Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.
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1. NMR Spectra of New Compounds

Figure S1. ^{1}H NMR spectrum (600 MHz, 298 K, THF-d_8) of $K^{+}\cdot\mathbf{5}^{-}$.

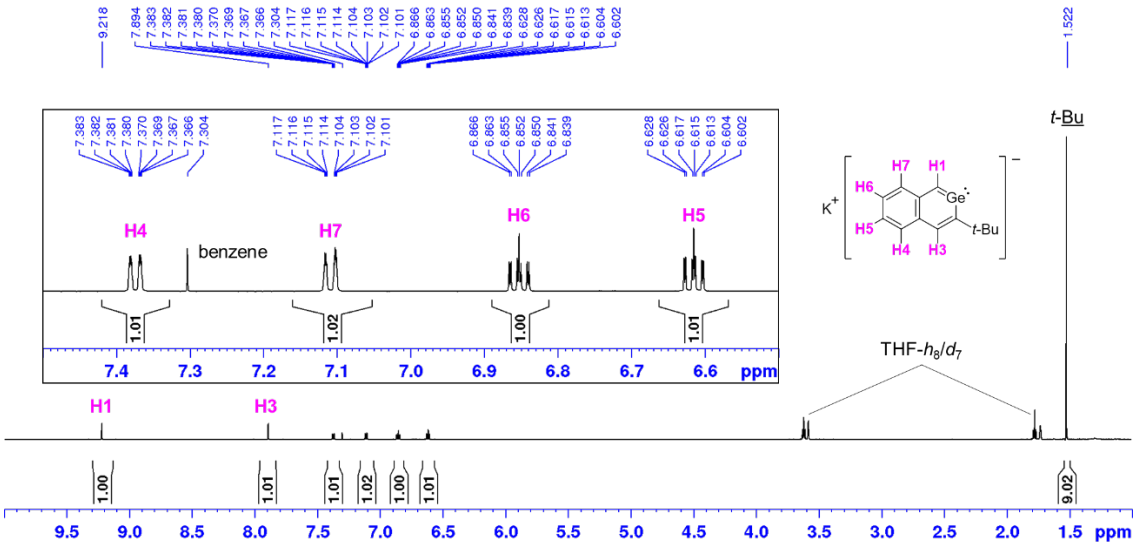


Figure S2. ^{13}C{^{1}H} NMR spectrum (151 MHz, 298 K, THF-d_8) of $K^{+}\cdot\mathbf{5}^{-}$.

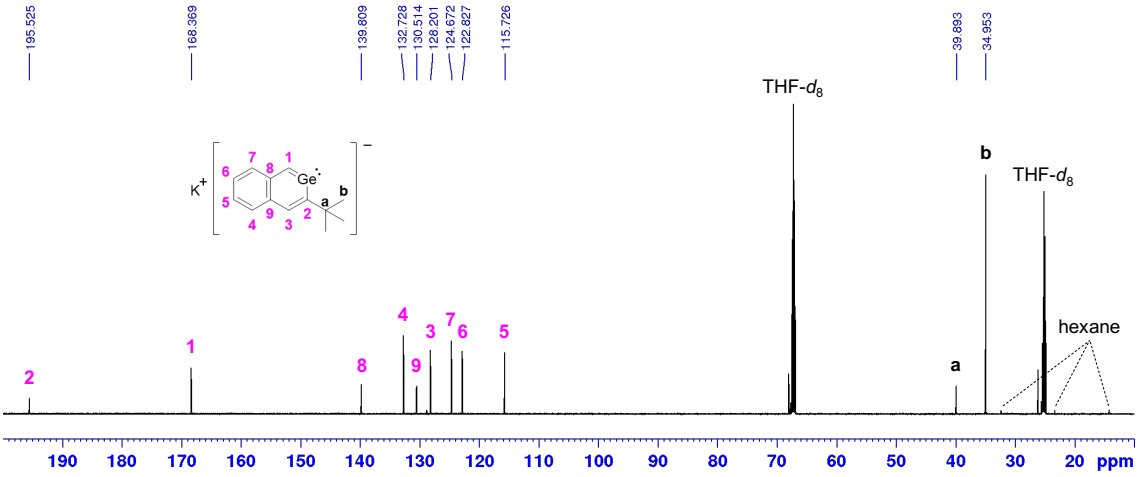


Figure S3. ^{1}H NMR spectrum (600 MHz, 298 K, THF-d_8) of K$^+$(crypt-222)·**5**$^-$.

