl}}$ ); 55.8 (N-C-(Bu $^t$ )); 35.1, 34.4 ( $C_{\text{quat}}$ ); 32.1, 31.5, 29.9 ( $\text{CH}_3(\text{Bu}^t)$ ).

**Synthesis of (Bu $^t$ Ap) $_4$ Ge $_4$ K $_2$ (THF) $_6$  (2).** To the yellow solution of complex **1** (0.66 g, 1.9 mmol) in 30 ml of THF a finely cutted potassium metal (37 mg, 0.95 mmol) was added under stirring. The color of reaction mixture became intense blue gradually. The process was proceeded at room temperature until full dissolution of metallic potassium pieces. It takes approximately 24 h. Compound **2** was isolated from concentrated THF solution (5 ml) as a deep blue crystalline product, which is extremely sensitive to air.

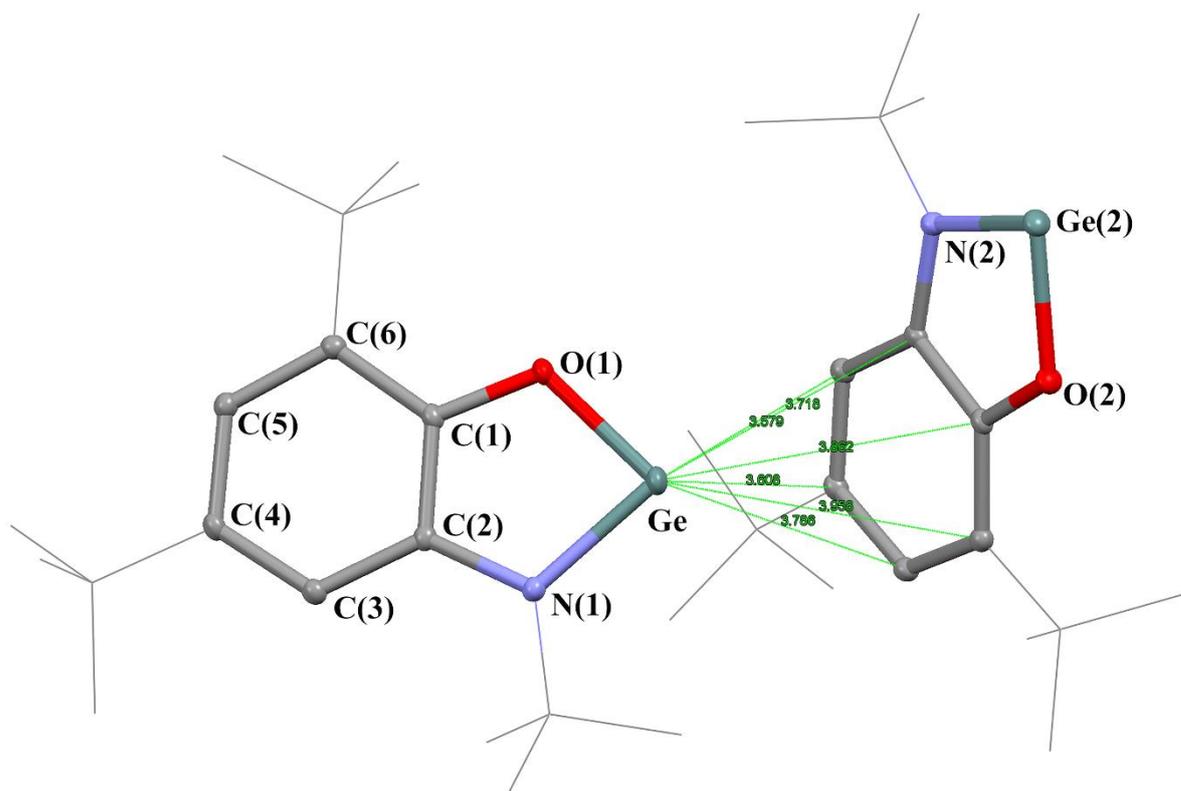
Yield 0.4 g (46%).  $\text{C}_{96}\text{H}_{164}\text{Ge}_4\text{K}_2\text{N}_4\text{O}_{10}$ . Calculated C, 60.59; H, 8.69. Found C, 60.72; H, 8.94.

$^1\text{H}$  (THF- $d_8$ , 20°C,  $\delta$ /ppm.,  $J$ /Hz): 6.84, 6.72, 6.59, 6.53 (d, 2H,  $H_{\text{AP}}$ ); 1.54, 1.26 (s, 18H, N-(Bu $^t$ )); 1.42, 1.20 (s, 36H, Bu $^t$ ).

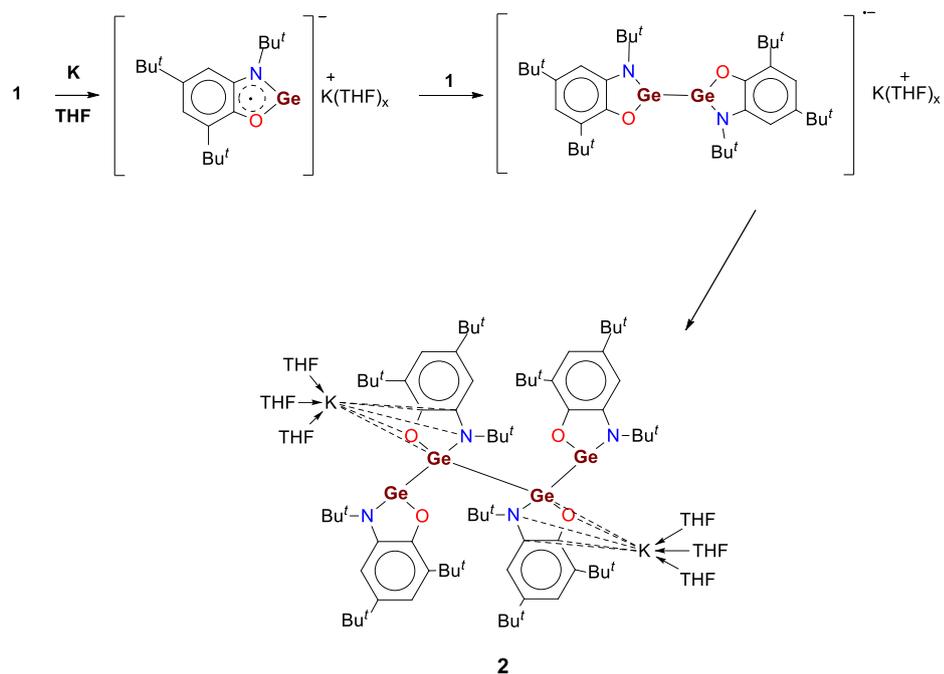
$^{13}\text{C}$  (THF- $d_8$ , 20 °C,  $\delta$ /ppm): 153.7, 147.5 (C-O); 139.7, 138.3, 137.0, 136.6 (C-(Bu $^t$ )); 128.6, 127.9 (C-N); 111.8, 110.4, 109.3, 108.7 ( $C_{\text{aryl}}$ ); 54.0, 50.2 (N-C-(Bu $^t$ )); 34.9, 34.5, 34.0, 33.7 ( $C_{\text{quat}}$ ); 31.5, 31.3, 30.9, 29.7, 29.4 ( $\text{CH}_3(\text{Bu}^t)$ ).

