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Supporting Information

Porous Ge@C materials via Twin polymerization of germanium(II) salicyl alcoholates for Li-ion batteries

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Syntheses

5-bromo-2-hydroxybenzaldehyde were purchased from Merck Schuchardt OHG (Hohenbrunn). 2-Hydroxybenzyl alcohol and 4-methylphenol were purchased from Alfa Aesar GmbH & Co KG (Karlsruhe). 2-Hydroxy-5-methylbenzaldehyde[1] were synthesized according to the literature procedures. 2-Hydroxy-5-methylbenzyl alcohol, 5-bromo-2-hydroxybenzyl alcohol[2] were synthesized according to modified literature procedures.

S.1 General synthesis procedure of substituted (in 5 position) 2-hydroxybenzyl alcohol[2]

The compounds were prepared according to the literature using a modified synthetic procedure – exemplified for 5-bromo-2-hydroxybenzyl alcohol here: 5-bromo-2-hydroxybenzaldehyde (10.1 g, 50 mmol) was dissolved in 250 mL of ethanol at 0 °C. $NaBH_4$ (1.88 g, 50 mmol) was added in portions (~ 0.3 g) to the stirred solution. The mixture was stirred at room temperature for 18 h. After removal of ethanol under reduced pressure (10^{-2} mbar) the resulting pale yellow solid was dissolved in 200 mL of a saturated, aqueous NH_4Cl solution. The crude product was extracted with diethyl ether (3 times 80 mL). The organic phase was washed with brine (3 times 20 mL) and dried with $MgSO_4$ for 2 h. After removal of $MgSO_4$ by filtration and excess solvent under reduced pressure (10^{-2} mbar) the product was purified by flash chromatography with silica (eluent: *n*-hexane / ethyl acetate – volume ratio of 8 / 2) to give a colorless solid after evaporation of the solvent. yield: 8.52 g, 84 %; mp 104–107 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C, TMS): δ = 2.21 [s, H; OH(CH_2OH)], 4.84 (s, 2 H, CH_2), 6.77 (d, H, H_α/C_6H_3, $^3J_{ortho}$ = 8.6 Hz), 7.16 (d, H, H_γ/C_6H_3, $^4J_{meta}$ = 2.4 Hz), 7.30 [s, H, OH(C_6H_3)], 7.30 ppm (d d, H, H_β/C_6H_3, $^3J_{ortho}$ = 8.6 Hz, $^4J_{meta}$ = 2.4 Hz); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 25 °C, TMS): δ = 64.2 (CH_2), 111.9 (C_6H_3), 118.5 (C_6H_3), 126.4 (C_6H_3), 130.3 (C_6H_3), 132.2 (C_6H_3), 155.3 ppm (C_6H_3). *for 2-hydroxy-5-methylbenzyl alcohol*: yield: 5.18 g, 75 %; mp 103–107 °C; ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C, TMS): δ = 2.11 [d, H; OH(CH_2OH), $^3J_{CH2OH}$ = 4.4 Hz], 2.26 (s, 3 H, CH_3), 4.83 (d, 2 H, CH_2, $^3J_{CH2OH}$ = 4.4 Hz), 6.79 (d, H, H_α/C_6H_3, $^3J_{ortho}$ = 8.2 Hz), 6.85 (d, H, H_γ/C_6H_3, $^4J_{meta}$ = 1.7 Hz), 6.96 [s, H, OH(C_6H_3)], 7.01 ppm (d d, H, H_β/C_6H_3, $^3J_{ortho}$ = 8.2 Hz, $^4J_{meta}$ = 1.7 Hz); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, 25 °C, TMS): δ =

20.4 (s, CH_3), 64.7 (CH_2), 116.5 (C_6H_3), 124.4 (C_6H_3), 128.3 (C_6H_3), 129.3 (C_6H_3), 129.9 (C_6H_3), 153.7 ppm (C_6H_3).

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2. B. Zeynizadeh and T. Behyar, *Z. Naturforsch. B*, 2005, **60**, 453-457.

Analyses

*A1 Single crystal X-ray diffraction analysis structure of (**1**)$_4$*

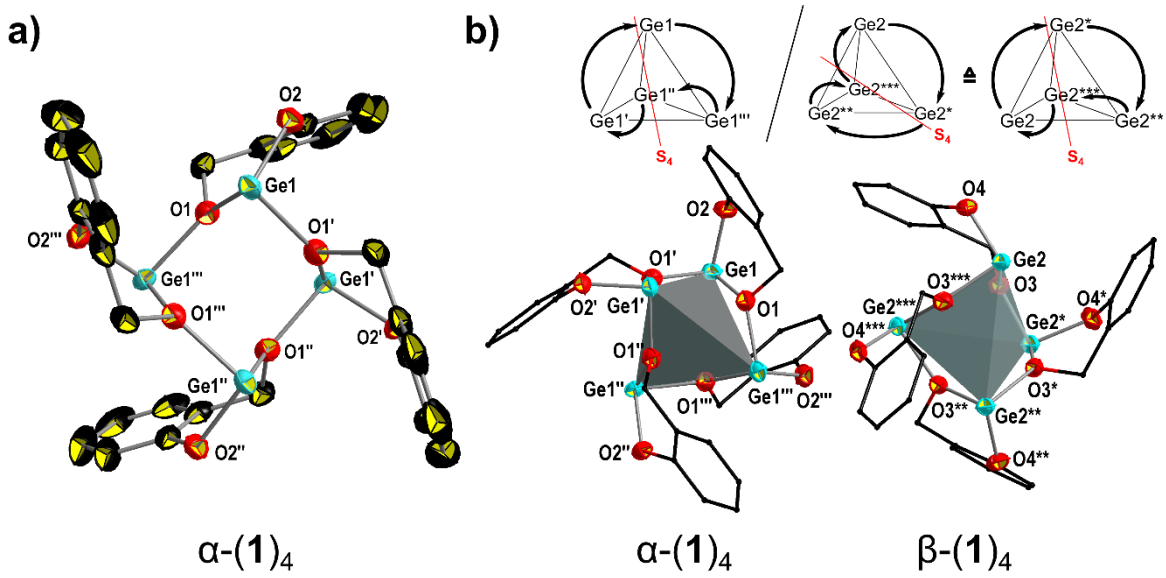

Figure S1 Molecular structure in the solid state of a) α-(**1**)$_4$ and b) α-(**1**)$_4$ and β-(**1**)$_4$ with salicyl alcoholate moieties depicted in wireframe style and the tetrahedron spanned by the germanium atoms highlighted in grey. The scheme in b) illustrates the coordination pattern of the bridging benzylic oxygen atoms as indicated by the direction of the arrows and the symmetry of α-(**1**)$_4$ and β-(**1**)$_4$. Thermal ellipsoids are drawn with 50% probability. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and bond angles [°]: Ge1-O1 1.987(3), Ge1-O2 1.884(3), Ge1-O1' 2.025(3), Ge2-O3 1.973(4), Ge2-O4 1.857(3), Ge2-O3*** 1.997(3); Ge1-O1-Ge1' 126.37(16), Ge2-O3-Ge2* 126.87(18), O1-Ge1-O2 91.36(13), O1-Ge1-O1' 85.29(14), O2-Ge1-O1' 94.14(12), O3-Ge2-O4 91.30(14), O3-Ge2-O3*** 87.53(15), O4-Ge2-O3*** 93.91(14). Symmetry transformations used to generate equivalent atoms: ' = x-0.5, -y+1.5, -z+0.5; '' = -x+2, -y+1, z; ''' = -x+1.5, y+0.5, -z+0.5; * = -x+1, y, -z+1; ** = -x+1, -y+1, z; *** = x, -y+1, -z+1.

A2 Temperature-dependent powder X-ray diffraction

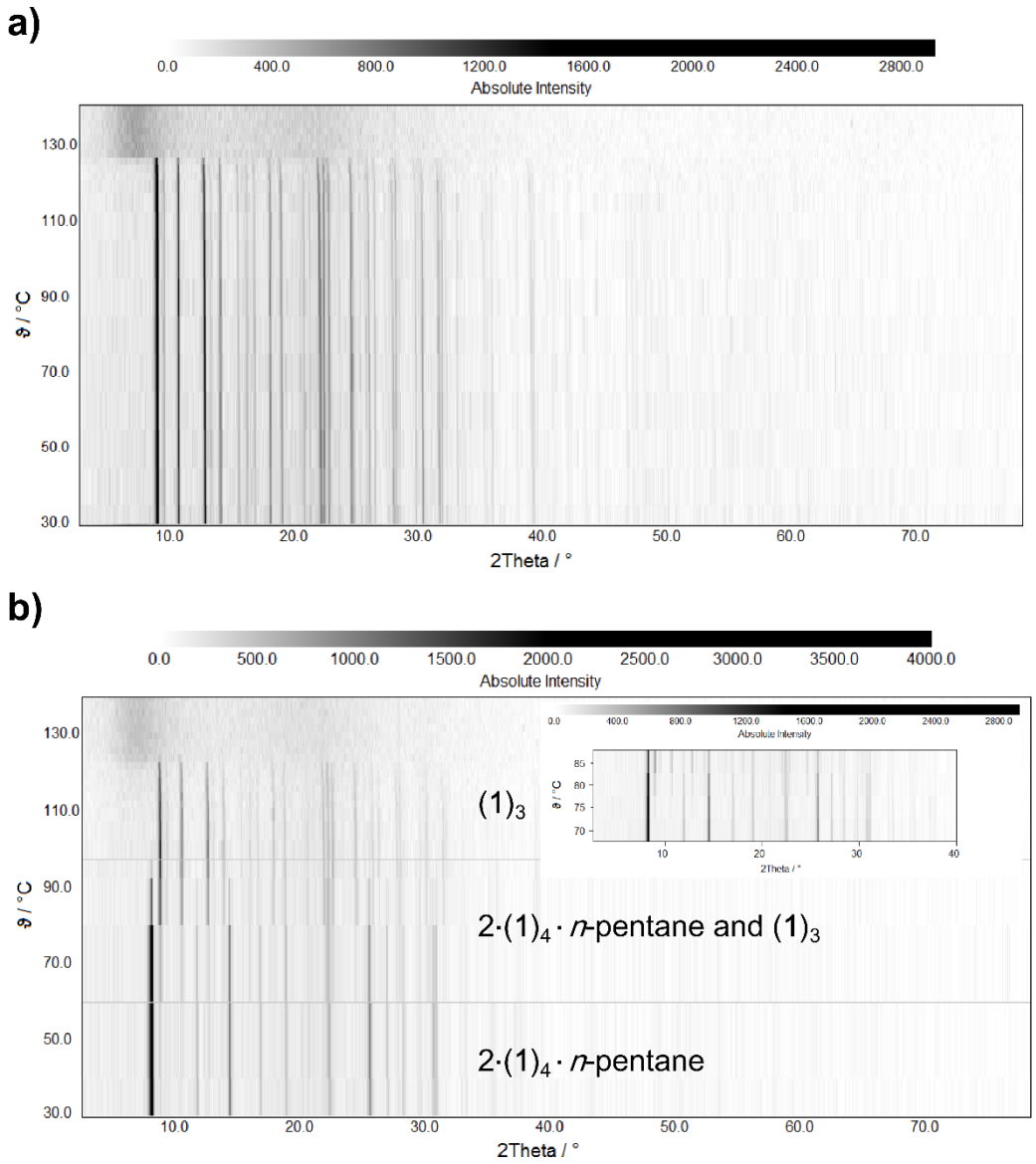

Figure S2 Temperature-dependent X-ray powder diffraction pattern starting from crystals of a) (**1**)$_3$ and b) 2·(**1**)$_4$ · *n*-pentane. The measurements were performed by holding the temperature constant for 6 min with a data collection time of 5 min from a) 30°C – 110 °C in 10 K steps, from 110 °C – 120 °C in 5 K steps and above 120 °C in 2 K steps with a heating rate of 5 K/min and b) 30°C – 90 °C in 10 K steps with a heating rate of 5 K/min, from 90 °C – 110 °C in 5 K steps and above 110 °C in 2 K steps with a heating rate of 1 K/min. The inlet in b) shows measurements performed from 70 °C – 85 °C in 5 K steps with a heating rate of 10 K/min in order to evaluate the transition temperature range more precisely.