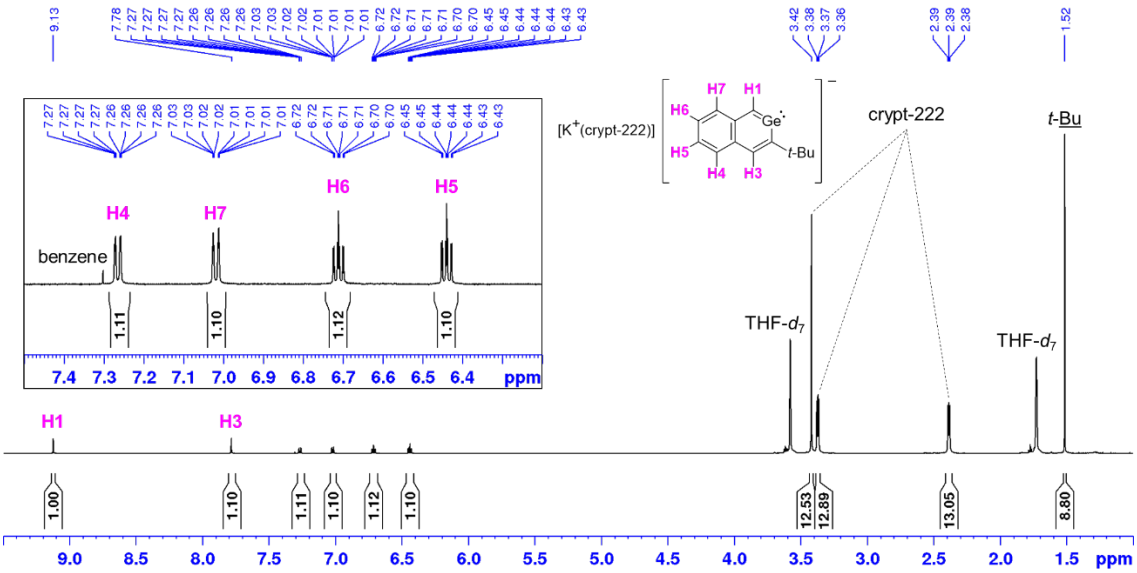


Figure S4. ^{13}C{^{1}H} NMR spectrum (151 MHz, 298 K, THF-d_8) of K$^+$(crypt-222)·**5**$^-$.