**Table S1** X-Ray crystallographic data and structure refinement for **1** and **2**.

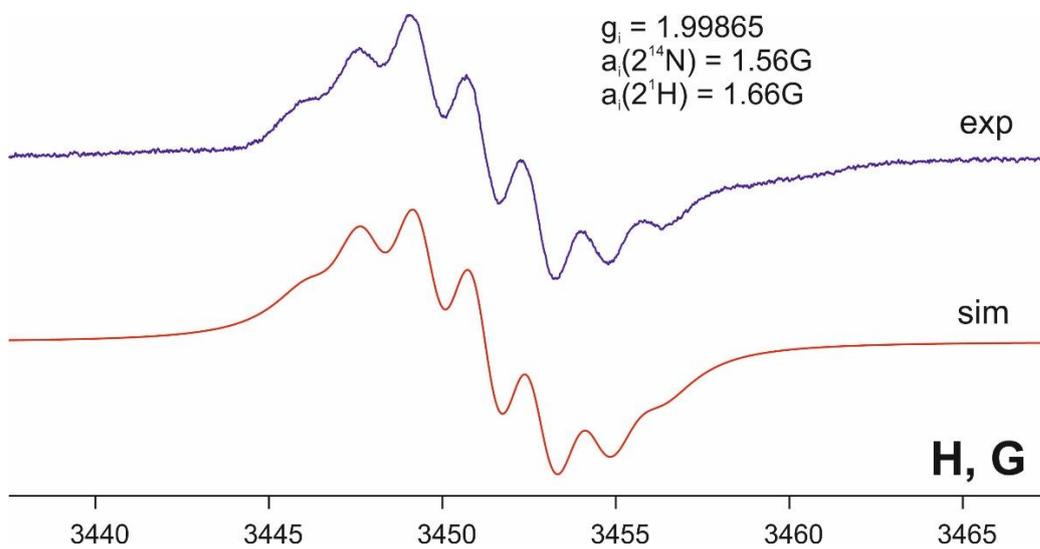
	C <sub>18</sub> H <sub>29</sub> GeNO ( <b>1</b> )	C <sub>96</sub> H <sub>164</sub> Ge <sub>4</sub> K <sub>2</sub> N <sub>4</sub> O <sub>10</sub> ( <b>2</b> )
Formula weight	348.01	1902.86
Crystal system	Orthorhombic	Monoclinic
Space group	P2(1)2(1)2(1)	C2/c
Unit cell dimensions		
<i>a</i> /Å	9.6783(3)	35.0133(8)
<i>b</i> /Å	10.0976(3)	12.05010(10)
<i>c</i> /Å	18.4011(5)	30.1745(7)
<i>a</i> /deg	90	90
<i>β</i> /deg	90	127.731(4)
<i>γ</i> /deg	90	90
<i>V</i> /Å <sup>3</sup>	1798.30(9)	10068.9(5)
<i>Z</i>	4	4
<i>d</i> <sub>calcd</sub> /g cm <sup>-3</sup>	1.285	1.255
Absorption coefficient/mm <sup>-1</sup>	1.703	1.320
<i>F</i> (000)	736	4056
Crystal size/mm	0.200×0.130×0.110	0.846×0.757×0.411
Θ range for data collection/deg	2.915 – 27.989	3.188 – 30.508
Reflections collected	21119	101330
Indep reflections	4285 [ <i>R</i> (int) = 0.0165]	15325 [ <i>R</i> (int) = 0.0249]
Completeness to Θ max	99.1 %	99.5 %
Data/ restraints/parameters	4285 / 0 / 200	15325 / 45 / 558
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0160	<i>R</i> <sub>1</sub> = 0.0253
	<i>wR</i> <sub>2</sub> = 0.0430	<i>wR</i> <sub>2</sub> = 0.0588
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0163	<i>R</i> <sub>1</sub> = 0.0333
	<i>wR</i> <sub>2</sub> = 0.0431	<i>wR</i> <sub>2</sub> = 0.0636
GOF on <i>F</i> <sup>2</sup>	1.077	1.065
Largest diff. peak and hole/e Å <sup>-3</sup>	0.361/-0.323	0.593 / -0.429



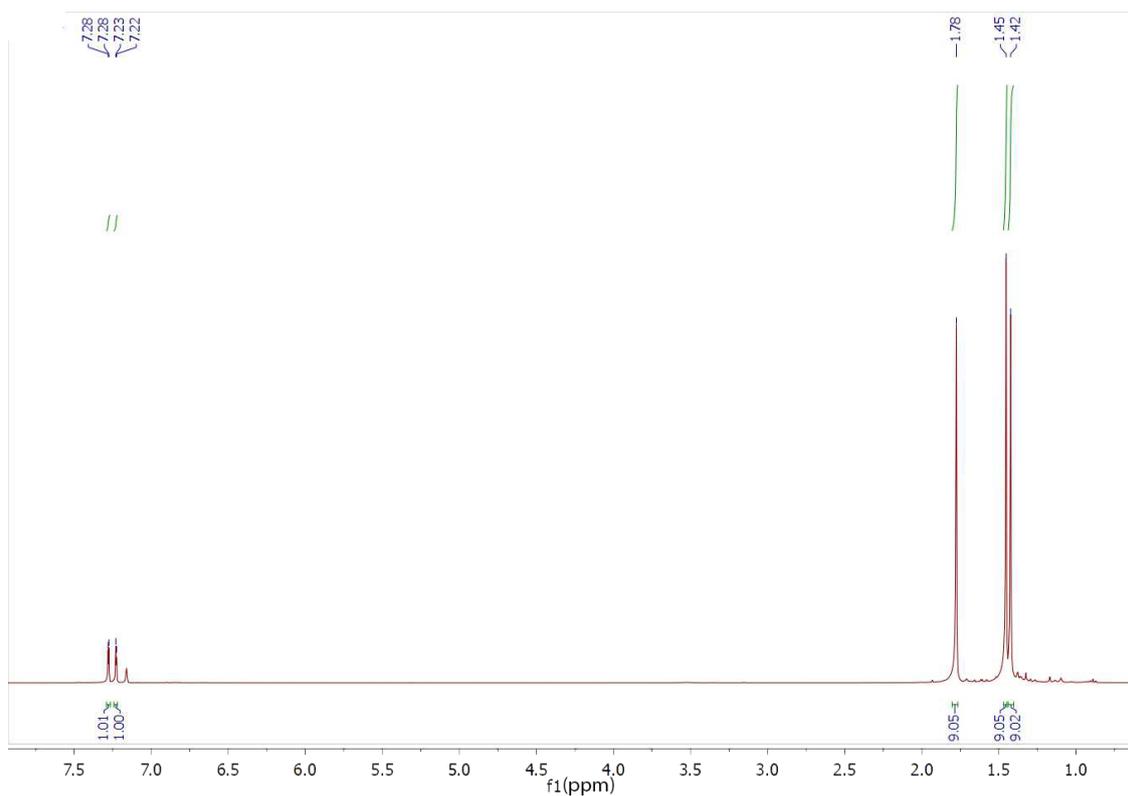
**Figure S1** Intermolecular contacts in the solid state structure of **1**.



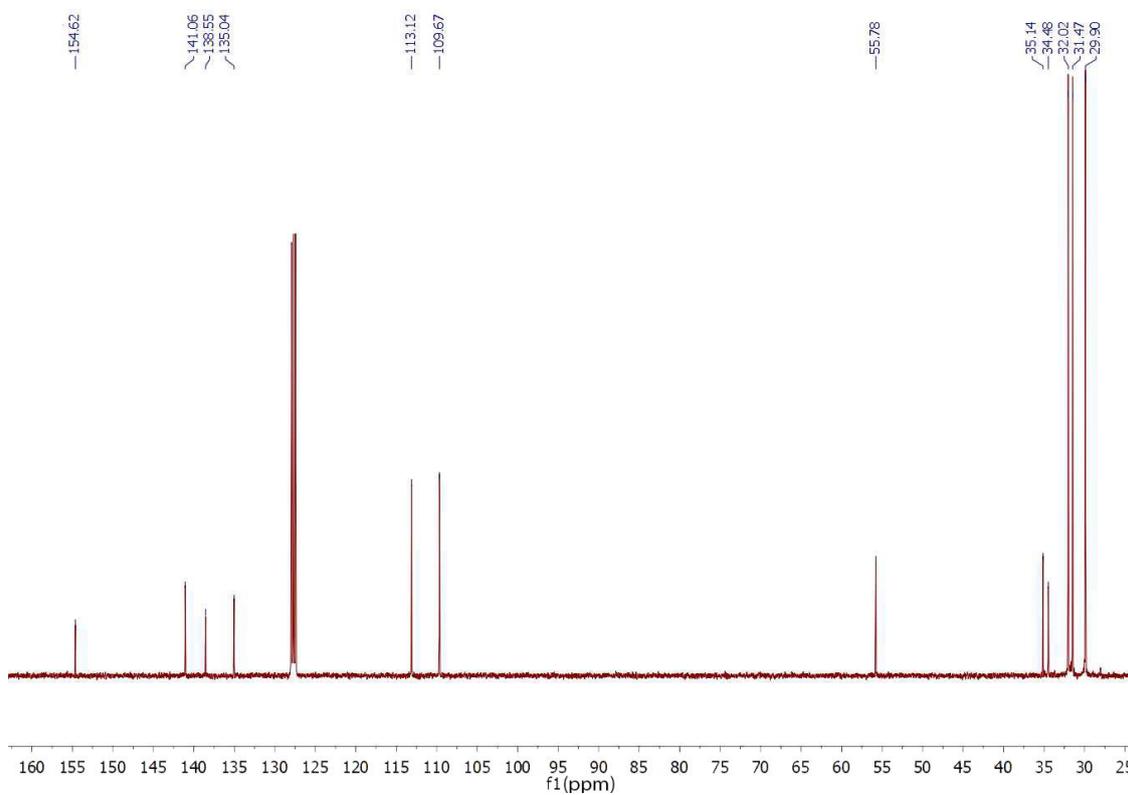
**Scheme S1** Probable mechanism of synthesis of compound **2**.