A3 TGA analyses

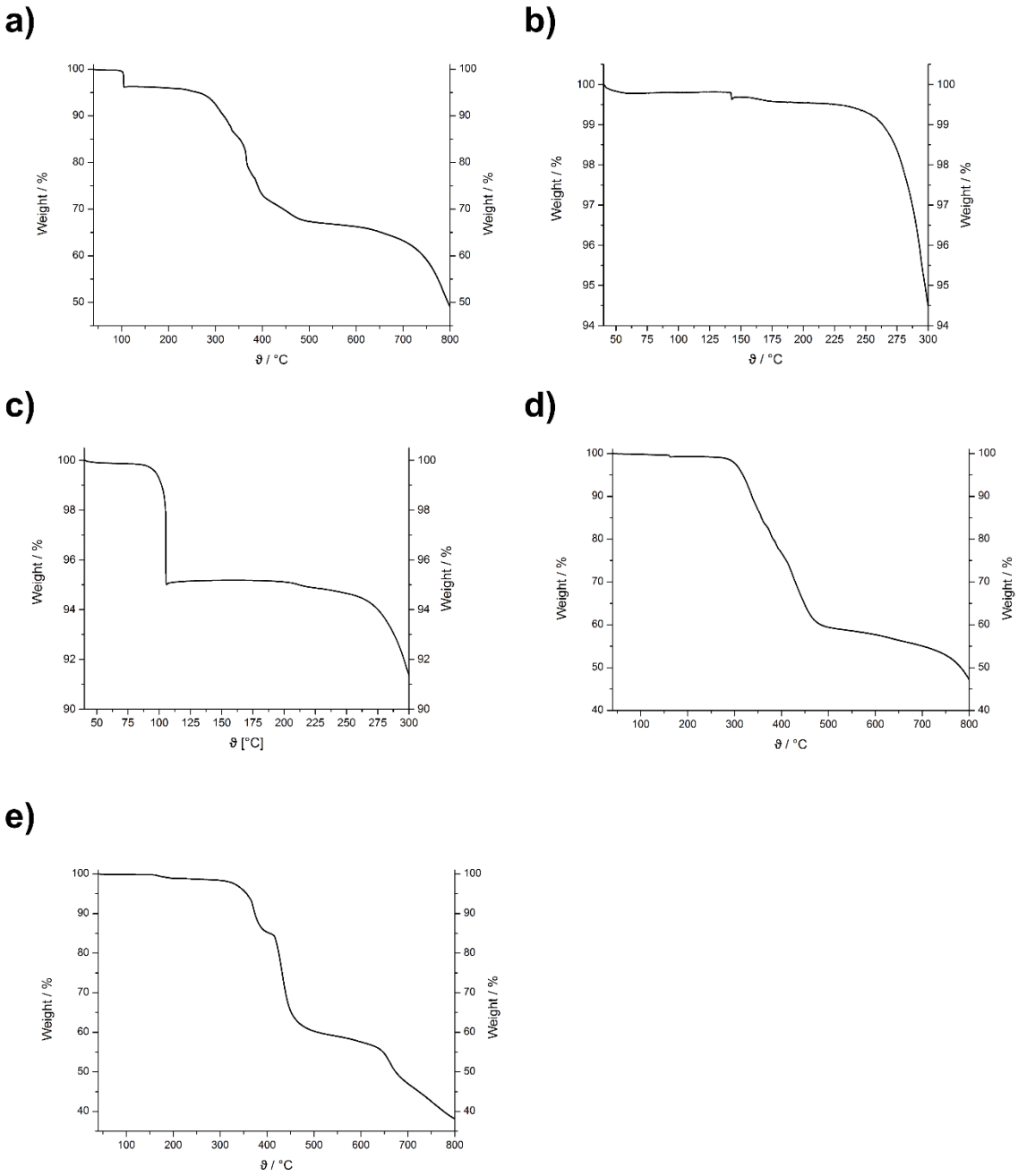

Figure S3 Thermal gravimetric analysis of a) amorphous material of **1**, b) crystals of $(\mathbf{1})_3$, c) crystals of $2\cdot(\mathbf{1})_4 \cdot$ *n*-pentane, d) amorphous material of **2** and e) amorphous material of **3**. The first weight loss step in a) with an onset temperature of 104 °C is assigned to the release of residual solvents within the amorphous material of **1** as similarly detected for crystals of $2\cdot(\mathbf{1})_4 \cdot$ *n*-pentane in c).

*A4 ^{1}H NMR spectroscopy of the germylene **1***

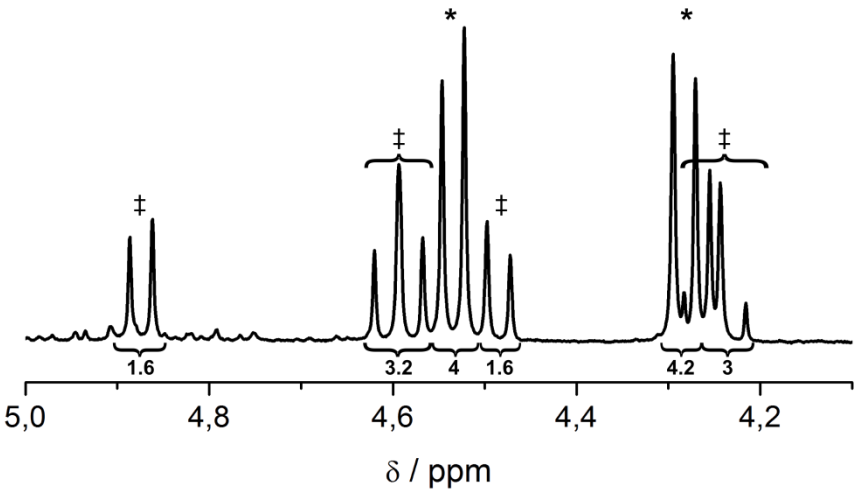

Figure S4 ^{1}H NMR spectra in the range of the chemical shifts for the resonance signals of the methylene group protons (δ = 4.1 – 5.0 ppm) of germylene 1 in $CDCl_3$ recorded at -60 °C. Resonance signals assigned to $(\mathbf{1})_3$ and $(\mathbf{1})_4$ are marked by ‡ and *. The integral ratios of the resonance signals are marked by curly brackets.

A5 Single crystal X-ray diffraction analysis structure of $(\mathbf{3})_2$

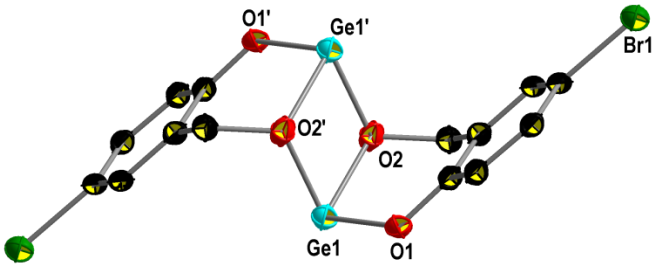

Figure S5 Molecular structure of $(\mathbf{3})_2$ in the solid state. Thermal ellipsoids are drawn with 50% probability. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and bond angles [°]: Ge1-O1 1.862(4), Ge1-O2 1.970(4), Ge1-O2' 2.012(4); Ge1-O2-Ge1' 103.76(17), O1-Ge1-O2 91.98(16), O1-Ge1-O2' 93.73(16), O2-Ge1-O2' 76.24(17). Symmetry transformations used to generate equivalent atoms: ' = -x, -y+1, -z.

A6 Solid state NMR spectroscopy

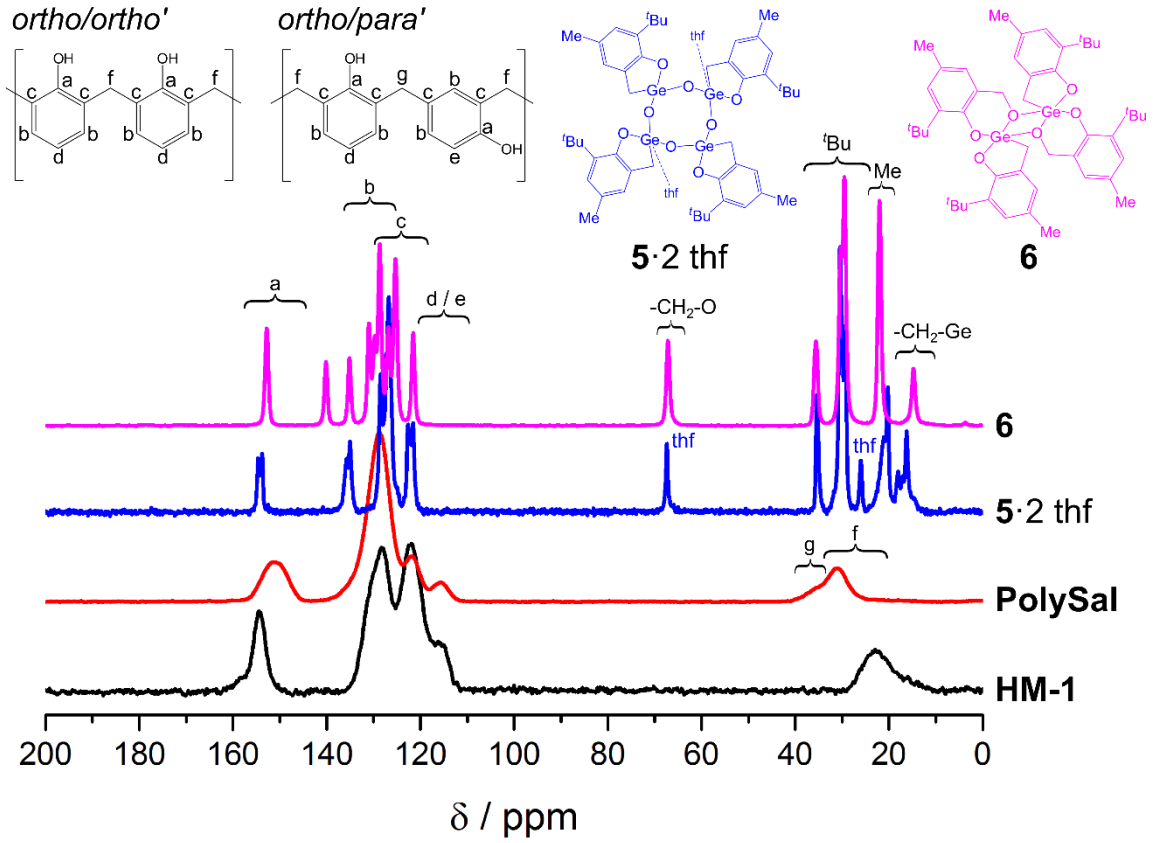

Figure S6 $^{13}C\{^{1}H\}$ CP-MAS NMR spectra of **HM-1** (black line), a phenolic resin obtained by thermal polymerization of 2-hydroxybenzyl alcohol (**PolySal**) (red line), 2,4,6,8-tetra-(3-*tert*-butyl-5-methyl-2-oxidophenyl)methanide-1,3,5,7,2,4,6,8-tetraoxidogermocane·2 thf (**5**·2 thf) (blue line) and {7,8'-di-*tert*-butyl-5,6'-dimethyl-3*H*,4'*H*-spiro[benzo[*d*][1,2]oxagermole-2,2'-benzo[*d*][1,3,2]dioxagermine]}$_2$ (**6**) (pink line). The compounds **5** and **6** were synthesized according to reference [3] as products of intramolecular insertion reactions starting from germylene **4**. Assignment of the resonance signals is given.

Reference

3. P. Kitschke, T. Rüffer, M. Korb, H. Lang, W. B. Schneider, A. A. Auer and M. Mehring, *Eur. J. Inorg. Chem.*, 2015, **2015**, 5467-5479.