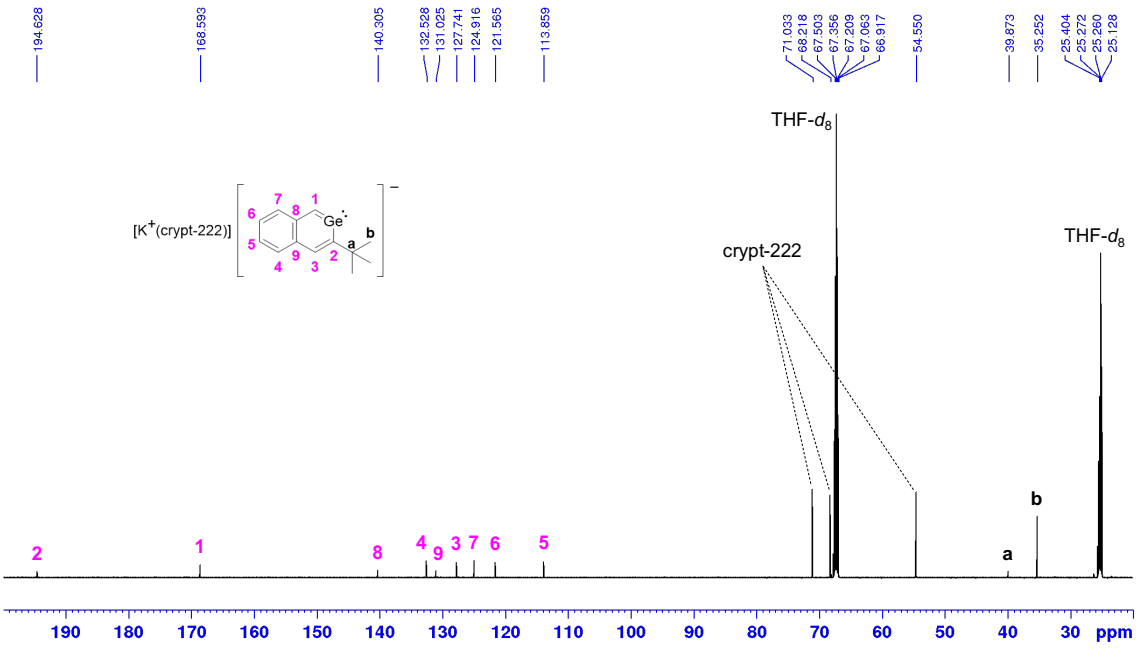
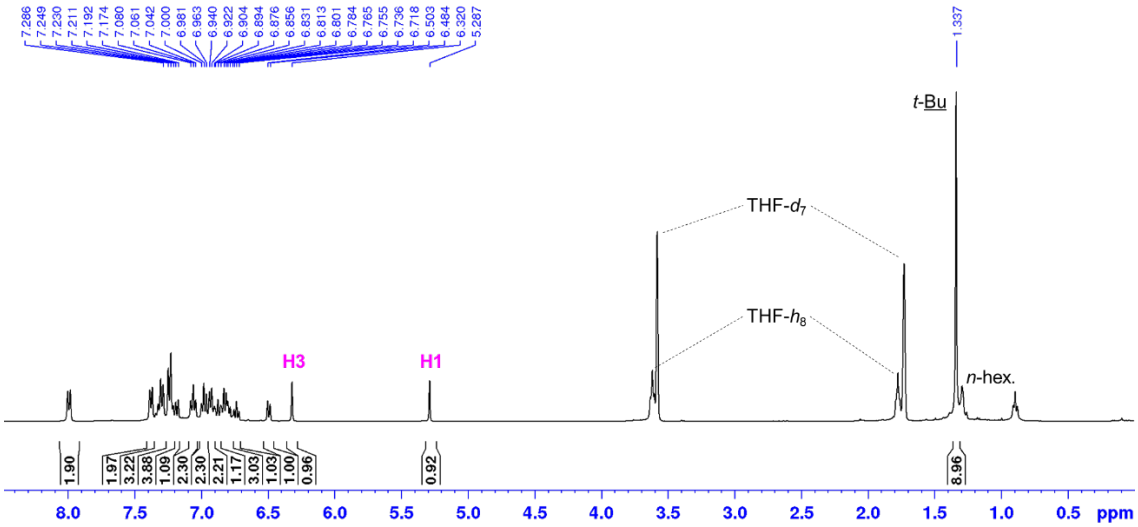
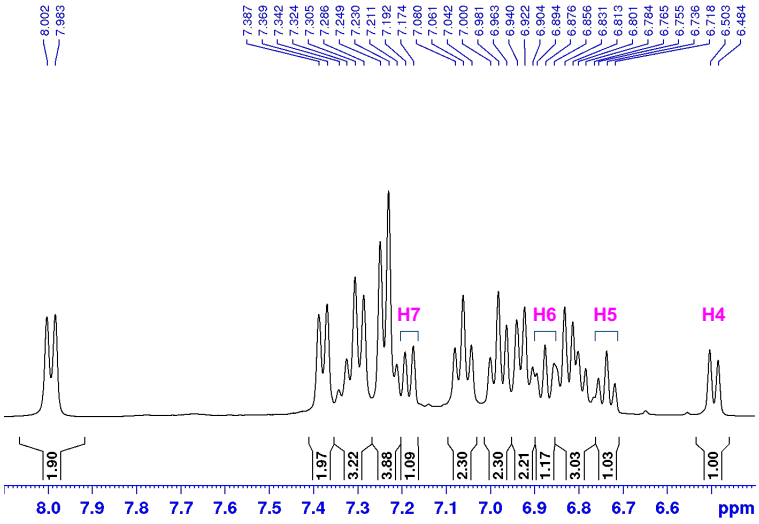


Figure S5. ^{1}H NMR spectrum (400 MHz, 298 K, THF-d_8) of K^{+}(thf)·**7**$^{-}$.



Aromatic region



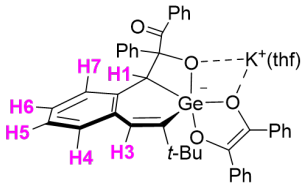


Figure S6. NOESY spectrum (400 MHz, 298 K, THF-d_8) of $K^+(thf)\cdot\mathbf{7}^-$.