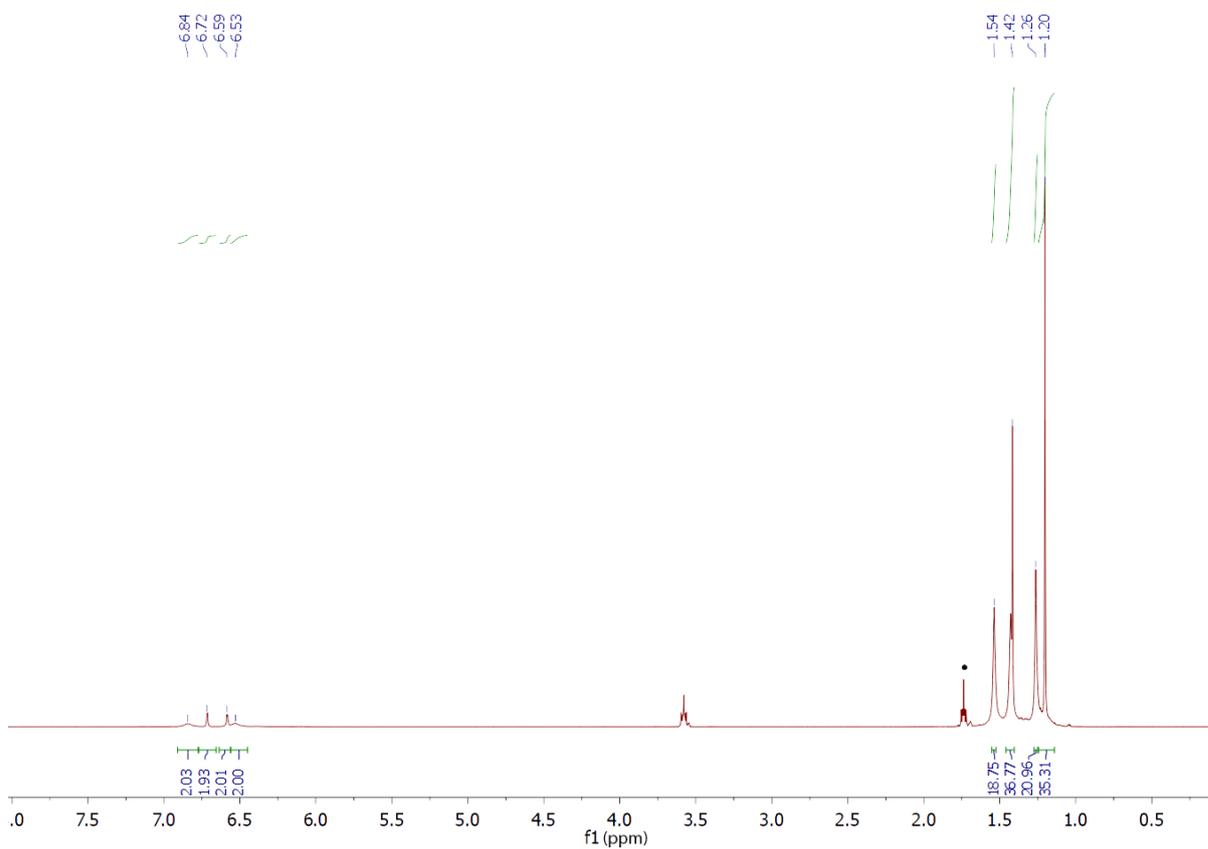
**Figure S2** Calculated and experimental EPR spectra of reaction mixture of **1** and potassium in THF solution at 290 K. HFS parameters are:  $a_i(2^1\text{H}) = 1.66\text{ G}$ ,  $a_i(2^{14}\text{N}) = 1.56\text{ G}$ , and  $g_i = 1.99865$ .



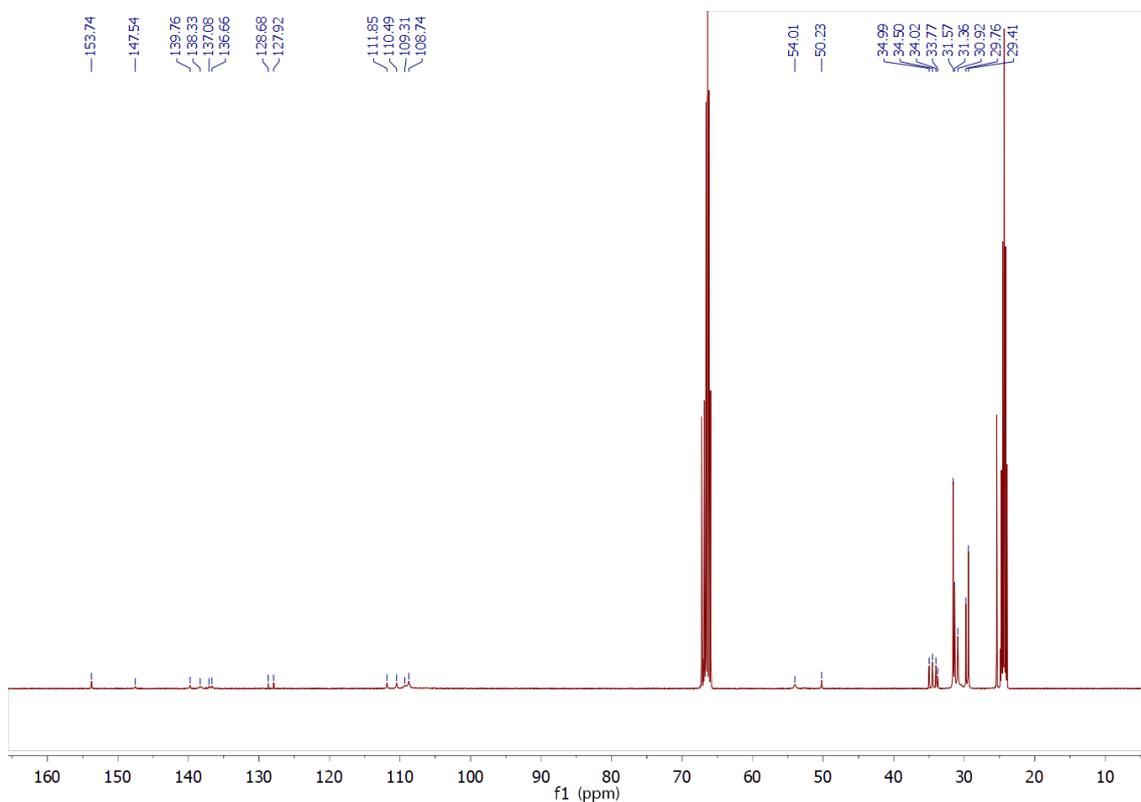
**Figure S3**  $^1\text{H}$  NMR spectra of  $\text{Bu}^t\text{ApGe}$  (**1**) in benzene- $d_6$ .