A7 X-ray photoelectron spectroscopy

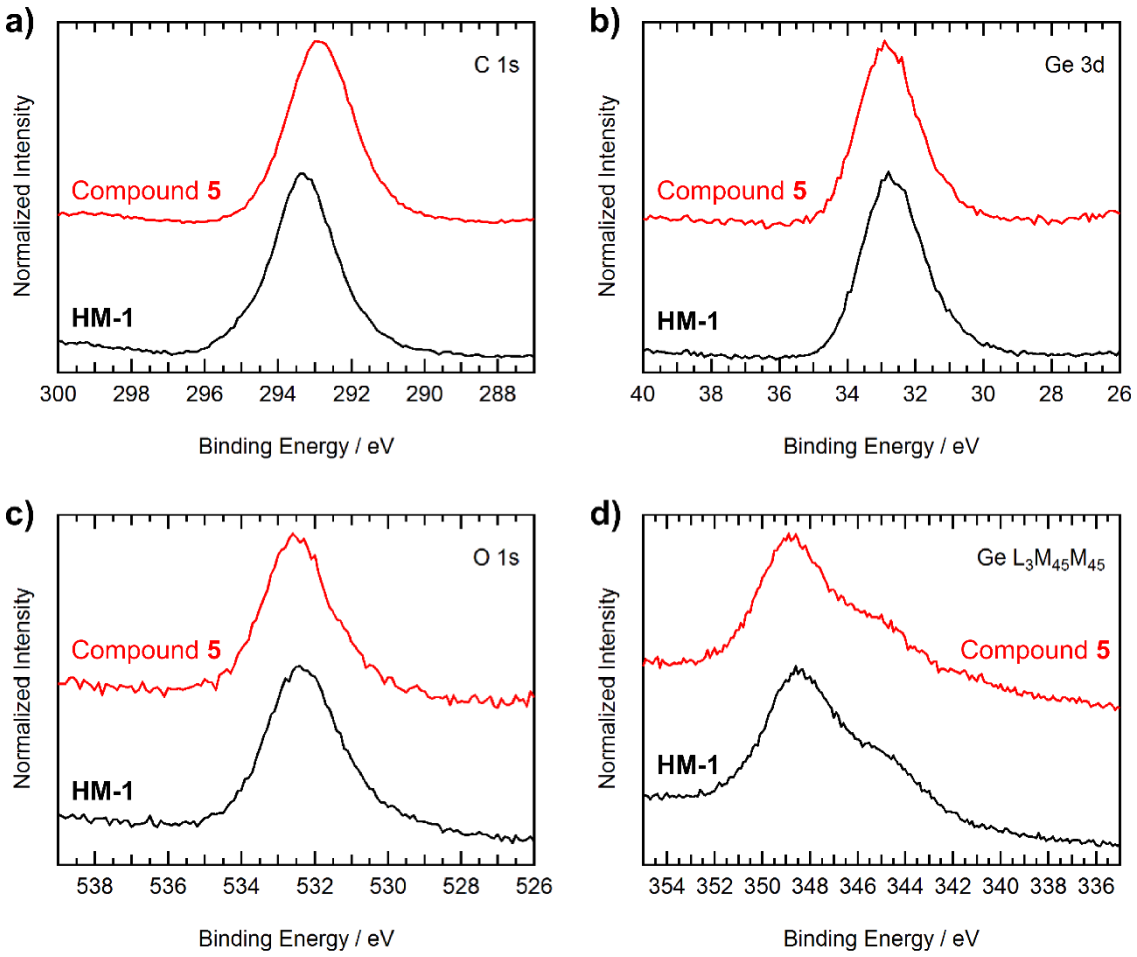

Figure S7 XPS core-level spectra of **HM-1** and compound **5**, showing emission from the a) C 1s, b) Ge 3d, and c) O 1s levels as well as d) Auger spectra arising from the Ge $L_3M_{45}M_{45}$ transition. Spectra are normalized to the same height and offset for clarity. In addition, the binding energy in b)-d) has been corrected for the shift caused by charging.

A comparative XPS analysis was carried out for **HM-1** and compound **5**. The latter is a product due to the oxidative intramolecular C-O insertion of germylene **4**.[3] Direct evaluation of core-level binding energies to determine the chemical state is hampered by a shift of the peaks to higher binding energies due to charging of the insulating samples upon photoemission. Assuming a binding energy of 285.0 eV in the absence of charging, the position of the C 1s line can be used as an internal energy reference.[4, 5] From the C 1s core-level spectra [Figure S7a)], the shift caused by charging can be estimated to amount to 8.3 eV and 7.8 eV for **HM-1** and **5**, respectively. This shift is then used to correct the binding

energy for Ge 3d and O 1s spectra [Figure S7b) and c)], yielding Ge 3d positions of 32.7 eV and 32.8 eV for **HM-1** and **5**, respectively, which is in the range reported for germanium oxides.[4, 6-14] Based on electronegativity arguments, smaller chemical shifts are expected to arise from carbon atoms bonded to germanium as compared to oxygen atoms, which is consistent with Ge 3d binding energies in a range between 28.5 eV to 32.0 eV that have been assigned to germanium atoms bonded to carbon.[10, 15-18] However, the lack of distinct spectral features in the Ge 3d signals (as well as in the C 1s spectra) of **HM-1** and **5** precludes the assignment of different chemically shifted components, likely because the substitution of an oxygen atom by a carbon atom only leads to minor changes in the binding energy of the germanium core-level. It should be mentioned that similar binding energies as for **HM-1** and **5** have also been reported for organogermanium films obtained by chemical vapor deposition.[4] Importantly, the comparison of the Ge 3d spectra of **HM-1** and **5** reveals almost identical positions, peak shapes and widths. This indicates a similar chemical environment of the germanium atoms in **HM-1** and compound **5**. The same holds for the O 1s spectra of the two samples.

These findings are supported by the Ge $L_3M_{45}M_{45}$ Auger spectra of **HM-1** and **5** [Figure S7d)], which also exhibit similar peak shapes and positions after correction for charging. The Auger parameters (i.e, the sum of the binding energy of the Ge 3d level and the kinetic energy of the sharp feature in the Ge $L_3M_{45}M_{45}$ line) are (1170 ± 0.3) eV and (1170.7 ± 0.3) eV for **HM-1** and compound **5**, respectively, in good agreement with literature data for Ge oxides.[4, 13, 14, 19] Note that the Auger parameter is independent of a reference to correct the energy scale for sample charging.

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A8 IR spectroscopy

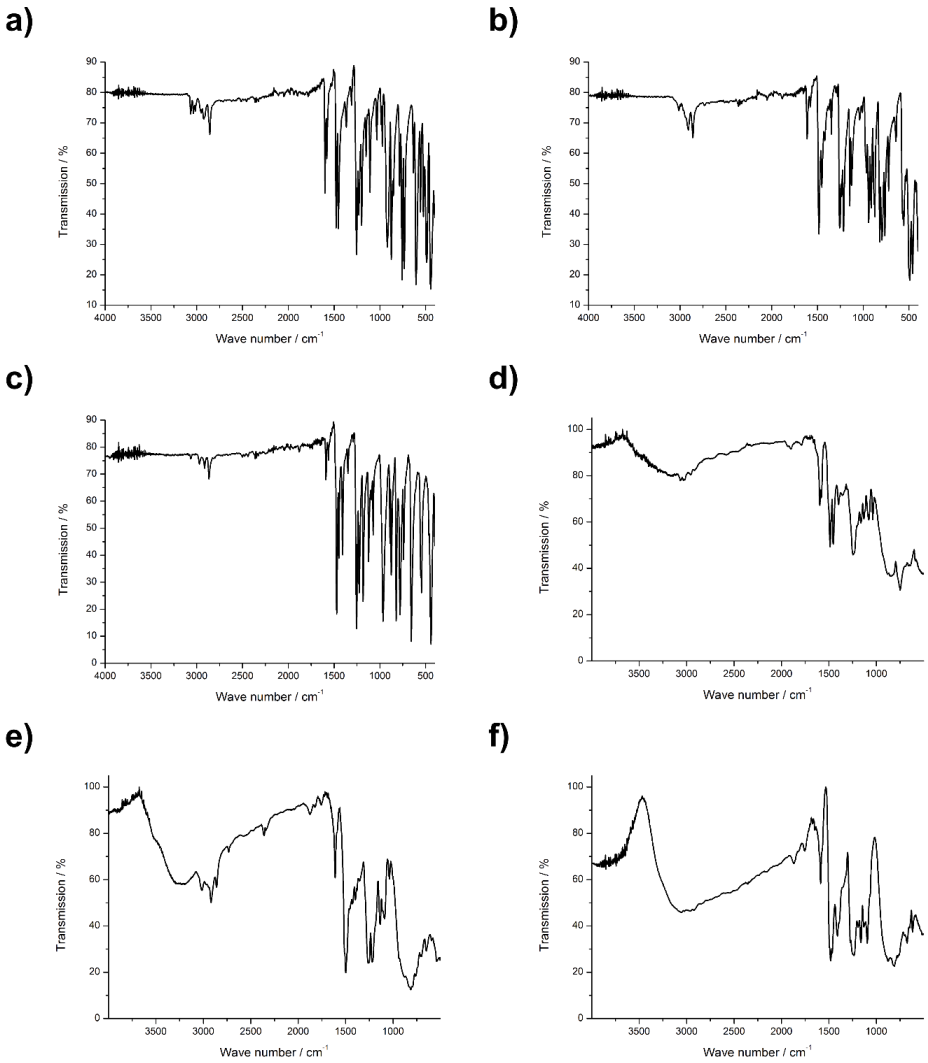

Figure S8 ATR-FT-IR spectra of a) **1**, b) **2**, c) **3** and FT-IR spectra of d) **HM-1**, e) **HM-2** and f) **HM-3**.

A9 N_2-sorption measurements

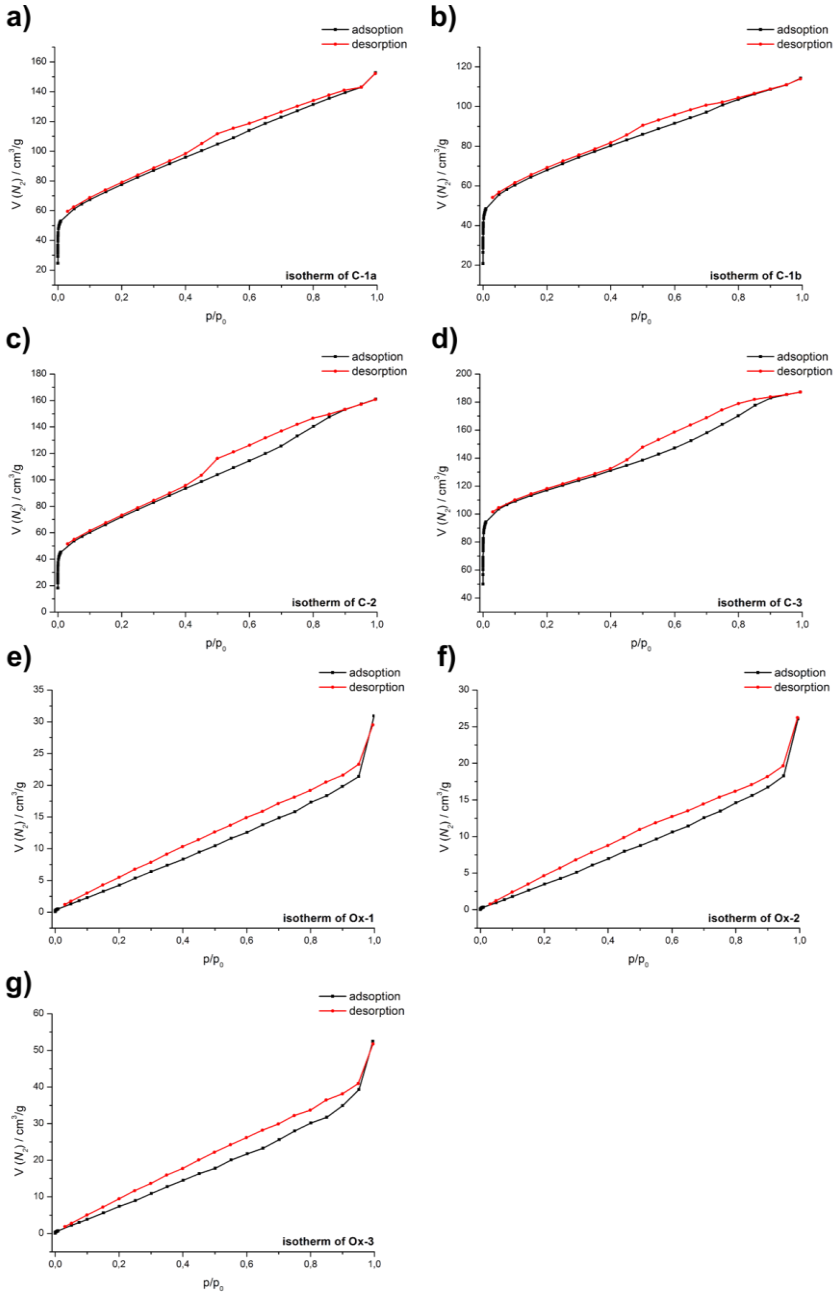

Figure S9 N_2 physisorption isotherms of a) **C-1a**, b) **C-1b**, c) **C-2**, d) **C-3**, e) **Ox-1**, f) **Ox-2** and g) **Ox-3**.