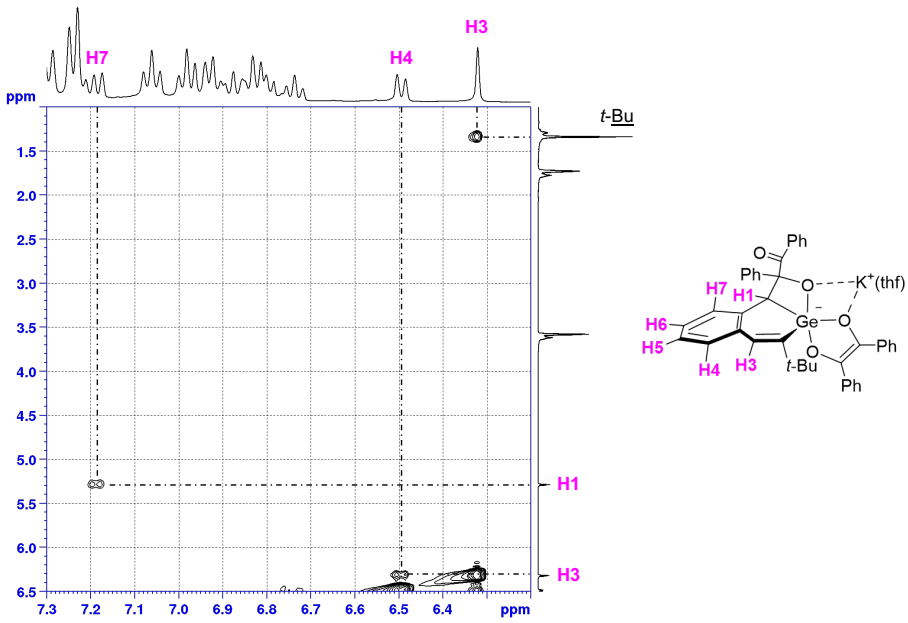


Figure S7. ^1H-^1H COSY spectrum (400 MHz, 298 K, THF-d_8) of $K^+(thf)\cdot\mathbf{7}^-$.

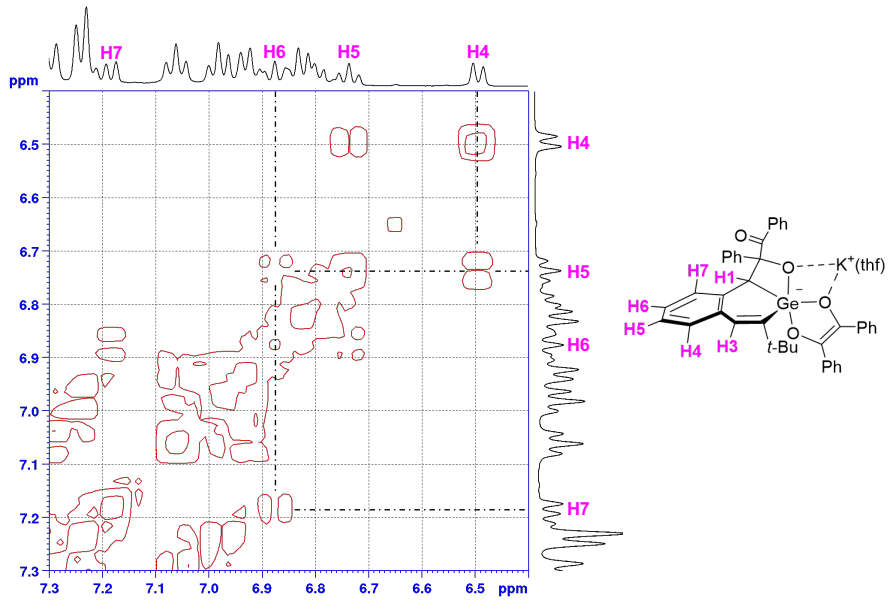
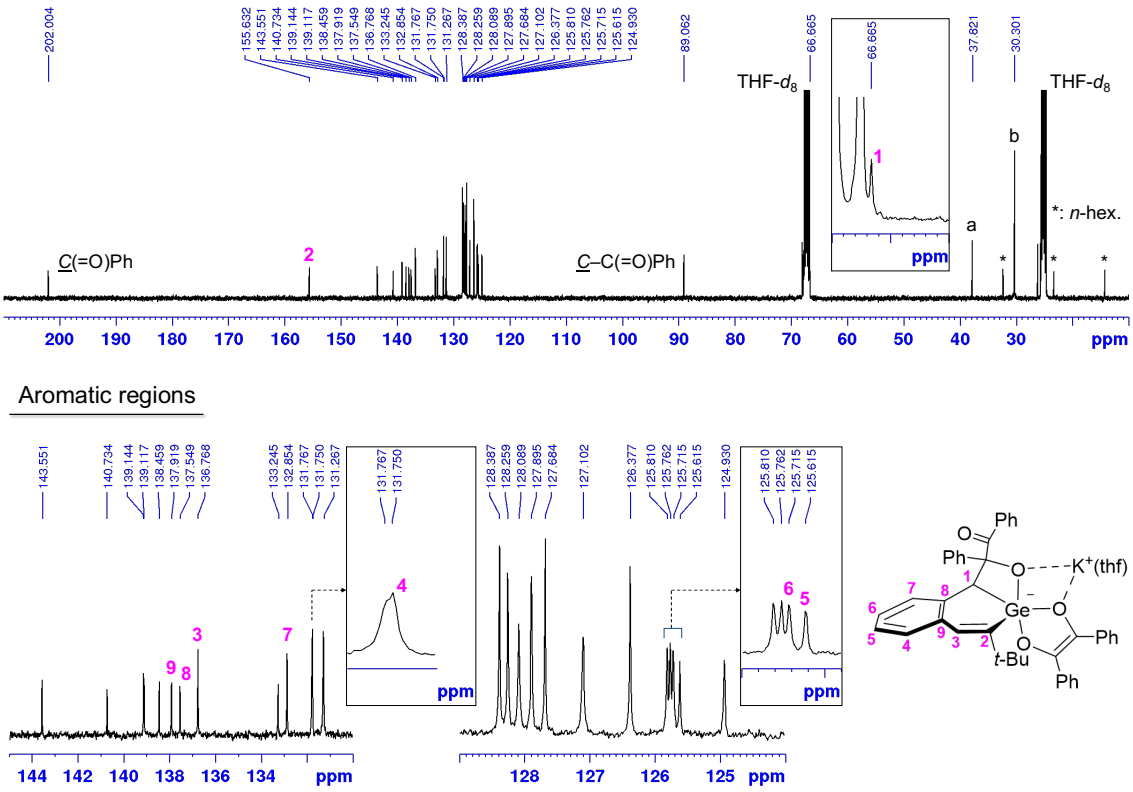
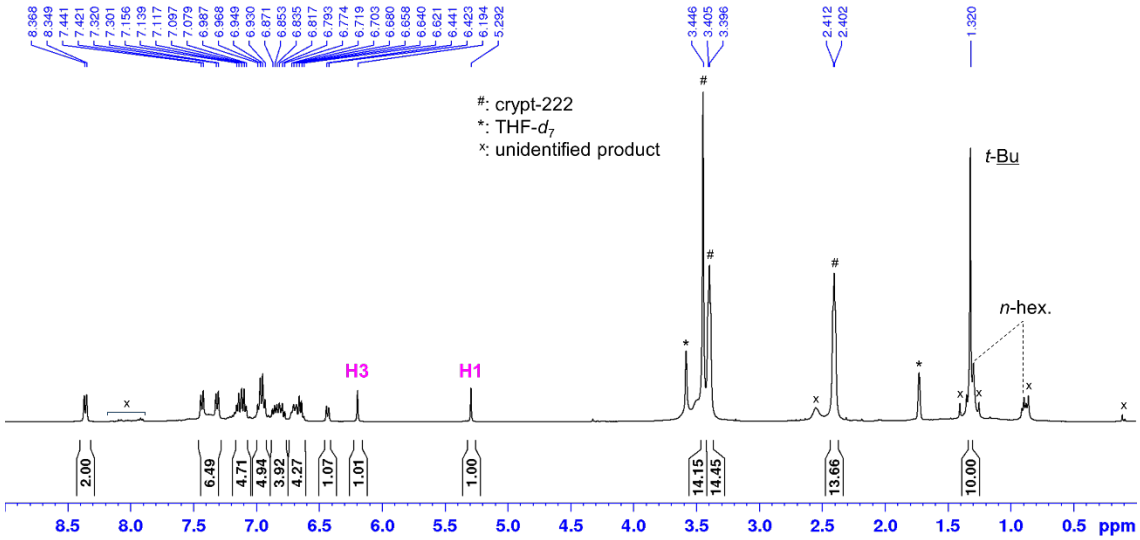