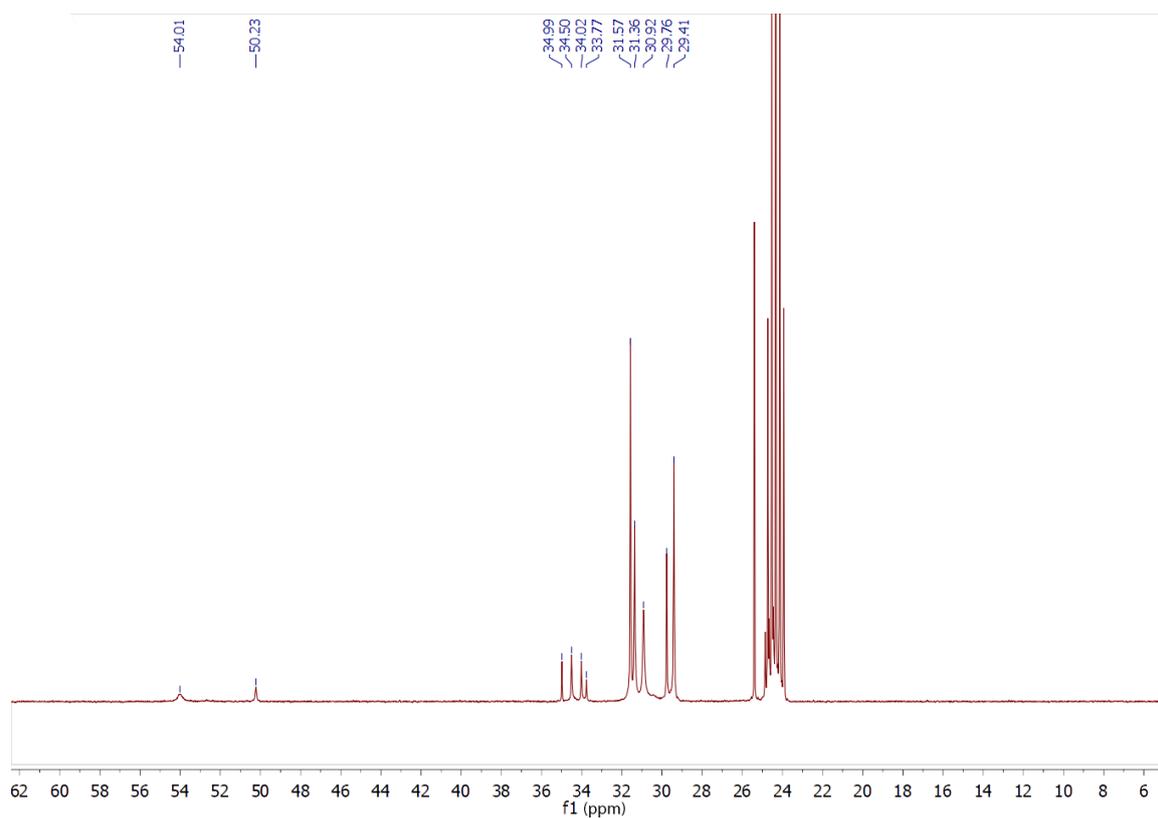
**Figure S4**  $^{13}\text{C}$  NMR spectra of  $\text{Bu}^t\text{ApGe}$  (**1**) in benzene- $d_6$ .



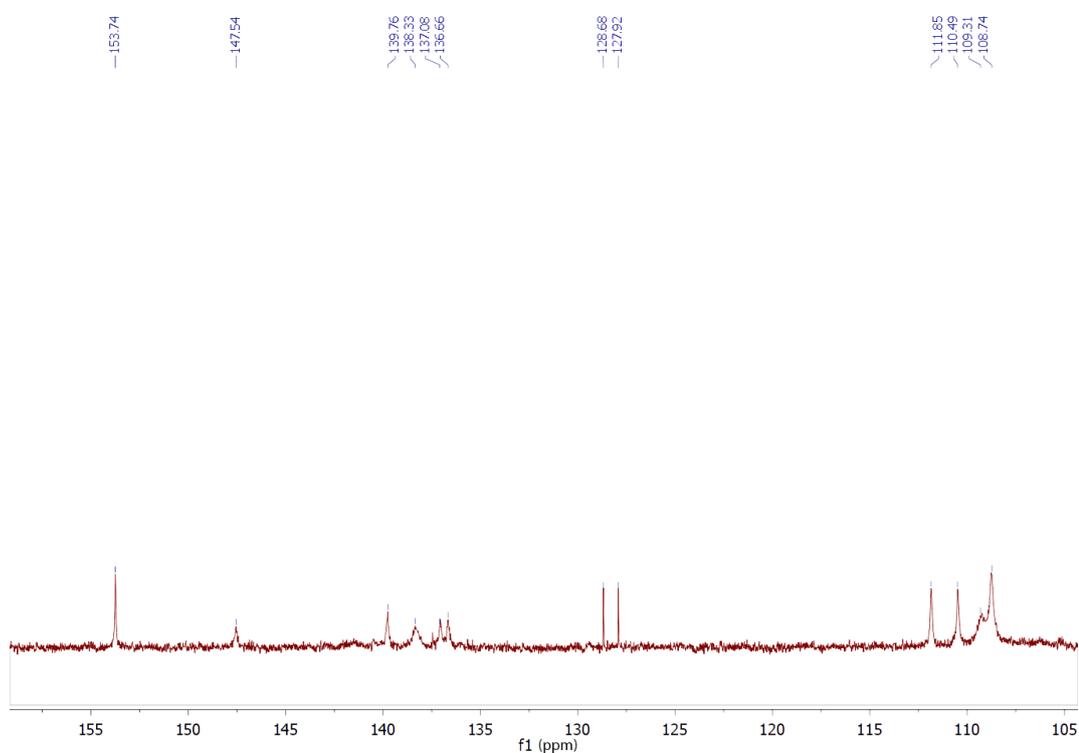
**Figure S5**  $^1\text{H}$  NMR spectra of  $(\text{Bu}^t\text{Ap})_4\text{Ge}_4\text{K}_2(\text{THF})_6(\mathbf{2})$  in tetrahydrofurane- $d_8$ . (●) indicates signals of THF.



**Figure S6**  $^{13}\text{C}$  NMR spectra of  $(\text{Bu}^t\text{Ap})_4\text{Ge}_4\text{K}_2(\text{THF})_6(\mathbf{2})$  in tetrahydrofurane- $d_8$ .



**Figure S7** Alkyl region of  $^{13}\text{C}$  NMR spectra of  $(\text{Bu}^t\text{Ap})_4\text{Ge}_4\text{K}_2(\text{THF})_6$  (**2**) in tetrahydrofuran- $\text{d}_8$ .



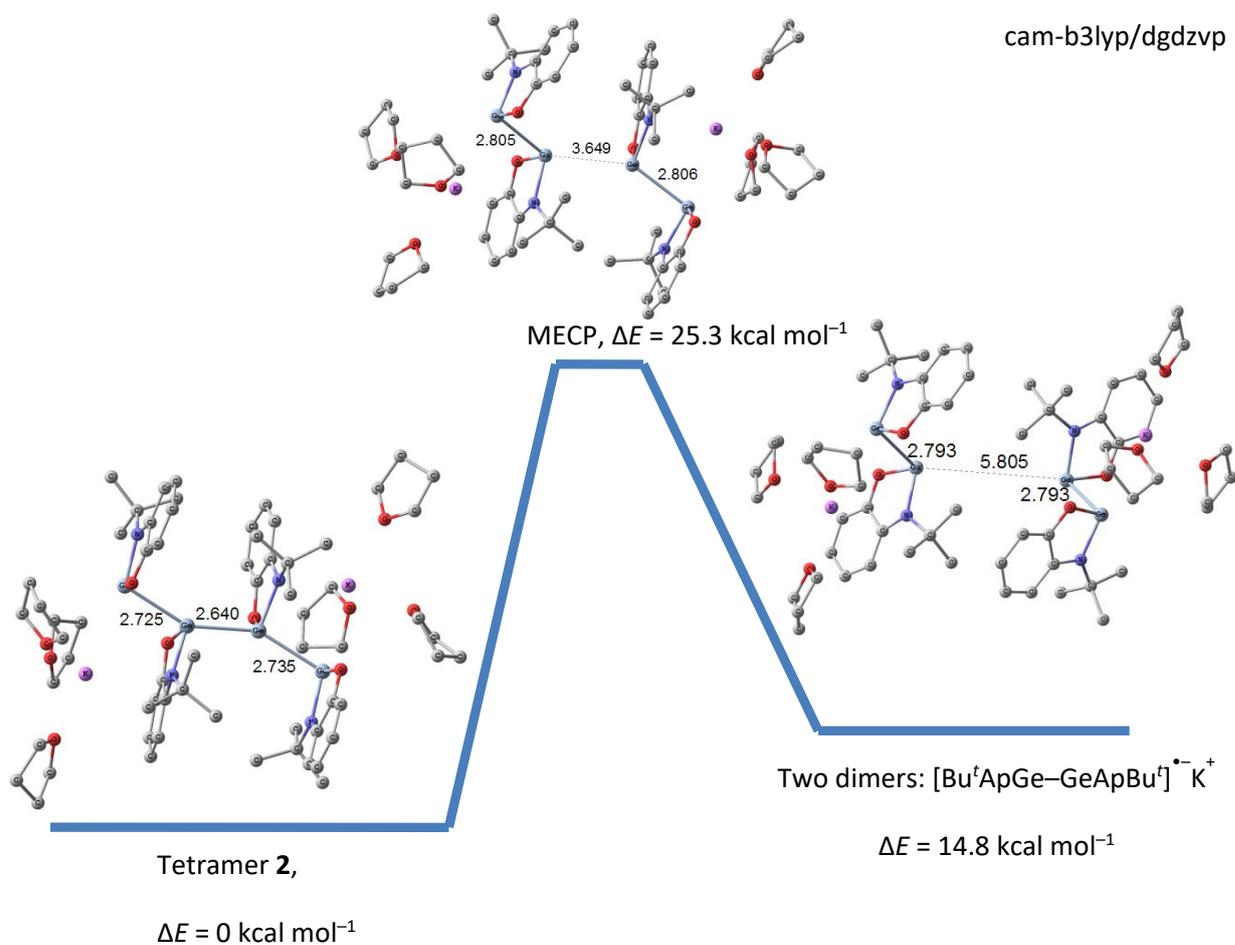
**Figure S8** Aryl region of  $^{13}\text{C}$  NMR spectra of  $(\text{Bu}^t\text{Ap})_4\text{Ge}_4\text{K}_2(\text{THF})_6$  (**2**) in tetrahydrofuran- $\text{d}_8$ .