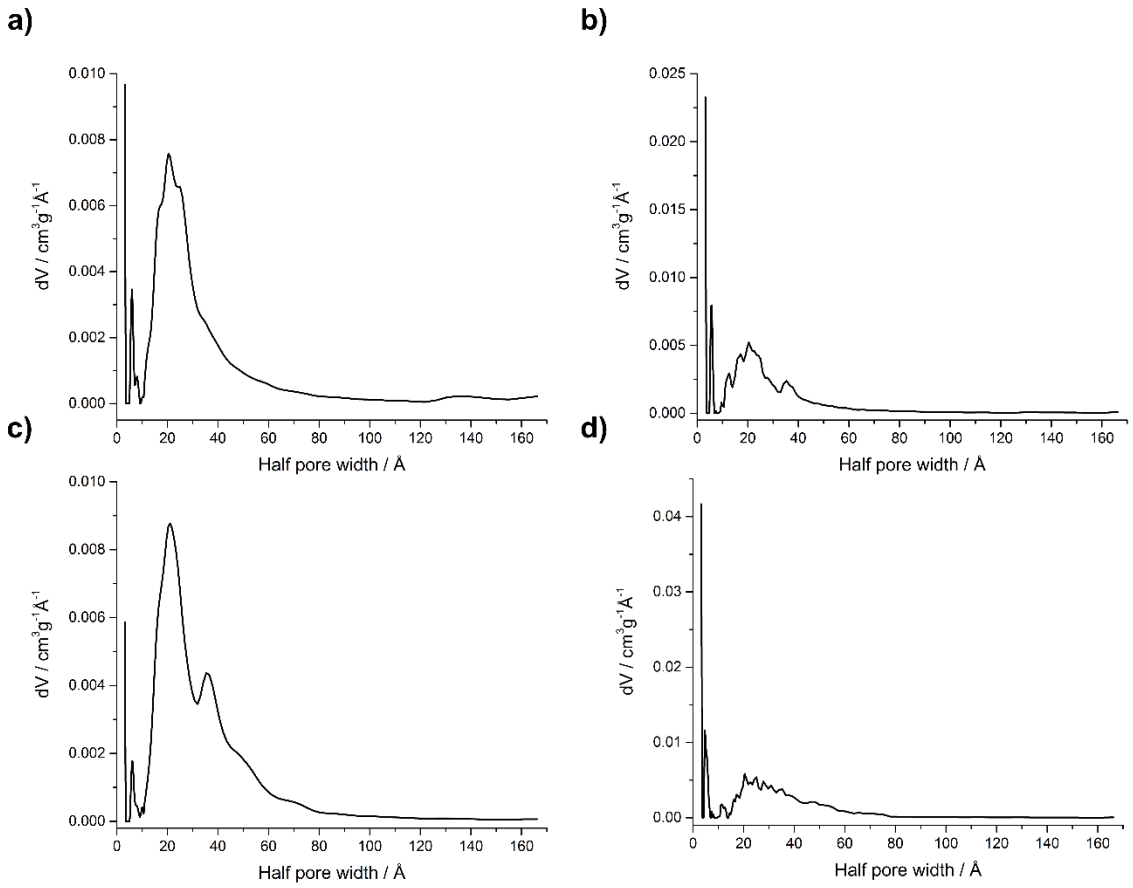

Figure S10 Pore size distributions of: a) **C-1a**, b) **C-1b**, c) **C-2** and d) **C-3**. The pore size distributions were estimated according to the QSDFT model for slit and cylindrical pores using the adsorption branch for carbon materials.

A10 DSC measurements

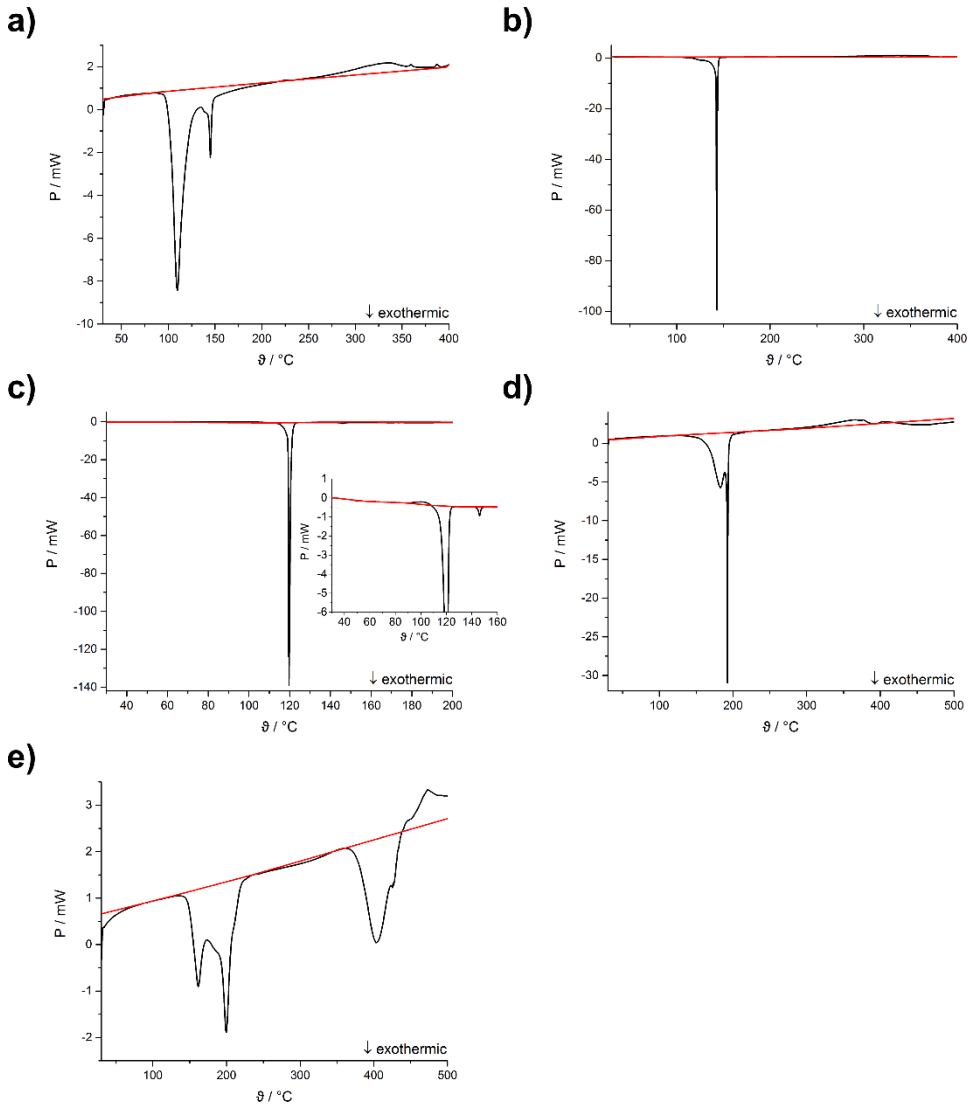

Figure S11 Differential scanning calorimetry (black curve) measurement of a) amorphous material of **1**, b) crystals of $(\mathbf{1})_3$, c) crystals of 2 $(\mathbf{1})_4 \cdot$ *n*-pentane, d) amorphous material of **2** and e) amorphous material of **3**. Baseline (red curve) was added in order to distinguish exothermic and endothermic processes.

A11 Raman spectroscopy

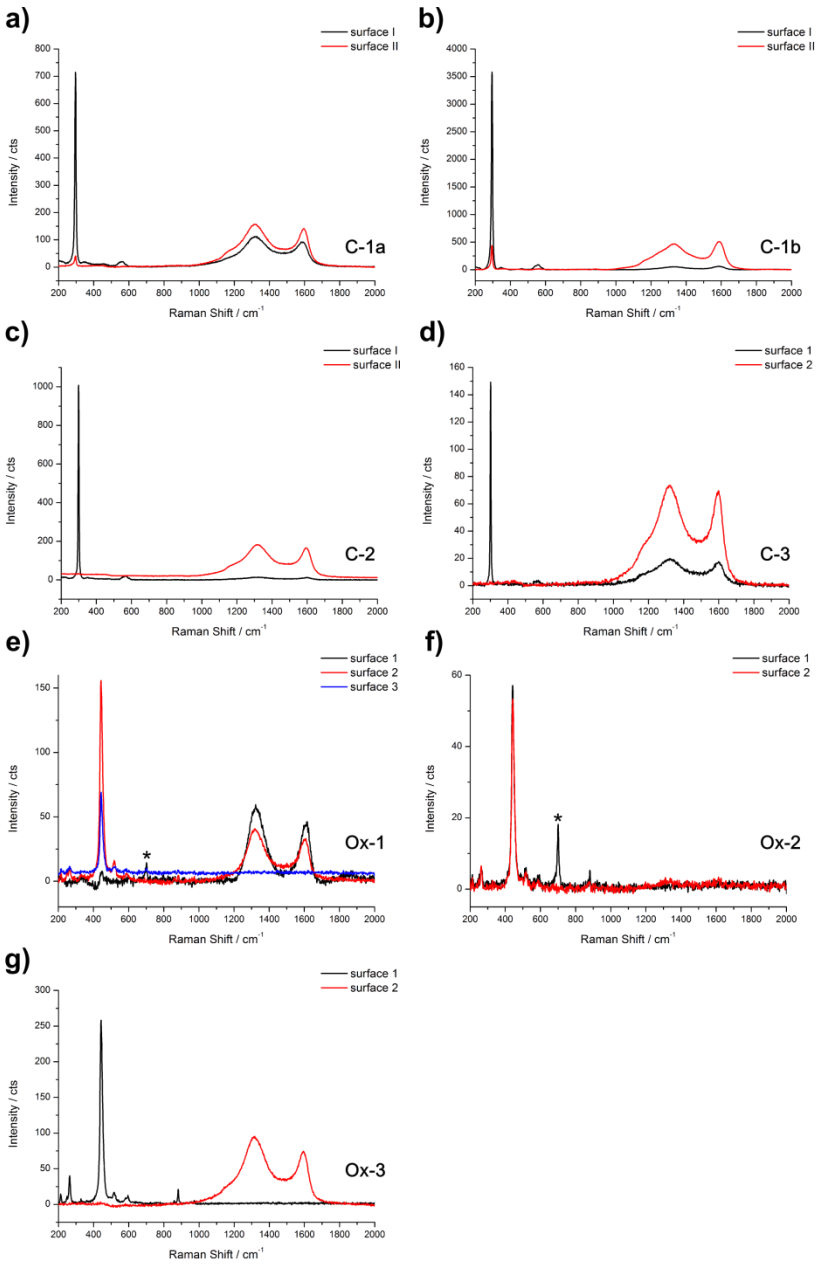

Figure S12 Raman spectra of a) **C-1a** b) **C-1b**, c) **C-2**, d) **C-3**, e) **Ox-1**, f) **Ox-2** and g) **Ox-3** at selected surfaces of the samples. The asterisks * in e) and f) mark Raman bands assigned to tetragonal GeO_2.

A12 Scanning electron microscopy including EDX mapping

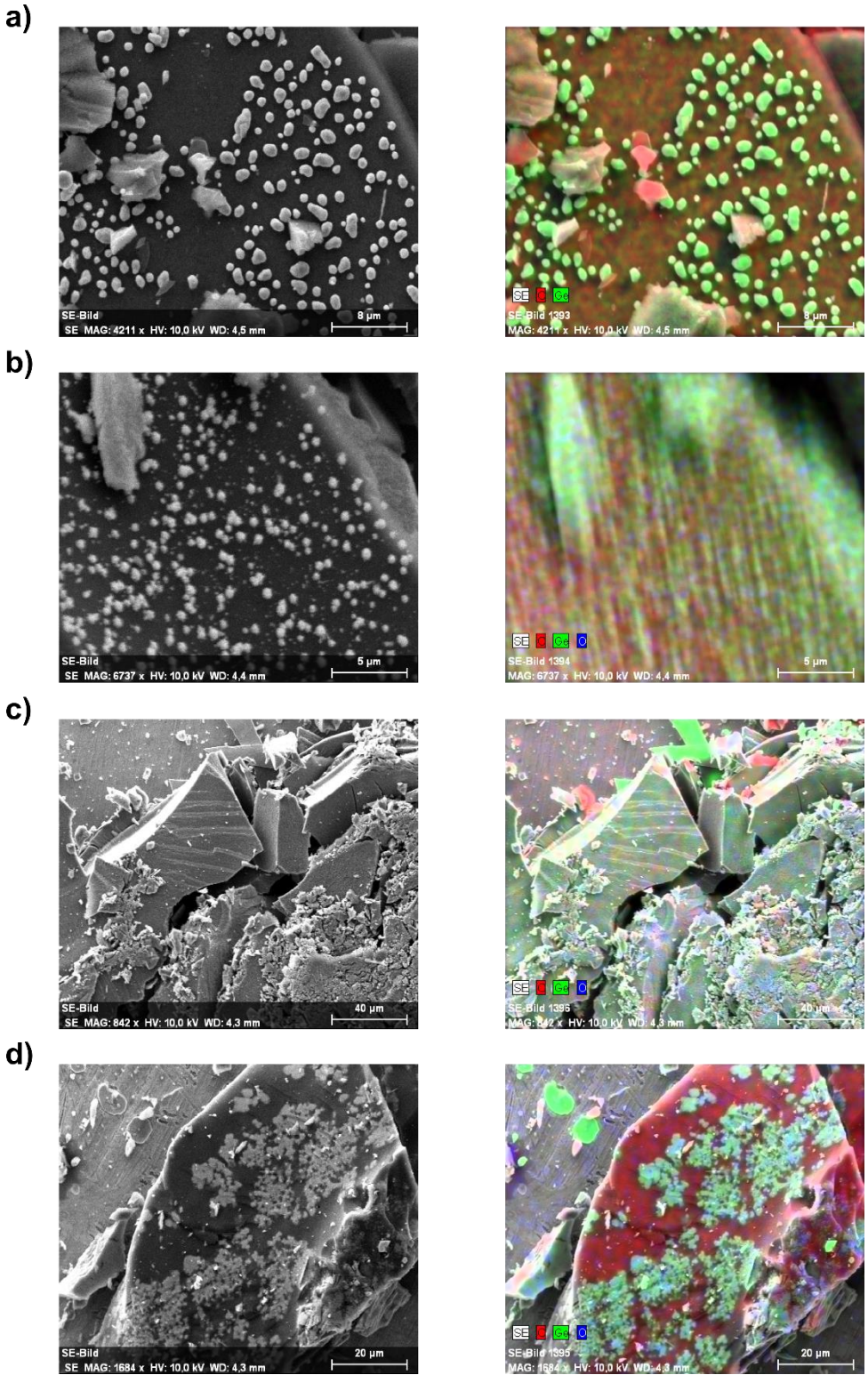

Figure S13 SEM images (left) with EDX mapping (right) of a) **C-1a**, b) **C-1b**, c) **C-2** and d) **C-3**. The EDX mapping colors green, red and blue denote germanium, carbon and oxygen, respectively.