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, THF-d_8) of $K^+(thf)\cdot\mathbf{7}^-$.

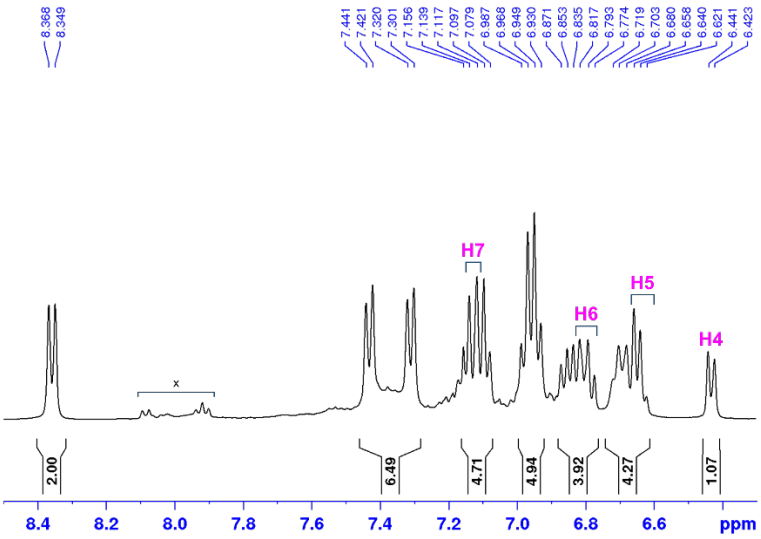


Aromatic regions

Figure S9. ^{1}H NMR spectrum (400 MHz, 298 K, THF-d_8) of K^+(crypt-222)·**7**$^-$.