## DFT Calculations

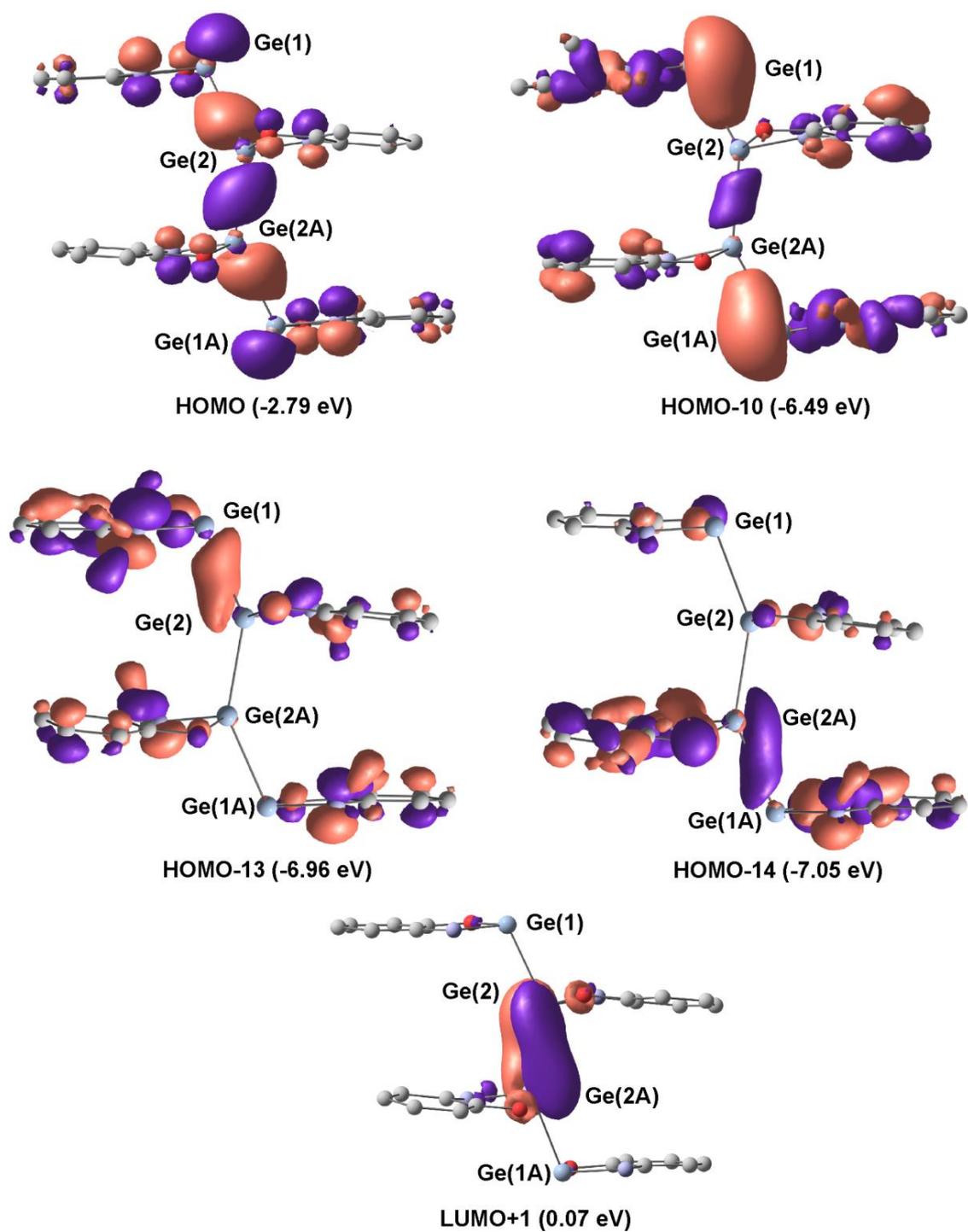
### Calculations of Minimum Energy Crossing Point<sup>S8</sup>

Investigation was carried out on the truncated structure, where Bu<sup>t</sup> substituents in benzene rings were replaced by hydrogen atoms. The truncations were made to minimize computational expense.

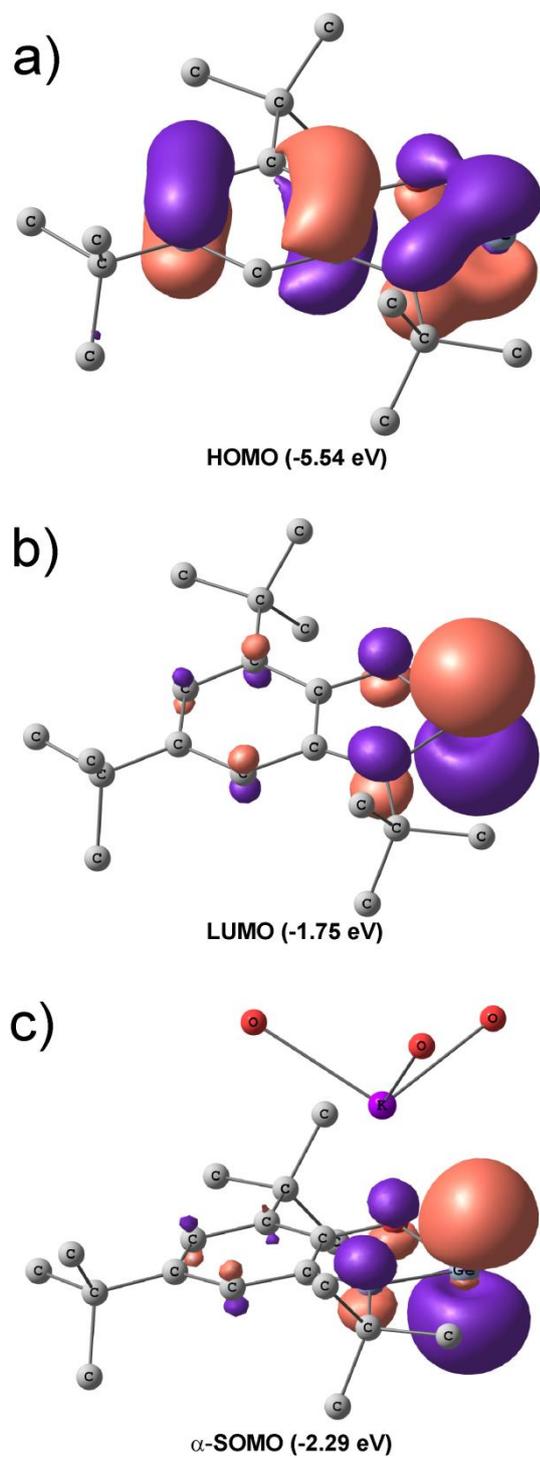
According to the calculations the MECP structure, which is characterized by elongated Ge(2)–Ge(2A) distance up to 3.6 Å, is destabilized by 25.3 kcal mol<sup>-1</sup> with respect to complex **2**, which is a ground state. The descent along the gradient line from MECP along the singlet PES (Potential energy surface) led to the initial compound **2**, while in case of triplet PES, to the structure with two separated radical-ionic [Bu<sup>t</sup>ApGe–GeApBu<sup>t</sup>]<sup>•-•+</sup> K<sup>+</sup> species, destabilized by 14.8 kcal mol<sup>-1</sup> with respect to the ground state.