A13 Powder X-ray diffraction

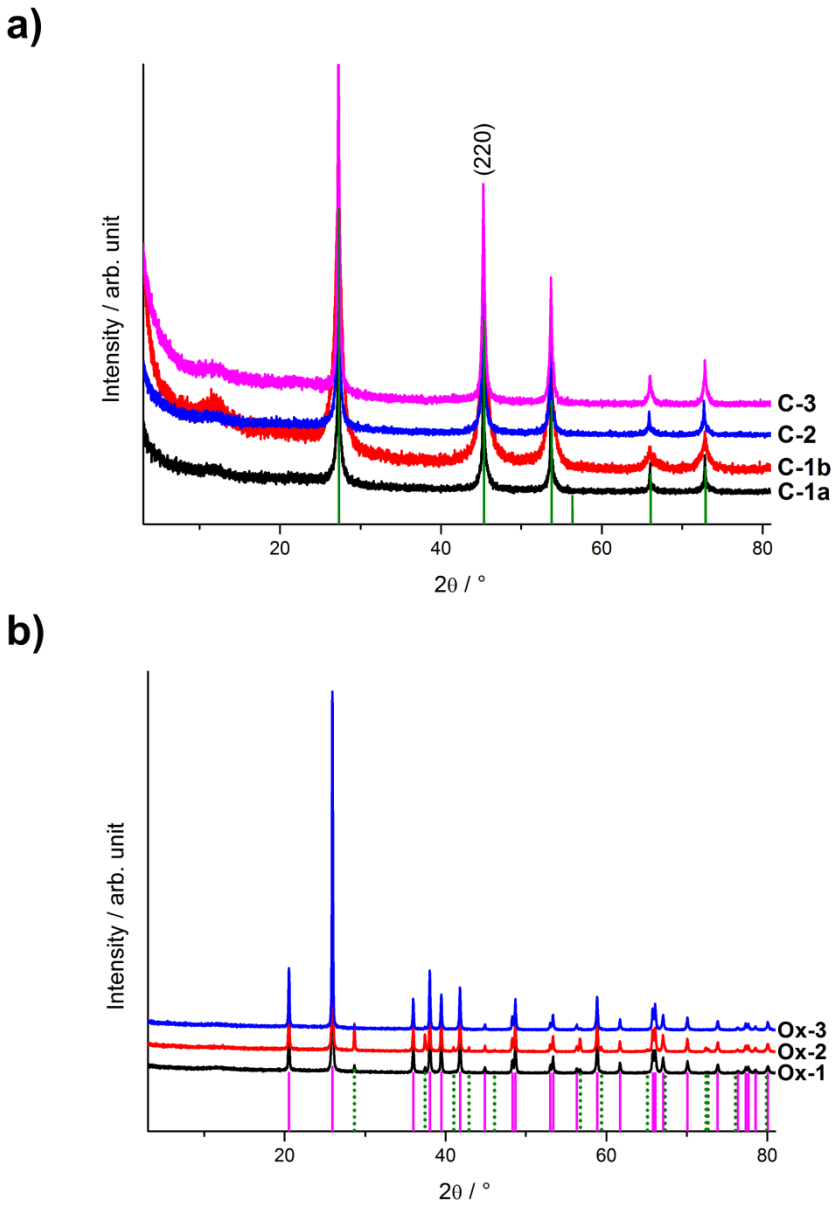

Figure S14 X-ray powder diffraction pattern of a) **C-1a** (black curve), **C-1b** (red curve), **C-2** (blue curve), **C-3** (pink curve) and b) **Ox-1** (black curve), **Ox-2** (red curve) and **Ox-3** (blue curve). The green bars in a) display the standard diffraction pattern of cubic Ge (ICDD no. C03-065-0333), whereas the pink bars and the green dots in b) depict the standard diffraction pattern of hexagonal (ICDD no. C00-036-1463) and tetragonal (ICDD no. C00-035-0729) GeO_2, respectively. Determination of the crystalline Ge particle sizes by applying the Scherrer equation was based on the (220) reflection marked in a).

A14 Transmission electron microscopy

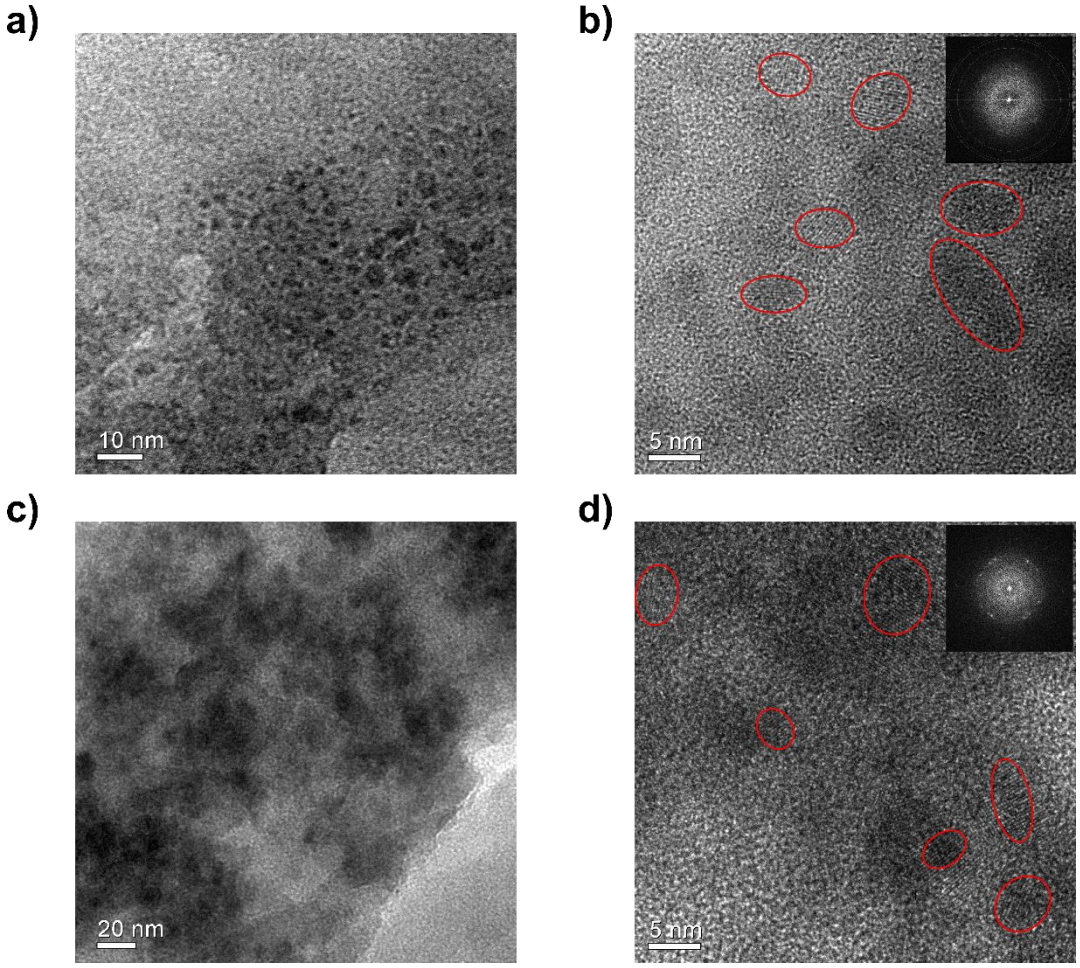

Figure S15 TEM images of selected carbon-rich areas of **C-1a** depicted in a) and b) and of **C-1b** depicted in c) and d). The images in b) and d) magnify areas exhibiting crystalline germanium, which are marked by red circles. The insets in b) and d) show the electron diffraction patterns of the crystalline germanium.

*A15 Comparison of the electrochemical performance of the Ge@C composite **C1-a** with other Ge/C materials reported in the literature*

Table S1 Comparison of the electrochemical performance of the herein presented Ge@C as Li-ion anode with previously reported results by others on Ge/C materials (currents and capacities related to Ge-content).

Reference	Current density (mAg^{-1})	Potential range (V vs. Li^+/Li)	Initial capacity ($mAhg^{-1}$)	Retained capacity ($mAhg^{-1}$)	Cycle number	Ge content in electrodes (%)
Present work	870	0.005-1.0	1360	1360	100	32
	3480		980	980	500	
[20]	1624	0.005-1.2	1250	825	250	40
[21]	272	0.01-1.5	1500	1200	50	81
[22]	69	0-1.0	1371	1234	50	53
[23]	706	0.01-1.0	1413	1192	400	36

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A16 Summary of analytical data of the as-obtained hybrid materials, carbonized and oxidized materials

Table S2 Summary of analytical data of the as-obtained hybrid materials (**HM-1** -**HM-3**), Ge@C composites (**C-1a** - **C-3**) and GeO_2 materials (**Ox-1** - **Ox-3**)

Compound	**HM-1**	**HM-2**	**HM-3**	**C-1a**	**C-1b**	**C-2**	**C-3**	**Ox-1**	**Ox-2**	**Ox-3**
BET surface[a] [m^2/g]	-	-	-	268	238	244	418	12	9	20
primary particle size[b] [nm]	-	-	-	51 ± 6	13 ± 1	39 ± 3	38 ± 3	-	-	-
CHN analysis [%] by weight	C 42.38 H 3.38	C 47.11 H 4.44	C 30.10 H 1.77	C 32.66 H 0.29	C 34.41 H 0.86	C 31.58 H 0.18	C 60.89 H 0.38	C 0.51 H -	C 0.22 H -	C 0.60 H -
EDX analysis [%] by weight	C 54.1±2.4 O 18.7±0.9 Ge 27.2±0.6	C 55.9±2.3 O 17.6±0.8 Ge 26.5±0.5	C 33.4±3.1 O 10.8±1.1 Ge 27.8±0.9 Br 28.0±0.9	C 44.3±4.1 O 9.2±1.4 Ge 46.5±2.8	C 58.5±7.5 O 1.7±0.3 Ge 39.8±2.4	C 55.2±6.7 O 8.2±1.2 Ge 36.6±2.0	C 70.4±8.7 O 3.1±0.5 Ge 26.5±1.6 Br -	C 3.5±0.7 O 31.0±3.7 Ge 65.5±3.7	C 3.1±0.8 O 28.7±3.9 Ge 68.2±4.1	C 3.3±0.6 O 31.2±3.4 Ge 65.5±3.3 Br -

[a] $p/p_0 = 0.150 \pm 0.002$; [b] determined by applying the Scherrer equation based on the (220) reflection of Ge (ICDD no. C03-065-0333) for the carbonized materials.

A17 xyz data of the optimized geometries

Table S3 xyz data of the optimized oligomers of compound **1**.