Aromatic region



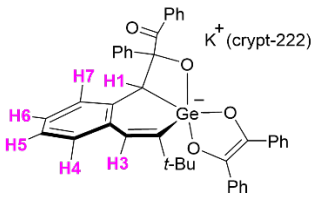


Figure S10. NOESY spectrum (400 MHz, 298 K, THF-d_8) of K^+(crypt-222)·**7**$^-$.

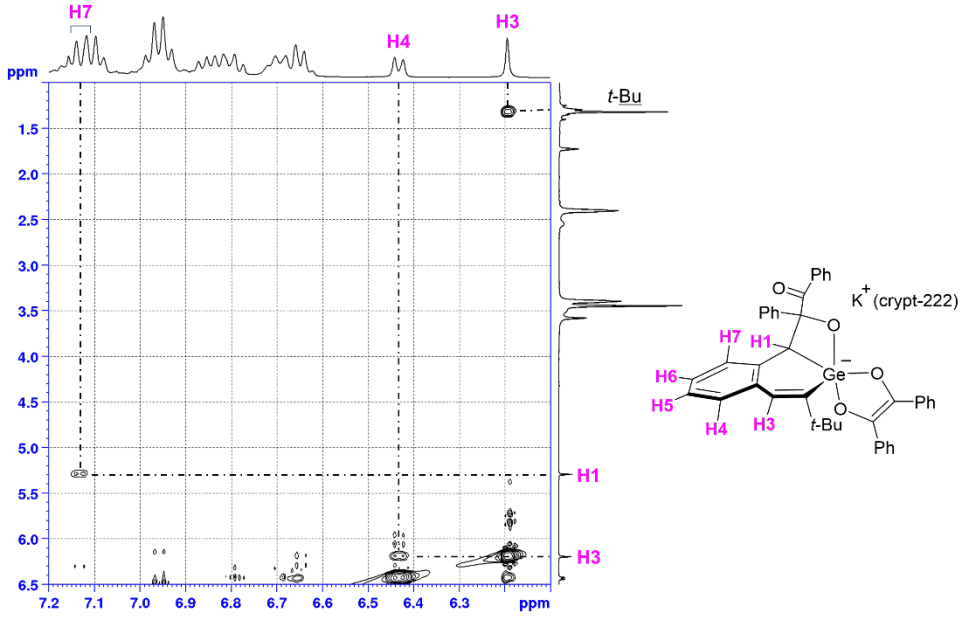


Figure S11. ^{1}H-^{1}H COSY spectrum (400 MHz, 298 K, THF-d_8) of K^+(crypt-222)·**7**$^-$.