**Figure S9** Energy profile for dissociation reaction of (Bu<sup>t</sup>Ap)<sub>4</sub>Ge<sub>4</sub>K<sub>2</sub>(THF)<sub>6</sub> producing two doublet particles.



**Figure S10** Selected canonical molecular orbitals for compound 2.



**Figure S11** Selected canonical molecular orbitals: (a) HOMO of **1**; (b) LUMO of **1**; (c)  $\alpha$ -SOMO of intermediate  $[\text{Bu}^t\text{ApGe}]^{\bullet-}\text{K}^+$

## Cartesian coordinates

### Complex 2

32	-3.249918000	-2.218807000	-0.201483000
32	-1.266689000	-0.356684000	-0.050506000
19	-5.108800000	0.608221000	0.655133000
8	-3.466334000	-2.270383000	-2.068628000
8	-1.627394000	0.122569000	1.750465000
8	-5.598675000	-0.193496000	3.223970000
7	-2.453613000	-3.947955000	-0.385553000
7	-2.283439000	1.279143000	-0.485611000
6	-2.825479000	-3.329699000	-2.625579000
6	-2.262502000	-4.275981000	-1.727592000
6	-1.617643000	-5.385757000	-2.290990000
1	-1.165079000	-6.143405000	-1.665748000
6	-1.536900000	-5.542728000	-3.679049000
6	-2.091060000	-4.602685000	-4.538181000
1	-2.021670000	-4.727595000	-5.615127000
6	-2.740993000	-3.486974000	-4.000621000
6	-2.004738000	-4.782541000	0.742576000
6	-2.689300000	-6.161280000	0.716998000
1	-2.453214000	-6.737460000	-0.177652000
1	-3.776136000	-6.038552000	0.752518000
1	-2.382190000	-6.752326000	1.586252000
6	-0.473252000	-4.917846000	0.780614000
1	-0.005572000	-3.935194000	0.875797000
1	-0.068541000	-5.388147000	-0.115791000
1	-0.164769000	-5.518335000	1.642468000
6	-2.427812000	-4.096709000	2.049361000
1	-1.987892000	-3.098185000	2.145910000
1	-2.083738000	-4.687236000	2.903472000
1	-3.516426000	-4.009961000	2.116990000
6	-2.044774000	1.398075000	1.863186000
6	-2.419747000	2.067400000	0.658561000
6	-2.924446000	3.370762000	0.783336000
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6	-2.623966000	3.339101000	3.189809000
1	-2.678367000	3.833454000	4.155954000
6	-2.131056000	2.030873000	3.095910000
6	-2.376517000	1.832783000	-1.855245000
6	-1.968090000	0.730507000	-2.839829000
1	-0.906550000	0.491401000	-2.734308000
1	-2.111303000	1.077129000	-3.867800000
1	-2.552105000	-0.184058000	-2.703622000
6	-3.829436000	2.218855000	-2.198020000
1	-4.268614000	2.921869000	-1.487688000

1	-4.460702000	1.324468000	-2.229739000
1	-3.873426000	2.682056000	-3.189376000
6	-1.425083000	3.021147000	-2.074398000
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1	-1.684517000	3.898382000	-1.481590000
1	-1.428083000	3.320206000	-3.127039000
6	-5.388528000	0.682867000	4.349585000
1	-6.354925000	0.897040000	4.819816000
1	-4.966058000	1.615181000	3.966608000
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1	-4.963209000	-0.404361000	6.188743000
1	-3.622740000	0.611262000	5.648486000
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1	-5.888053000	-2.065896000	4.083976000
32	3.245416000	2.231641000	-0.277842000
32	1.279645000	0.339486000	-0.091991000
19	5.068440000	-0.603999000	0.626502000
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8	1.695103000	-0.136182000	1.699879000
8	5.607942000	0.212998000	3.182022000
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7	2.275883000	-1.303929000	-0.546803000
6	2.761176000	3.343371000	-2.688047000
6	2.197456000	4.276762000	-1.777176000
6	1.527128000	5.379142000	-2.324863000
1	1.071940000	6.126188000	-1.688796000
6	1.423358000	5.541628000	-3.710707000
6	1.979389000	4.614445000	-4.582679000
1	1.892747000	4.743994000	-5.657829000
6	2.654319000	3.506233000	-4.060864000
6	1.982102000	4.774590000	0.699528000
6	2.654242000	6.159073000	0.660338000
1	2.392290000	6.734555000	-0.227575000
1	3.742576000	6.045130000	0.670023000
1	2.362757000	6.746174000	1.537597000
6	0.450768000	4.897174000	0.772347000
1	-0.006456000	3.910804000	0.879224000
1	0.021841000	5.363285000	-0.114812000
1	0.157317000	5.495956000	1.640612000
6	2.439285000	4.091111000	1.996002000
1	2.011074000	3.088264000	2.099998000
1	2.107168000	4.677081000	2.857955000
1	3.529860000	4.015071000	2.040894000
6	2.081176000	-1.422993000	1.804726000
6	2.416760000	-2.098745000	0.592233000
6	2.895891000	-3.412712000	0.706199000
1	3.167609000	-3.981290000	-0.172614000
6	3.007717000	-4.040001000	1.955643000
6	2.647717000	-3.375626000	3.118823000
1	2.712242000	-3.871672000	4.083445000
6	2.180655000	-2.057294000	3.035589000

6	2.357539000	-1.850504000	-1.919642000
6	1.963274000	-0.737966000	-2.898664000
1	0.904253000	-0.486432000	-2.795826000
1	2.105538000	-1.080970000	-3.928015000
1	2.556423000	0.169891000	-2.757318000
6	3.804896000	-2.254342000	-2.265252000
1	4.234372000	-2.966243000	-1.558074000
1	4.448901000	-1.368428000	-2.290583000
1	3.843220000	-2.712186000	-3.259266000
6	1.388757000	-3.024413000	-2.143709000
1	0.368754000	-2.732428000	-1.882262000
1	1.634983000	-3.908255000	-1.555155000
1	1.387331000	-3.318670000	-3.197730000
6	5.400147000	-0.645547000	4.321455000
1	6.366604000	-0.847023000	4.797131000
1	4.983866000	-1.586412000	3.952828000
6	4.432337000	0.091659000	5.264532000
1	4.965395000	0.468867000	6.142020000
1	3.630715000	-0.560945000	5.615628000
6	3.915938000	1.256417000	4.408792000
1	3.056464000	0.953028000	3.804777000
1	3.636485000	2.130631000	5.001874000
6	5.107160000	1.519327000	3.501050000
1	4.851062000	2.014967000	2.562333000
1	5.888165000	2.100044000	4.012784000
8	-6.759639000	-0.748337000	-1.133558000
6	-6.512667000	-0.850764000	-2.555347000
1	-5.433461000	-0.917154000	-2.719858000
1	-6.906182000	0.051486000	-3.032830000
6	-7.204022000	-2.131557000	-3.009879000
6	-7.079172000	-3.011045000	-1.763979000
6	-7.282381000	-1.997938000	-0.642883000
1	-8.345250000	-1.863686000	-0.404641000
1	-6.746537000	-2.262588000	0.273315000
1	-6.722523000	-2.565964000	-3.888240000
1	-8.256387000	-1.943540000	-3.247408000
1	-7.810926000	-3.821708000	-1.728580000
1	-6.075579000	-3.440020000	-1.709994000
8	-6.824537000	2.683870000	0.304813000
6	-7.025357000	3.832552000	1.149687000
1	-6.046397000	4.233475000	1.422990000
1	-7.539454000	3.508808000	2.062877000
6	-7.885968000	4.800942000	0.342741000
6	-8.709932000	3.844819000	-0.524211000
6	-7.690354000	2.756700000	-0.843183000
1	-8.126646000	1.767913000	-1.002958000
1	-7.088429000	3.020819000	-1.721674000
1	-7.257783000	5.439501000	-0.285846000
1	-8.495789000	5.445028000	0.980137000
1	-9.544013000	3.430539000	0.050536000
1	-9.114293000	4.313652000	-1.424103000
8	6.790227000	0.740483000	-1.096192000
6	6.535989000	1.036805000	-2.489217000
1	5.482780000	0.847275000	-2.703855000
1	7.161650000	0.371702000	-3.097199000