Dimer $(\mathbf{1})_2$	Trimer $(\mathbf{1})_3$	Tetramer $(\mathbf{1})_4$
32	48	64
Energy = -4995.467629603 Hartree	Energy = -7493.225737920 Hartree	Energy = -9990.972886351 Hartree
C 0.3494197 3.3640098 16.5244050	C 3.2030388 -0.0902732 9.9751462	Ge 7.1017036 5.2491696 8.4719961
H 0.4309373 4.3885181 16.1588731	C 2.6876484 -1.3014208 10.4353152	O 7.7795648 3.6501827 7.8007818
H 1.2996553 2.8620268 16.3147834	C 3.9394462 0.7297177 10.8447013	O 6.3219637 5.7409787 6.7051881
O -0.4333693 0.7894410 17.3589341	O 3.0077926 0.3012998 8.6953754	O 8.7603559 6.3247594 7.9281699
O 0.2023784 3.3999083 17.9660808	H 2.1235486 -1.9195307 9.7499342	H 9.4914688 5.7085667 9.7730603
Ge 0.3118068 1.6085807 18.8430654	C 2.9008882 -1.6883327 11.7524183	C 8.2712831 3.5567968 6.5439026
C -0.8010536 2.6460542 15.8831080	C 4.1556218 0.3200735 12.1565719	Ge 5.2457465 7.3992099 6.1611125
C -1.1501322 1.3743927 16.3722756	C 4.4691223 2.0129420 10.2914133	C 6.1783550 4.6314195 5.7696609
C -1.5423888 3.2037104 14.8445386	Ge 4.4368589 0.8211064 7.6118705	Ge 9.2530374 7.1050273 6.1619923
C -2.2325721 0.6928740 15.8142880	H 2.4952898 -2.6283700 12.1040069	C 9.8692880 6.1816103 8.8645304
C -2.6098505 2.5185176 14.2798315	C 3.6361282 -0.8831725 12.6185686	C 7.5084482 4.0231148 5.4624024
H -1.2786232 4.1898562 14.4808927	H 4.7367488 0.9503377 12.8194021	C 9.5354050 3.0136043 6.3179531
H -2.4853489 -0.2816116 16.2091160	H 3.6569582 2.6570721 9.9454157	O 3.6477532 6.7192938 6.8330889
C -2.9510114 1.2609448 14.7718316	H 5.0350071 2.5610635 11.0462467	O 5.7374215 8.1790136 7.9278530
H -3.7858962 0.7213415 14.3433231	O 5.3476177 1.7658641 9.1495607	H 5.7059873 5.0088982 4.8606224
Ge -1.5286208 4.1921226 18.7188841	H 4.2577530 -1.8682172 6.8369055	H 5.4983408 3.9044905 6.2217094
O -0.7838362 5.0113635 20.2032712	O 5.5128265 -0.8120707 8.1065322	O 10.8513850 7.7832491 6.8346109
O -1.4192619 2.4007415 19.5958072	H 3.8053517 -1.1926024 13.6407882	O 8.1768089 8.7632317 6.7062208
C -0.0659704 4.4263885 21.1891097	Ge 7.2615186 2.4014905 9.3973715	H 8.7943928 9.4957813 4.8623109
C -1.5655353 2.4369663 21.0376532	C 5.1844125 -2.0270929 7.3918187	C 10.4755779 7.5123938 9.1725511
C 1.0166366 5.1080668 21.7465461	Ge 6.9917750 -1.0293817 9.4196549	H 10.5972924 5.5025457 8.4128298
C -0.4143879 3.1545043 21.6781567	O 7.4471755 3.2156316 7.7488960	C 8.0204686 3.9314049 4.1724224
H -1.6473590 1.4125343 21.4033195	O 7.8697338 0.6493012 8.6855867	H 10.1101633 2.6674113 7.1661546
H -2.5153827 2.9394680 21.2477029	C 6.2977318 -2.4244981 6.4730230	C 10.0281577 2.9230574 5.0223419
H 1.2689482 6.0827094 21.3518079	H 4.9811063 -2.8044313 8.1358653	C 3.5580524 6.2255395 8.0895083
C 1.7357738 4.5399575 22.7885084	O 7.8478702 -2.2433314 8.2997901	Ge 7.3955842 9.2550731 8.4723724
C 0.3275128 2.5968890 22.7163398	C 7.2211314 2.5840794 6.5694953	C 4.6278864 8.3205163 8.8638578
H 2.5708224 5.0796327 23.2166087	C 8.6045550 0.7143077 7.4243812	C 10.9426085 8.2754521 8.0915190
C 1.3951063 3.2822722 23.2805709	C 7.5972465 -2.5096842 6.9977653	C 8.3205945 9.8728756 5.7707590
H 0.0641559 1.6106351 23.0799796	C 6.0867816 -2.6990433 5.1262768	C 10.5625415 8.0258340 10.4622833
H 1.9613457 2.8383287 24.0878600	C 6.4525971 3.2004856 5.5830790	C 9.2743340 3.3782271 3.9439395
H -3.1755711 2.9625147 13.4722088	C 7.7635327 1.3096293 6.3426005	H 7.4334081 4.3061229 3.3423422
	H 8.9352384 -0.2885064 7.1731909	H 11.0100128 2.4996819 4.8541364
	H 9.4898398 1.3287818 7.6105981	C 4.0238602 6.9885182 9.1711343
	C 8.6533384 -2.8843632 6.1653754	C 3.0223187 4.9580501 8.3145485
	C 7.1370790 -3.0745634 4.2973109	O 6.7171726 10.8534474 7.8000983
	H 5.0854499 -2.6090628 4.7219731	H 5.0046456 8.7939103 9.7726386
	H 6.0487518 4.1844372 5.7785142	H 3.8990472 8.9985340 8.4119608
	C 6.2146440 2.5426789 4.3836523	C 11.4827911 9.5408139 8.3178236
	C 7.4979872 0.6563787 5.1432953	C 6.9900526 10.4794095 5.4621215
	H 9.6459064 -2.9476999 6.5903385	H 8.9992836 10.6005617 6.2235641
	C 8.4210997 -3.1694818 4.8263647	C 11.1116824 9.2813934 10.6910331
	H 6.9578964 -3.2861885 3.2520919	H 10.1867518 7.4387496 11.2918419
	H 5.6147878 3.0243518 3.6221789	H 9.6645776 3.3104899 2.9377307
	C 6.7268771 1.2672120 4.1621589	C 3.9397341 6.4729942 10.4602315
	H 7.8910418 -0.3388593 4.9832110	H 2.6765655 4.3831518 7.4662382
	H 9.2483894 -3.4602821 4.1919849	C 2.9399647 4.4615043 9.6092664
	H 6.5256875 0.7494805 3.2342293	C 6.2259447 10.9453585 6.5428808
		H 11.8302312 10.1154913 7.4700625
		C 11.5683305 10.0351238 9.6131955
		C 6.4778243 10.5676137 4.1719875
		H 11.1751259 9.6730279 11.6969714
		C 3.3950740 5.2152689 10.6877183
		H 4.3148262 7.0599295 11.2902059
		H 2.5234275 3.4765920 9.7766451
		C 4.9603555 11.4847609 6.3160151
		H 11.9886869 11.0182400 9.7816039
		C 5.2222580 11.1165179 3.9426346
		H 7.0659124 10.1930978 3.3425506
		H 3.3341889 4.8218848 11.6931208
		H 4.3845851 11.8307001 7.1636417
		C 4.4671824 11.5713837 5.0202857
		H 4.8316196 11.1810456 2.9363711
		H 3.4839266 11.9912415 4.8514309

Table S4 xyz data of the optimized oligomers of compound **2**.

Dimer $(\mathbf{2})_2$	Trimer $(\mathbf{2})_3$	Tetramer $(\mathbf{2})_4$
38	57	76
Energy = -5074.0777226850 Hartree	Energy = -7611.1423491950 Hartree	Energy = -10148.19358828 Hartree
C 0.3864928 3.3339173 16.5270473	C 3.1901067 -0.0517167 9.9220522	Ge 7.0617908 5.2139101 8.4436978
H 0.4700229 4.3517437 16.1435961	C 2.6723948 -1.2645160 10.3747389	O 7.7271117 3.6297582 7.7271045
H 1.3415043 2.8314679 16.3417690	C 3.9105303 0.7598917 10.8069907	O 6.2943314 5.7669128 6.6875720
O -0.3951678 0.7699107 17.3986452	O 3.0210095 0.3410473 8.6368169	O 8.7322781 6.2921789 7.9467034
O 0.2161187 3.3961658 17.9650016	H 2.1220925 -1.8866924 9.6817351	H 9.4136164 5.66068309.8052856
Ge 0.3150773 1.6217234 18.8790901	C 2.8692711 -1.6538711 11.6913197	C 8.2206643 3.5746585 6.4666809
C -0.7508451 2.5988039 15.8816522	C 4.1082275 0.3421653 12.1205203	Ge 5.2164006 7.4376677 6.1907976
C -1.1010039 1.3357253 16.3904803	C 4.4574149 2.0425343 10.2690330	C 6.1359033 4.6826529 5.7257201
C -1.4763092 3.1342340 14.8230540	Ge 4.4867170 0.8346779 7.5930447	Ge 9.2844528 7.0589213 6.1900012
C -2.1717494 0.6484139 15.8246157	H 2.4595196 -2.5985518 12.0294723	C 9.8169580 6.1347918 8.9082992
C -2.5398029 2.4499925 14.2369812	C 3.5916553 -0.8623467 12.5892509	C 7.4614733 4.0756772 5.3985138
H -1.2052365 4.1161366 14.4496787	H 4.6834257 0.9722898 12.7901428	C 9.4827172 3.0451181 6.2163188
H -2.4347345 -0.3201344 16.2276615	H 3.6558518 2.6914029 9.9078556	O 3.6321496 6.7723721 6.9071075
C -2.8724191 1.2001942 14.7602019	H 5.0109037 2.5851472 11.0367501	O 5.7694185 8.2046048 7.9471286
H -3.6995711 0.6480378 14.3304273	O 5.3579595 1.7949035 9.1441696	H 5.6615923 5.0865620 4.8290911
Ge -1.5306547 4.1970849 18.6729615	H 4.2807486 -1.8684624 6.8874316	H 5.4538176 3.9484283 6.1624577
O -0.8164441 5.0462087 20.1539210	O 5.5306374 -0.7997104 8.1508076	O 10.8686025 7.7252029 6.9057401
O -1.4338791 2.4218320 19.5838240	Ge 7.2689304 2.4181242 9.4267550	O 8.2066721 8.7297613 6.6868961
C -0.1144029 4.4756178 21.1618033	C 5.2029333 -2.0227489 7.4506917	H 8.8381098 9.4097840 4.8278980
C -1.6052417 2.4829843 21.0220690	Ge 6.9901985 -1.0135807 9.4860175	C 10.4229909 7.4610318 9.2345505
C 0.9610850 5.1607940 21.7286885	O 7.4890402 3.2156831 7.7738230	H 10.5514843 5.4529922 8.4716397
C -0.4672034 3.2157957 21.6684902	O 7.8860000 0.6551969 8.7487124	C 7.9749824 4.0311312 4.1090449
H -1.6903143 1.4648154 21.4041908	C 6.3233988 -2.4327160 6.5467635	H 10.0641667 2.6695958 7.0474008
H -2.5600254 2.9861280 21.2067484	H 4.9924837 -2.7895162 8.2037364	C 9.9734338 3.0045260 4.9161641
H 1.2257237 6.1288435 21.3253953	O 7.8513882 -2.2486122 8.3950489	C 3.5767580 6.2786277 8.1674451
C 1.6594662 4.6072618 22.7896041	C 7.2774577 2.5709238 6.5982981	Ge 7.4402290 9.2826468 8.4434734
C 0.2587877 2.6761897 22.7289413	C 8.6393147 0.7027852 7.4964197	C 4.6851848 8.3630058 8.9090015
H 2.4892563 5.1557538 23.2200343	C 7.6151871 -2.5210926 7.0890592	C 10.9232737 8.2198391 8.1657666
C 1.3225960 3.3551660 23.3132667	C 6.1267577 -2.7035114 5.1993718	C 8.3647119 9.8139366 5.7249007
H -0.0160580 1.6951697 23.1008464	C 6.5254664 3.1770681 5.5967598	C 10.4668512 7.9757248 10.5235769
C -3.3023376 3.0536342 13.0863743	C 7.8173655 1.2903219 6.3975211	C 9.2329887 3.4927198 3.8399549
H -4.1083520 2.3982053 12.7566214	H 8.9673901 -0.3047573 7.2606440	H 7.3846492 4.4376131 3.2946589
H -2.6497732 3.2349354 12.2293839	H 9.5251716 1.3140237 7.6901909	H 10.9580417 2.5894834 4.7376643
H -3.7455059 4.0130524 13.3624778	C 8.6706612 -2.9029378 6.2645192	C 4.0778234 7.0375031 9.2358171
C 2.0982172 2.7683187 24.4636787	C 7.1743161 -3.0842116 4.3605546	C 3.0463907 5.0168740 8.4175729
H 1.7181230 1.7850858 24.7403011	H 5.1281542 -2.6033564 4.7871714	O 6.7752068 10.8672272 7.7275215
H 2.0406815 3.4077325 25.3474749	H 6.1239780 4.1655798 5.7807886	H 5.0892083 8.8369275 9.8057881
H 3.1561081 2.6586960 24.2144483	C 6.2836029 2.5205527 4.3908279	H 3.9511331 9.0454216 8.4724698
	C 7.5579623 0.6306732 5.2029067	C 11.4511019 9.4828318 8.4150450
	H 9.6616252 -2.9739272 6.6922288	C 7.0392894 10.4217810 5.3986451
	C 8.4465984 -3.1839058 4.9217656	H 9.0475427 10.5478128 6.1610580
	C 6.8011062 1.2378251 4.2080800	C 11.0035086 9.2347076 10.7915698
	H 7.9432593 -0.3694806 5.0536176	H 10.0606108 7.3858210 11.3383953
	H 9.2825302 -3.4768326 4.2980343	C 4.0323001 6.5240549 10.5252820
	H 6.6082558 0.7068291 3.2847321	H 2.6707631 4.4357086 7.5863394
	C 3.8069939 -1.3128824 14.0107851	C 3.0050280 4.5261387 9.7176934
	H 4.3902102 -0.5852343 14.5747052	C 6.2810561 10.9230713 6.4673706
	H 4.3394155 -2.2658708 14.0479576	H 11.8258628 10.0640552 7.5834613
	H 2.8574308 -1.4537314 14.5317721	C 11.4906450 9.9749036 9.7147153
	C 6.9266711 -3.3625857 2.9008735	C 6.5254334 10.4678457 4.1093640
	H 7.8478629 -3.6336786 2.3855864	C 3.4930010 5.2663774 10.7941376
	H 6.5077096 -2.4889031 2.3961442	H 4.4386440 7.1141937 11.3398780
	H 6.2167900 -4.1817078 2.7667139	H 2.5895568 3.5416749 9.8959776
	C 5.4586279 3.1895168 3.3230472	C 5.0196078 11.4543966 6.2177649
	H 5.3756493 2.5657698 2.4337343	H 11.9040568 10.9603579 9.8923172
	H 5.8993218 4.1435061 3.0264925	C 5.2682428 11.0085209 3.8409683
	H 4.4485921 3.3993139 3.6820837	H 7.1149572 10.0611236 3.2945135
		H 4.4389094 11.8301218 7.0492842
		C 4.5287493 11.4969352 4.9177279
		H 3.5448327 11.9138338 4.7397434
		C 11.0362852 9.7717290 12.1988298
		H 11.4819651 10.7653828 12.2340943
		H 11.6168096 9.1227967 12.8581953
		H 10.0310836 9.8426930 12.6205024
		C 4.7325946 11.0448181 2.4332727
		H 3.7410566 11.4951392 2.3975019
		H 4.6573029 10.0402670 2.0107974
		H 5.3847840 11.6227888 1.7748822
		C 3.4580586 4.7308671 12.2019184
		H 3.0097164 3.7384420 12.2379414
		H 2.8788885 5.3820150 12.8602894
		H 4.4628230 4.6576654 12.6242444
		C 9.7686621 3.4590534 2.4322048
		H 10.7609386 3.0104063 2.3958325
		H 9.8422997 4.4642680 2.0110147
		H 9.1173981 2.8808628 1.7730926