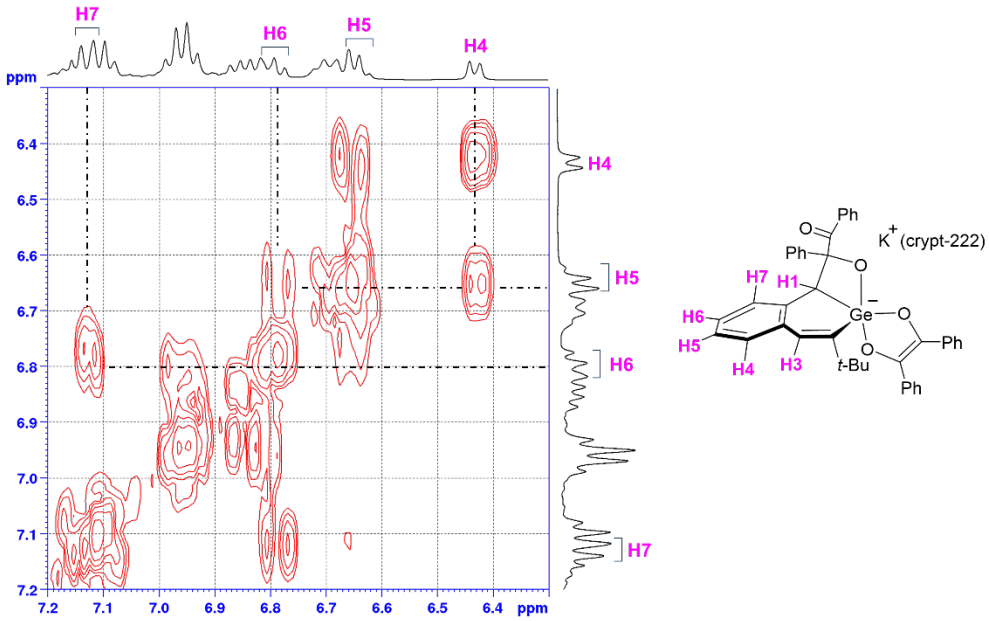
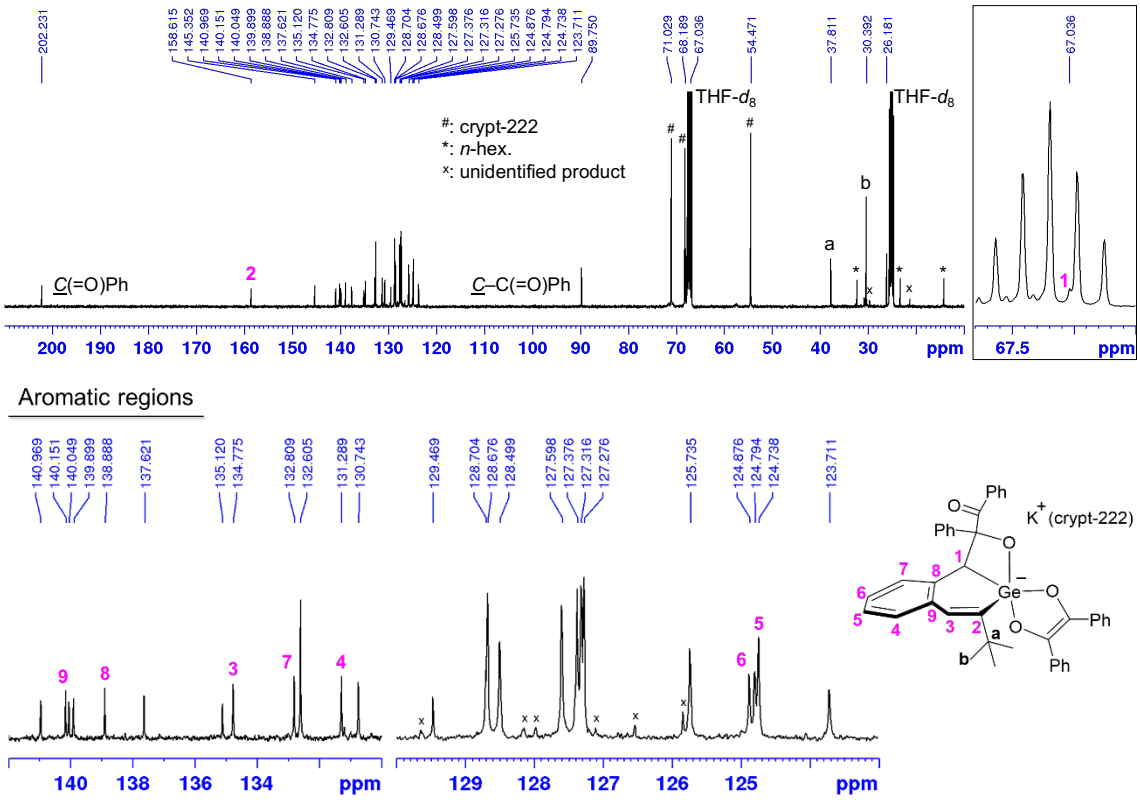


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, 298 K, THF-d_8) of K^+(crypt-222)·**7**$^-$.



2. X-Ray Diffraction Studies

All single crystals were obtained by slow evaporation technique using the solvent, and the crystal data were summarized in Table S1. The intensity data were collected at 103 K on Rigaku Saturn70 CCD diffractometer with the VariMax Optix [for K^+·**5**$^-$ and K^+(crypt-222)·**5**$^-$] or at 90 K on Bruker D8 VENTURE system (PHOTONIII 14 with IμS Diamond), using Mo Kα radiation (λ = 0.71073 Å). The intensity data were corrected for Lorentz and polarization effects and for absorption (multi-scan). The structure was solved by SHELXT-2018/2[1] and refined by least-squares calculations on F^2 for all reflections (SHELXL-2019/3).[2] All non-hydrogen atoms were refined anisotropically. All calculations were performed using Yadokari-XG 2011 software package[3] and Olex2-1.5.[4] In the crystal structure of K^+(thf)·**7**$^-$, THF molecule in a unit structure was highly disordered and treated by SQUEEZE.[5]

Figure S13. Atomic displacement parameter plot for the crystal packing of K^+(crypt-222)·**5**$^-$ at 50% probability.