6	6.902365000	2.504124000	-2.685504000
6	7.979925000	2.717978000	-1.619778000
6	7.460787000	1.853107000	-0.476931000
1	8.249603000	1.459408000	0.170386000
1	6.739323000	2.405578000	0.138169000
1	6.027754000	3.128901000	-2.488401000
1	7.251126000	2.710783000	-3.699894000
1	8.949380000	2.348030000	-1.969072000
1	8.097519000	3.763865000	-1.327203000
8	6.789656000	-2.676468000	0.284329000
6	7.630534000	-2.769939000	-0.880447000
1	8.065646000	-1.784934000	-1.064188000
1	7.010193000	-3.044799000	-1.742668000
6	8.651702000	-3.857387000	-0.565660000
6	7.837942000	-4.801202000	0.324067000
6	6.991627000	-3.821830000	1.133645000
1	6.013128000	-4.215327000	1.419310000
1	7.516968000	-3.495334000	2.039404000
1	9.495800000	-3.439543000	-0.008274000
1	9.040598000	-4.337429000	-1.466482000
1	7.198868000	-5.444766000	-0.288227000
1	8.455192000	-5.440365000	0.959281000
1	-1.027784000	-6.415217000	-4.080290000
1	-3.186094000	-2.727944000	-4.638512000
1	3.356463000	-5.068886000	1.997741000
1	1.874870000	-1.505899000	3.920465000
1	3.103490000	2.758415000	-4.708894000
1	0.895002000	6.408077000	-4.100004000
1	-1.794719000	1.486269000	3.973889000
1	-3.392742000	5.017114000	2.085508000

**MECP structure**

32	-3.835013000	-2.196164000	-0.384005000
32	-1.787443000	-0.345135000	0.113835000
19	-5.450987000	0.696502000	0.486010000
8	-3.518211000	-2.532547000	-2.199775000
8	-2.430527000	0.049747000	1.862742000
8	-7.351014000	-0.654812000	1.964495000
7	-2.882268000	-3.817276000	-0.045075000
7	-2.481176000	1.440676000	-0.311625000
6	-2.754705000	-3.636411000	-2.388854000
6	-2.392552000	-4.370377000	-1.226579000
6	-1.622052000	-5.526830000	-1.411876000
1	-1.311131000	-6.126875000	-0.567839000
6	-1.229074000	-5.931519000	-2.691249000
6	-1.587889000	-5.195353000	-3.813991000
1	-1.274801000	-5.512256000	-4.805126000
6	-2.357025000	-4.038628000	-3.655837000
6	-2.625090000	-4.364609000	1.298785000
6	-3.228734000	-5.772732000	1.448854000
1	-2.789388000	-6.500681000	0.767319000
1	-4.303502000	-5.738604000	1.245546000
1	-3.082505000	-6.137676000	2.470800000
6	-1.123338000	-4.358210000	1.637701000
1	-0.725494000	-3.341127000	1.586949000
1	-0.531443000	-4.975053000	0.961321000
1	-0.963832000	-4.731434000	2.654658000
6	-3.325364000	-3.466149000	2.329339000

1	-2.951845000	-2.437443000	2.306691000
1	-3.145832000	-3.855863000	3.335846000
1	-4.408017000	-3.451532000	2.166565000
6	-2.779428000	1.340774000	2.021891000
6	-2.788533000	2.150973000	0.847472000
6	-3.134377000	3.502554000	1.006510000
1	-3.121621000	4.181416000	0.164716000
6	-3.478953000	4.016684000	2.263116000
6	-3.495268000	3.202617000	3.388146000
1	-3.756285000	3.608398000	4.361751000
6	-3.141466000	1.853899000	3.261341000
6	-2.294393000	2.079135000	-1.633218000
6	-1.902472000	0.986441000	-2.636924000
1	-0.929568000	0.553918000	-2.390175000
1	-1.818289000	1.417225000	-3.638804000
1	-2.639876000	0.177991000	-2.676499000
6	-3.607543000	2.700987000	-2.145764000
1	-4.000545000	3.478212000	-1.489301000
1	-4.379809000	1.932459000	-2.261972000
1	-3.442342000	3.154325000	-3.128479000
6	-1.161092000	3.116949000	-1.608639000
1	-0.235339000	2.651687000	-1.262495000
1	-1.368008000	3.960183000	-0.949091000
1	-0.976676000	3.518515000	-2.609720000
6	-8.030317000	-0.203598000	3.144910000
1	-9.062481000	0.064409000	2.886626000
1	-7.516898000	0.694656000	3.495563000
6	-7.988401000	-1.367702000	4.158290000
1	-9.001425000	-1.681369000	4.422055000
1	-7.479595000	-1.086727000	5.082101000
6	-7.241957000	-2.484380000	3.406234000
1	-6.177260000	-2.473837000	3.651353000
1	-7.632721000	-3.480839000	3.624495000
6	-7.433640000	-2.085428000	1.949274000
1	-6.663217000	-2.455224000	1.269374000
1	-8.420997000	-2.393950000	1.575234000
32	3.846066000	2.214601000	-0.363408000
32	1.791126000	0.367287000	0.125679000
19	5.452492000	-0.680668000	0.533285000
8	3.545556000	2.541858000	-2.183379000
8	2.413923000	-0.015158000	1.884330000
8	7.301173000	0.720551000	2.034117000
7	2.884576000	3.834372000	-0.040535000
7	2.483392000	-1.423528000	-0.278441000
6	2.782487000	3.643639000	-2.384868000
6	2.406140000	4.381124000	-1.229534000
6	1.634544000	5.535236000	-1.427900000
1	1.312625000	6.137298000	-0.589747000
6	1.255460000	5.934278000	-2.713193000
6	1.628866000	5.195231000	-3.829047000
1	1.326814000	5.508113000	-4.824883000
6	2.398467000	4.040511000	-3.657971000
6	2.605280000	4.383388000	1.298573000
6	3.198541000	5.795375000	1.453942000
1	2.766334000	6.518999000	0.763345000
1	4.276665000	5.766673000	1.268194000
1	3.033610000	6.162184000	2.472393000
6	1.098837000	4.368917000	1.615783000
1	0.708565000	3.348882000	1.564864000
1	0.512690000	4.978144000	0.927559000
1	0.922186000	4.746397000	2.628352000
6	3.296126000	3.491775000	2.341185000
1	2.929102000	2.460784000	2.316517000