Table S5 xyz data of the optimized oligomers of compound **3**.

Dimer $(\mathbf{3})_2$	Trimer $(\mathbf{3})_3$	Tetramer $(\mathbf{3})_4$
32 Energy = -10142.3577011900 C 0.3668711 3.3639903 16.5234344 H 0.4523302 4.3874009 16.1566111 H 1.3160239 2.8588337 16.3179580 O -0.4361427 0.7921810 17.3609123 O 0.2083107 3.4004548 17.9622480 Ge 0.3093074 1.6115863 18.8467453 C -0.7809484 2.6452073 15.8760148 C -1.1385879 1.3771260 16.3670393 C -1.5044397 3.2086077 14.8287696 C -2.2178798 0.7004436 15.7976646 C -2.5639277 2.5142421 14.2661382 H -1.2401406 4.1901629 14.4593028 H -2.4821107 -0.2726312 16.1877698 C -2.9274530 1.2615043 14.7462757 Br -3.5448924 3.2970041 12.8225455 H -3.7594018 0.7311974 14.3056834 Ge -1.5235374 4.2053803 18.7056168 O -0.7774268 5.0245674 20.1913475 O -1.4228335 2.4164826 19.5900185 C -0.0735395 4.4388588 21.1837601 C -1.5807880 2.4534559 21.0289874 C 1.0081086 5.1138975 21.7505578 C -0.4317638 3.1711738 21.6754177 H -1.6671433 1.4302097 21.3960795 H -2.5293073 2.9596852 21.2347377 H 1.2737139 6.0860050 21.3590054 C 1.7187440 4.5521000 22.8008339 C 0.2926959 2.6070640 22.7216198 H 2.5519898 5.0814972 23.2400368 C 1.3543324 3.3000112 23.2819684 H 0.0273107 1.6262122 23.0922059 Br 2.3374463 2.5158058 24.7233063	48 Energy = -15213.5627383200 Hartree C 3.1888089 -0.0622290 9.9355623 C 2.6746377 -1.2771747 10.3852704 C 3.9145700 0.7527755 10.8178893 O 3.0084405 0.3341595 8.6571611 H 2.1157471 -1.8948501 9.6956299 C 2.8791776 -1.6816021 11.6976953 C 4.1292498 0.3392435 12.1281522 C 4.4507766 2.0394058 10.2766531 Ge 4.4558137 0.8499490 7.5943528 H 2.4814135 -2.6240734 12.0455480 C 3.6083265 -0.8716512 12.5602250 H 4.7031083 0.9577425 12.8049986 H 3.6414002 2.6808287 9.9200227 H 5.0021462 2.5877427 11.0414513 O 5.3466248 1.7920139 9.1505979 H 4.2753005 -1.8487726 6.8297166 O 5.5215500 -0.7867271 8.1044760 Br 3.9091850 -1.4385222 14.3621023 Ge 7.2611843 2.4219562 9.4435318 C 5.1954475 -2.0048060 7.3954852 Ge 6.9836071 -1.0090041 9.4421940 O 7.4794891 3.2482101 7.8026171 O 7.8746220 0.6731188 8.7250894 C 6.3177771 -2.4143769 6.4913197 H 4.9836646 -2.7781176 8.1413800 O 7.8589232 -2.2088157 8.3246258 C 7.2503963 2.6243039 6.6224188 C 8.6160358 0.7375714 7.4701235 C 7.6135890 -2.4887890 7.0253487 C 6.1041250 -2.7191930 5.1515827 C 6.4863597 3.2471905 5.6371304 C 7.7799162 1.3457762 6.3908077 H 8.9389416 -0.2663154 7.2140494 H 9.5057085 1.3442482 7.6586254 C 8.6724721 -2.8706951 6.2010777 C 7.1654169 -3.1159888 4.3502853 H 5.1098774 -2.6422058 4.7334827 H 6.0951990 4.2369794 5.8276211 C 6.2250697 2.5946165 4.4408028 C 7.5001631 0.6870289 5.1983237 H 9.6660815 -2.9223629 6.6243931 C 8.4518776 -3.1904091 4.8682997 Br 6.8526904 -3.5725749 2.5226226 H 5.6261272 3.0725694 3.6789181 C 6.7214827 1.3128093 4.2361907 H 7.8801241 -0.3106478 5.0293941 H 9.2748608 -3.4942405 4.2375831 Br 6.3112427 0.3811729 2.6193104	64 Energy = -20284.753453650 Hartree Ge 7.0551169 5.2131059 8.4455523 O 7.7180733 3.6284922 7.7210585 O 6.2861471 5.7689939 6.6870985 O 8.7294839 6.2855798 7.9462872 H 9.4068184 5.6577517 9.8085006 C 8.2164612 3.5805976 6.4663677 Ge 5.2140460 7.4435679 6.1878273 C 6.1316448 4.6879871 5.7216304 Ge 9.2850904 7.0544392 6.1876273 C 9.8106973 6.1304091 8.9113763 C 7.4615110 4.0876630 5.3981993 C 9.4844591 3.0543711 6.2247955 O 3.6289010 6.7817991 6.9120544 O 5.7699881 8.2128475 7.9461795 H 5.6584492 5.0917457 4.8247498 H 5.4534394 3.9476451 6.1534261 O 10.8703102 7.7165188 6.9114188 O 8.2130854 8.7291025 6.6867705 H 8.8404969 9.4059195 4.8242145 C 10.4128931 7.4594969 9.2345842 H 10.5501734 5.4513219 8.4794611 C 7.9792616 4.0640888 4.1083951 H 10.0581162 2.6716191 7.0575660 C 9.9966253 3.0263226 4.9344443 C 3.5792523 6.2845996 8.1671172 Ge 7.4444930 9.2851424 8.4453242 C 4.6889302 8.3685305 8.9113465 C 10.9199539 8.2142409 8.1662673 C 8.3678346 9.8099849 5.7212429 C 10.4401173 7.9758767 10.5248678 C 9.2400484 3.5318070 3.8842581 H 7.4059865 4.4718228 3.2869311 H 10.9805799 2.6207219 4.7478752 C 4.0865305 7.0396780 9.2350914 C 3.0492054 5.0183793 8.4095380 O 6.7820029 10.8700148 7.7210941 H 5.0930051 8.8414243 9.8082575 H 3.9495210 9.0476060 8.4792994 C 11.4496132 9.4807358 8.4081006 C 7.0383548 10.4113408 5.3981056 H 9.0466696 10.5499071 6.1527761 C 10.9761308 9.2350566 10.7493170 H 10.0330981 7.4024908 11.3466320 Br 9.9539185 3.5163462 2.1105269 C 4.0592074 6.5238913 10.5256050 H 2.6655515 4.4449541 7.5770354 C 3.0172047 4.5082467 9.7006053 C 6.2837838 10.9187211 6.4663911 H 11.8329764 10.0539377 7.5753127 C 11.4814834 9.9914670 9.6989278 C 6.5209852 10.4364293 4.1081748 Br 10.9973526 9.9467733 12.5238748 C 3.5228074 5.2649819 10.7506443 H 4.4663654 7.0975582 11.3471014 H 2.6082765 3.5257991 9.8879027 C 5.0166169 11.4469097 6.2248095 H 11.8901401 10.9741106 9.8857713 C 5.2609480 10.9705252 3.8840447 H 7.0941594 10.0289354 3.2865130 Br 3.5013411 4.5541124 12.5255406 H 4.4435383 11.8305184 7.0575763 C 4.5048380 11.4765027 4.9343403 Br 4.5475353 10.9880026 2.1101357 H 3.5215633 11.8837427 4.7477431

Table S6 xyz data of the optimized oligomers of compound **4**.