1	3.100198000	3.883390000	3.343935000
1	4.381076000	3.483410000	2.193666000
6	2.760597000	-1.304962000	2.056879000
6	2.779958000	-2.124578000	0.889273000
6	3.122263000	-3.475058000	1.062257000
1	3.117132000	-4.160603000	0.225809000
6	3.453180000	-3.979875000	2.326442000
6	3.459400000	-3.156918000	3.445057000
1	3.710605000	-3.555446000	4.424442000
6	3.109286000	-1.808828000	3.304043000
6	2.303161000	-2.073249000	-1.595245000
6	1.919457000	-0.988478000	-2.610769000
1	0.946893000	-0.550592000	-2.372335000
1	1.838189000	-1.428116000	-3.609064000
1	2.659802000	-0.183039000	-2.654412000
6	3.617507000	-2.702681000	-2.095214000
1	4.004102000	-3.476700000	-1.431152000
1	4.392694000	-1.937315000	-2.211605000
1	3.456959000	-3.162284000	-3.075810000
6	1.167453000	-3.108247000	-1.568095000
1	0.241269000	-2.638005000	-1.230073000
1	1.369318000	-3.946667000	-0.900852000
1	0.987060000	-3.517210000	-2.566880000
6	7.993847000	0.268573000	3.205683000
1	9.029032000	0.020594000	2.938839000
1	7.497445000	-0.641391000	3.550070000
6	7.938684000	1.422852000	4.229941000
1	8.947908000	1.731874000	4.512757000
1	7.415140000	1.133094000	5.142748000
6	7.202735000	2.548165000	3.478951000
1	6.138259000	2.547841000	3.724927000
1	7.603304000	3.540482000	3.698183000
6	7.388791000	2.150628000	2.020522000
1	6.618735000	2.523992000	1.342750000
1	8.376665000	2.456014000	1.644633000
8	-6.761281000	0.159585000	-1.887196000
6	-6.332563000	-0.594744000	-3.032461000
1	-5.259797000	-0.770234000	-2.945918000
1	-6.531059000	-0.004590000	-3.937463000
6	-7.157361000	-1.889600000	-3.011544000
6	-8.359167000	-1.556904000	-2.096566000
6	-8.166152000	-0.072497000	-1.770323000
1	-8.701531000	0.564037000	-2.490710000
1	-8.468208000	0.209557000	-0.759625000
1	-6.563385000	-2.708190000	-2.603295000
1	-7.468884000	-2.174227000	-4.019196000
1	-9.323309000	-1.741855000	-2.576884000
1	-8.323180000	-2.153004000	-1.182064000
8	-7.285607000	2.714636000	0.334186000
6	-8.082363000	3.337362000	1.358234000
1	-7.433337000	3.629354000	2.189644000
1	-8.799557000	2.592431000	1.718430000
6	-8.778365000	4.539631000	0.704973000
6	-8.685582000	4.217724000	-0.790559000
6	-7.343433000	3.504628000	-0.862857000
1	-7.231128000	2.826223000	-1.710637000
1	-6.512654000	4.222845000	-0.870335000
1	-8.234558000	5.462463000	0.925507000
1	-9.804842000	4.663864000	1.056373000
1	-9.488499000	3.538331000	-1.093356000
1	-8.727369000	5.105704000	-1.425345000
8	6.774319000	-0.198674000	-1.854425000
6	6.285589000	0.481564000	-3.030486000

1	5.261521000	0.809744000	-2.845877000
1	6.294500000	-0.220488000	-3.874670000
6	7.249496000	1.636750000	-3.256011000
6	8.580468000	1.027534000	-2.807471000
6	8.158211000	0.136741000	-1.637143000
1	8.739420000	-0.788683000	-1.571569000
1	8.238620000	0.657726000	-0.676447000
1	6.968119000	2.481890000	-2.621416000
1	7.256737000	1.976284000	-4.294035000
1	9.011995000	0.424172000	-3.612405000
1	9.322254000	1.772912000	-2.511537000
8	7.263446000	-2.720518000	0.420019000
6	7.334443000	-3.516858000	-0.771825000
1	7.226705000	-2.843553000	-1.624532000
1	6.506071000	-4.237786000	-0.782571000
6	8.677846000	-4.226396000	-0.683807000
6	8.759514000	-4.537012000	0.814646000
6	8.060010000	-3.328946000	1.452633000
1	7.410150000	-3.612371000	2.286322000
1	8.775574000	-2.578596000	1.804973000
1	9.482540000	-3.548027000	-0.984668000
1	8.726762000	-5.118712000	-1.311972000
1	8.212865000	-5.457503000	1.038058000
1	9.783179000	-4.659645000	1.174761000
1	-0.630607000	-6.833017000	-2.796401000
1	-2.658642000	-3.435974000	-4.508249000
1	3.693746000	-5.035535000	2.422535000
1	3.073933000	-1.136240000	4.156882000
1	2.710973000	3.435572000	-4.504448000
1	0.656290000	6.834161000	-2.828440000
1	-3.113664000	1.188277000	4.119900000
1	-3.721381000	5.072974000	2.348672000

**2[<sup>t-Bu</sup>ApGe-GeAp<sup>t-Bu</sup>]<sup>-</sup>K<sup>+</sup>**

32	-4.042511000	-2.273834000	-0.244821000
32	-2.835760000	-0.674531000	1.701625000
19	-6.173562000	0.505505000	-0.252415000
8	-2.966365000	-1.885167000	-1.737593000
8	-4.339700000	-0.672692000	2.865761000
8	-8.234464000	-0.927808000	0.814242000
7	-3.011079000	-3.881148000	-0.091017000
7	-3.430146000	1.133035000	1.245942000
6	-2.002545000	-2.816293000	-1.932292000
6	-1.994664000	-3.924603000	-1.040633000
6	-0.999545000	-4.893869000	-1.236072000
1	-0.930848000	-5.759153000	-0.590937000
6	-0.069971000	-4.772621000	-2.274908000
6	-0.102905000	-3.686021000	-3.140188000
1	0.620654000	-3.596792000	-3.945749000
6	-1.078992000	-2.700717000	-2.960813000
6	-3.197284000	-4.884462000	0.972208000
6	-3.510396000	-6.272122000	0.383403000
1	-2.702154000	-6.669026000	-0.230533000
1	-4.404409000	-6.215556000	-0.244910000
1	-3.701659000	-6.989789000	1.187970000
6	-1.981803000	-4.934427000	1.915630000
1	-1.812224000	-3.950132000	2.360980000
1	-1.063037000	-5.227581000	1.407001000
1	-2.159018000	-5.650165000	2.725168000
6	-4.412725000	-4.473029000	1.816516000
1	-4.275941000	-3.494074000	2.287492000
1	-4.567709000	-5.200378000	2.618640000
1	-5.324054000	-4.446757000	1.210754000

6	-4.957799000	0.519088000	2.932089000
6	-4.476334000	1.546428000	2.065923000
6	-5.122935000	2.791897000	2.124555000
1	-4.796887000	3.614023000	1.501671000
6	-6.184816000	3.014159000	3.011624000
6	-6.632415000	2.003756000	3.852791000
1	-7.443359000	2.185931000	4.552638000
6	-6.011970000	0.750263000	3.807617000
6	-2.614161000	2.056637000	0.425166000
6	-1.461504000	1.256513000	-0.195450000
1	-0.769577000	0.902759000	0.573659000
1	-0.891134000	1.891341000	-0.878404000
1	-1.827424000	0.394754000	-0.765020000
6	-3.431475000	2.639897000	-0.743592000
1	-4.331576000	3.168082000	-0.421918000
1	-3.727471000	1.839331000	-1.430465000
1	-2.815610000	3.341963000	-1.314247000
6	-1.989503000	3.175401000	1.275910000
1	-1.408178000	2.736539000	2.091787000
1	-2.728134000	3.845921000	1.717784000
1	-1.311129000	3.773412000	0.660092000
6	-9.052826000	-0.394296000	1.872954000
1	-10.065125000	-0.221751000	1.489410000
1	-8.619151000	0.562798000	2.171834000
6	-9.039414000	-1.430461000	3.013656000
1	-10.024241000	-1.892880000	3.122951000
1	-8.776104000	-0.976590000	3.970702000
6	-8.003569000	-2.466883000	2.552267000
1	-6.999707000	-2.197180000	2.890886000
1	-8.228458000	-3.477917000	2.900410000
6	-8.081413000	-2.335669000	1.038807000
1	-7.180687000	-2.659558000	0.513063000
1	-8.950012000	-2.871979000	0.629996000
32	4.021568000	2.264737000	-0.195422000
32	2.818025000	0.641602000	1.733253000
19	6.168940000	-0.489004000	-0.214502000
8	2.958397000	1.872712000	-1.696079000
8	4.322086000	0.631894000	2.897506000
8	8.229667000	0.933809000	0.866071000
7	2.979147000	3.864998000	-0.044181000
7	3.419673000	-1.159223000	1.257655000
6	1.994283000	2.801395000	-1.898897000
6	1.973389000	3.907902000	-1.005017000
6	0.978633000	4.875416000	-1.210069000
1	0.900612000	5.739414000	-0.564231000
6	0.061547000	4.754429000	-2.260126000
6	0.106997000	3.669758000	-3.127118000
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1	-6.317261000	-0.058323000	4.466070000
1	-6.643158000	3.999274000	3.049276000

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