Dimer $(4)_2$	Trimer $(4)_3$	Tetramer $(4)_4$
62	93	124
Energy = -5388.5009449310 Hartree	Energy = -8082.7777355370 Hartree	Energy = -10777.04695060 Hartree
C 0.4399215 3.4757740 16.5867251	C 8.1918927 5.9912453 18.5074663	Ge 6.8100714 4.8803915 8.0018117
H 0.5284353 4.5071926 16.2443862	H 7.9650070 5.8399214 19.5637530	O 7.4728480 3.6581088 6.7493421
H 1.4021799 2.9839276 16.4116693	H 8.8887636 5.2021127 18.2136471	O 6.0481639 6.0167575 6.5526414
O -0.2600765 0.8934859 17.2912427	C 6.9339984 5.9282894 17.6976255	O 8.4860179 6.0478244 8.0730713
O 0.2281239 3.4876693 18.0218807	O 8.8836773 7.2561650 18.3646900	H 8.4586307 5.4803667 10.0663750
Ge 0.3813736 1.6761544 18.8398138	Ge 8.9525131 8.4365924 20.0057541	C 8.0161394 4.0241612 5.5607700
C -0.6779341 2.7635680 15.8844713	C 5.7280994 5.5604539 18.2813428	Ge 4.8755784 7.6888075 6.6260958
C -1.0150953 1.4696231 16.3195788	C 7.0030350 6.2026873 16.3260536	C 5.9496799 5.3507520 5.2598716
C -1.3928244 3.3672682 14.8584801	Ge 9.5271981 7.6384680 16.5310985	Ge 9.6235591 6.8112993 6.6257058
C -2.0976952 0.7797599 15.7370812	O 9.9812889 9.7628217 18.8871690	C 9.1527213 5.9465776 9.3651541
C -2.4451595 2.7041137 14.2411382	O 10.5327582 7.7100884 20.6867155	C 7.2919492 4.9251712 4.7650096
H -1.1259722 4.3710747 14.5464079	H 5.6954768 5.3667605 19.3477027	C 9.2613048 3.5282588 5.1239191
C -2.7732128 1.4297761 14.7019719	C 4.5740977 5.4518403 17.5193885	O 3.6575631 7.0218146 7.8802960
H -3.6038560 0.9316232 14.2251634	C 5.8616567 6.0500998 15.5071862	O 6.0132764 8.4523293 8.0732343
Ge -1.5898414 4.1464154 18.7024121	O 8.1931996 6.5829291 15.7908356	H 5.4868705 0.0460618 4.5577010
O -0.9451003 4.9236829 20.2532851	O 8.5074559 9.4091644 16.5624829	H 5.2866845 4.4890604 5.3722441
O -1.4396940 2.3333325 19.5147225	C 11.3484390 9.9438057 19.3605577	O 10.8420448 7.4777189 7.8798422
C -0.1968702 4.3414542 21.2262681	Ge 9.4902354 10.9460877 17.3107792	O 8.4508056 8.4833508 6.5522009
C -1.6553767 2.3417294 20.9494724	C 11.6891501 7.5752525 19.9855820	H 9.0122739 8.4541018 4.5573153
C 0.8879381 5.0289517 21.8158793	C 4.6752449 5.6894250 16.1473312	C 9.5757569 7.2881816 9.8638457
C -0.5380689 3.0499305 21.6562090	C 3.2458769 5.1148279 18.1442908	H 10.0154549 5.2853110 9.2505014
H -1.7465439 1.3094372 21.2885001	C 5.9354636 6.2019968 13.9770539	C 7.8133232 5.3851921 3.5657708
H -2.6175665 2.8344377 21.1229924	C 7.0581009 9.5855261 16.5077118	C 9.7378790 4.0181780 3.9051706
C 1.5577344 4.3750276 22.8479668	H 11.2929081 10.2802509 20.3993161	C 4.0253717 6.4828626 9.0703164
C 0.1736541 2.4403499 22.6852250	H 11.8092922 10.7404588 18.7752530	Ge 7.6891227 9.6198515 8.0014812
H 2.3892874 4.8679694 23.3297048	C 12.1365801 8.6796262 19.2475370	C 5.3467380 8.5537104 9.3653564
C 1.2242587 3.0974283 23.3049827	O 7.9633030 11.6590458 18.0659188	C 10.4746732 8.0169597 9.0698856
H -0.0982859 1.4372879 22.9942251	C 12.4515379 6.3877452 20.0227788	C 8.5494485 9.1494271 5.2594676
C -3.2129589 3.3492639 13.1169096	H 3.7765034 5.5754714 15.5595079	C 9.1149728 7.8045827 11.0649332
H -4.0449531 2.7239396 12.7929891	H 3.3730244 4.6356824 19.1153415	C 9.0538972 4.9452240 3.1205638
H -2.5727343 3.5245447 12.2491879	H 2.6650845 4.4436970 17.5100158	H 7.2399575 6.0895373 2.9744229
H -3.6200918 4.3171101 13.4171086	H 2.6456678 6.0148800 18.3022545	H 10.6942428 3.6734845 3.5413475
C 2.0013324 2.4663211 24.4305752	C 6.9457798 5.1770262 13.4170639	C 4.9239247 7.2121251 9.8642280
H 1.6618934 1.4495109 24.6277965	C 6.3628936 7.6273360 13.5724330	C 3.5335436 5.2373366 9.5106363
H 1.8929815 3.0379772 25.3552742	C 4.5798788 5.9270963 13.3056174	O 7.0257049 10.8416592 6.7490218
H 3.0685478 2.4241783 24.2023863	H 6.6296568 8.6979826 16.0590159	H 6.0408592 9.0200812 10.0664262
C -2.5209058 -0.6169858 16.2211858	H 6.8734928 10.4302025 15.8385463	H 4.4839186 9.2148532 9.2507520
C -3.7177132 -1.1662896 15.4269701	C 6.4722848 9.8317305 17.8596096	C 10.9671684 9.2622563 9.5101397
H -3.9751898 -2.1555979 15.8078796	C 13.2848752 8.5947957 18.4698196	C 7.2073133 9.5752131 4.7644048
H -3.4890542 -1.2724213 14.3653205	C 6.9680791 10.9058551 18.6123323	H 9.2125316 10.0110279 5.3719721
H -4.6024652 -0.5354832 15.5277340	C 13.5976763 6.3562528 19.2272371	C 9.5519254 9.0449453 11.5137437
C -1.3567262 -1.6159577 16.0515710	C 12.0793199 5.2097830 20.9377429	H 8.4123793 7.2275734 11.6548626
H -1.6621996 -2.6052535 16.3999390	H 6.6294270 4.1597272 13.6551064	C 5.3848518 6.6961048 11.0654146
H -0.4805859 -1.3078517 16.6145068	H 7.9399270 5.3319527 13.8276223	C 4.0244338 4.7660454 10.7310833
H -1.0771122 -1.7014063 14.9997099	H 7.0032400 5.2664419 12.3300699	C 6.4824953 10.4754319 5.5604955
C -2.9465060 -0.5447811 17.7034190	H 5.6336717 8.3632260 13.9168555	C 10.4765767 9.7338187 10.7305849
H -3.2564250 -1.5328176 18.0511794	H 6.4184994 7.7007416 12.4844377	C 6.6869399 9.1163929 3.5642778
H -3.7885336 0.1383836 17.8280223	H 7.3371552 7.8871079 13.9767314	C 4.9486003 5.4555244 11.5143015
H -2.1373426 -0.1974687 18.3384651	H 4.2246083 4.9150550 13.5041543	H 6.0870985 7.2735516 11.6553307
C 1.3128019 6.4272833 21.3379248	H 4.6881742 6.0314724 12.2252512	H 3.6828740 3.8095083 11.0973963
C 0.1485393 7.4259942 21.5094925	H 3.8120613 6.6323269 13.6285297	C 5.2373331 10.9711764 5.1234794
H 0.4553086 8.4165933 21.1660785	C 5.4600732 9.0284575 18.3615286	H 10.8188326 10.6900663 11.0969666
H -0.1333798 7.5071457 22.5610798	H 13.6019167 9.4568831 17.8932524	C 5.4464048 9.5562444 3.1188311
H -0.7265196 7.1208806 20.9432453	C 14.0262848 7.4224010 18.4346808	H 7.2610942 8.4131511 2.9723609
C 1.7415369 6.3619854 19.8561680	C 6.4400131 11.1949770 19.8857840	C 4.7615596 10.4821297 3.9040612
H 2.0519117 7.3518441 19.5140840	H 14.2021935 5.4613460 19.2181470	H 3.8051654 10.8266311 3.5401333
H 0.9338963 6.0176905 19.2175753	C 12.0426739 5.6939321 22.4035719	C 9.0404491 9.6153763 12.8108574
H 2.5842590 5.6799577 19.7299544	C 10.7041200 4.6358473 20.5492046	H 9.4871480 10.5862832 13.0243242
C 2.5079939 6.9725215 22.1370814	C 13.0995737 4.0635126 20.8521489	H 9.2623459 8.9537987 13.6508169
H 2.7669620 7.9632755 21.7610702	H 5.1029002 8.1947028 17.7712936	H 7.9561614 9.7479621 12.7856188
H 3.3925679 6.3415499 22.0356729	C 4.9171936 9.2803090 19.6146126	C 4.8710335 9.0460758 1.8233956
H 2.2769623 7.0741440 23.1986633	C 15.2474852 7.2889941 17.5625153	H 3.9008852 9.4956179 1.6124047
	C 5.4182597 10.3584493 20.3419607	H 4.7350447 7.9622400 1.8495409
	C 6.9556380 12.3712379 20.7296520	H 5.5309171 9.2655117 0.9814682
	H 11.3179020 6.4927269 22.5395207	C 5.4602452 4.8855411 12.8115489
	H 13.0234318 6.0629838 22.7092515	H 5.0141869 3.9143304 13.0250216
	H 11.7731283 4.8665959 23.0642652	H 5.2377589 5.5470302 13.6514333
	H 9.9251148 5.3815728 20.6643542	H 6.5446381 4.7537140 12.7864830
	H 10.4569900 3.7849368 21.1876728	C 9.6302594 5.4565414 1.8260262
	H 10.7085451 4.2896016 19.5142764	H 10.6002823 5.0067276 1.6150775
	H 12.7979047 3.2650149 21.5313994	H 9.7668039 6.5402714 1.8534549
	H 14.0999030 4.3843788 21.1461653	H 8.9707352 5.2383937 0.9834973
	H 13.1548468 3.6380920 19.8486677	C 12.0018141 10.0557886 8.6966085
	C 3.8177747 8.4081438 20.1602992	C 12.4197406 11.3543682 9.4039041
	H 16.0141703 6.6767014 18.0396554	H 13.1664511 11.8679009 8.7969655
	H 15.6854587 8.2621287 17.3382601	H 12.8659220 11.1604723 10.3803897
	H 15.0010331 6.8142990 16.6088417	H 11.5798857 12.0380596 9.5390252
	H 4.9876973 10.5411695 21.3153462	C 13.2698163 9.1973726 8.5028418
	C 6.1875144 12.5114858 22.0534116	H 14.0098189 9.7488759 7.9187701
	C 8.4428269 12.1613018 21.0833191	H 13.0433158 8.2694879 7.9838216
	C 6.7832899 13.6919149 19.9493091	H 13.7167930 8.9518873 9.4680238
	H 3.5858376 8.6577025 21.1954881	C 11.4250249 10.4449932 7.3202204
	H 4.0957298 7.3535863 20.1187574	H 12.1642034 11.0139507 6.7526367
	H 2.8997821 8.5172143 19.5778772	H 10.5372552 11.0706509 7.4317544
	H 5.1235361 12.6887541 21.8899916	H 11.1584259 9.5666388 6.7414735
	H 6.5819423 13.3641572 22.6079911	C 2.4993851 4.4431687 8.6971006
	H 6.2974513 11.6291671 22.6853202	C 1.2308363 5.3008046 8.5034480
	H 9.0591429 12.0811666 20.1931221	H 0.4911590 4.7488655 7.9193797
	H 8.5726639 11.2520163 21.6735003	H 1.4567297 6.2288581 7.9844722
	H 8.8087199 13.0012479 21.6775110	H 0.7837418 5.5459501 9.4686616
	H 5.7289108 13.8684309 19.7278050	C 3.0763735 4.0543985 7.3206733
	H 7.3320683 13.6753654 19.0122209	H 2.3375434 3.4849746 6.7530986
	H 7.1457226 14.5296905 20.5493254	H 3.9645654 3.4293172 7.4321438
		H 3.3423887 4.9329413 6.7419487
		C 2.0823193 3.1443066 9.4043842

		H 1.3359725 2.6302724 8.7974196 H 1.6359687 3.3378952 10.3808610 H 2.9226402 2.4611817 9.5395382 C 10.0494897 2.4909577 5.9393299 C 10.4368920 3.0664747 7.3166910 H 11.0031883 2.3259952 7.8852565 H 9.5577902 3.3346000 7.8935992 H 11.0645166 3.9530677 7.2066404 C 9.1865786 1.2257116 6.1307616 H 9.7341320 0.4840521 6.7164651 H 8.9423690 0.7793727 5.1649504 H 8.2579724 1.4552295 6.6471747 C 11.3486398 2.0690760 5.2353633 H 11.8579495 1.3202915 5.8433390 H 12.0355976 2.9066758 5.1026665 H 11.1559892 1.6241477 4.2580583 C 4.4484686 12.0077762 5.9391275 C 3.1495609 12.4297091 5.2347495 H 2.6396377 13.1778429 5.8430021 H 2.4630030 11.5919521 5.1010324 H 3.3425899 12.8754525 4.2578929 C 5.3108295 13.2732044 6.1318152 H 4.7627206 14.0142772 6.7177317 H 5.5553260 13.7202652 5.1664232 H 6.2392529 13.0436915 6.6484990 C 4.0605637 11.4312882 7.3159328 H 3.4937455 12.1712277 7.8846670 H 4.9394701 11.1631214 7.8930877 H 3.4332857 10.5445724 7.2050530