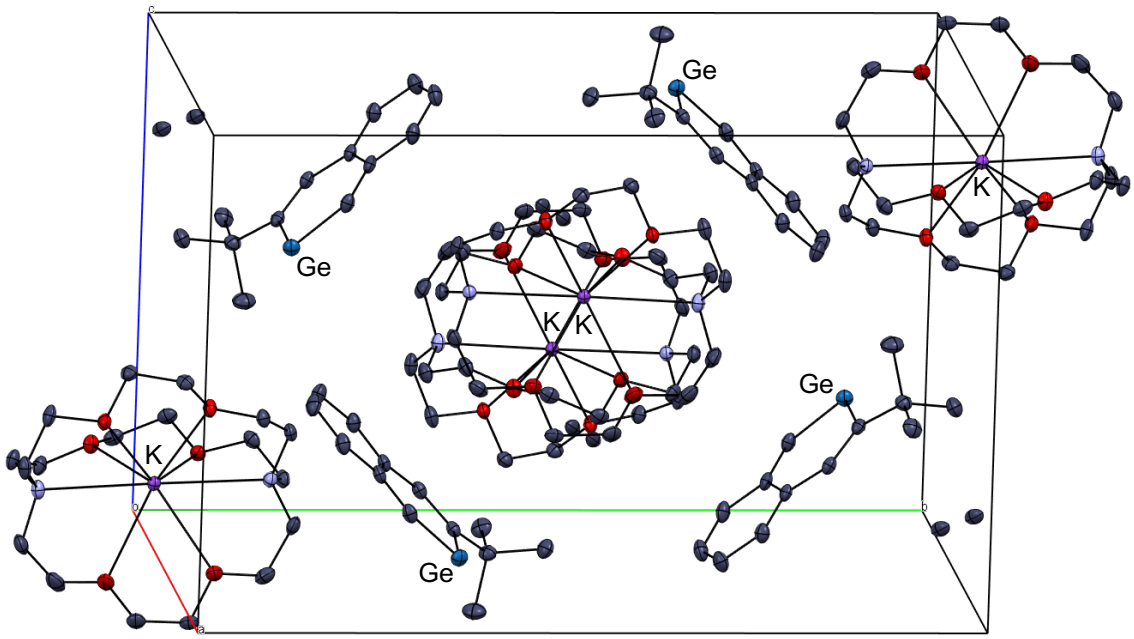


Figure S14. Atomic displacement parameter plot for the crystal packing of K^+(thf)·**7**$^-$ at 50% probability.

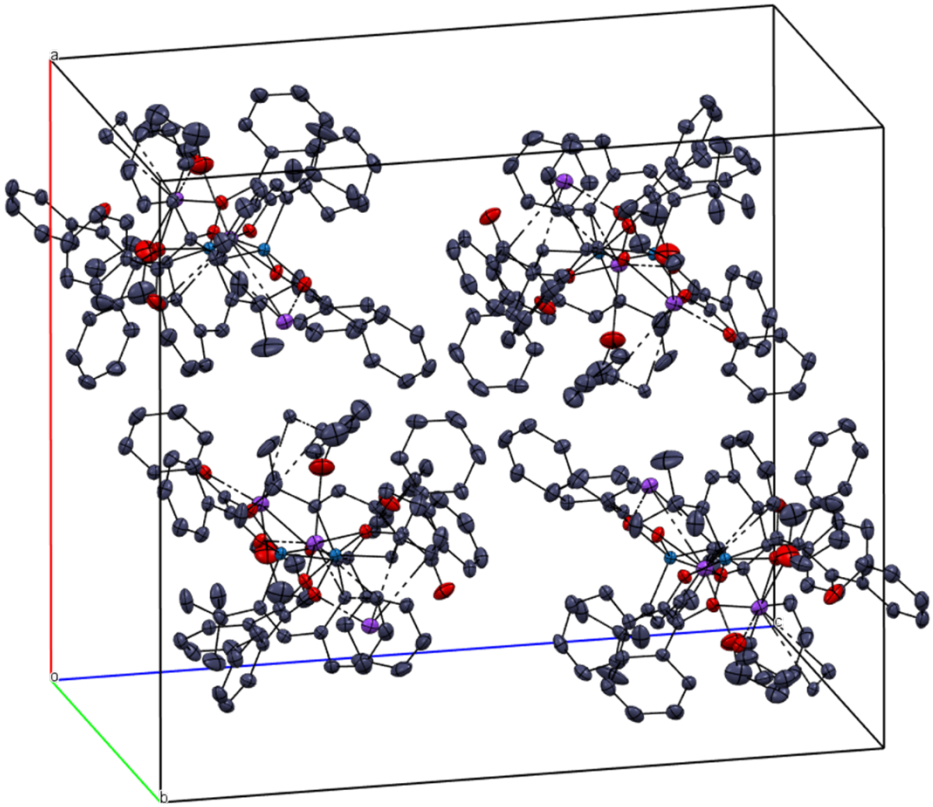


Figure S15. Chain structure of K^+(thf)·**7**$^-$ along b-axis.

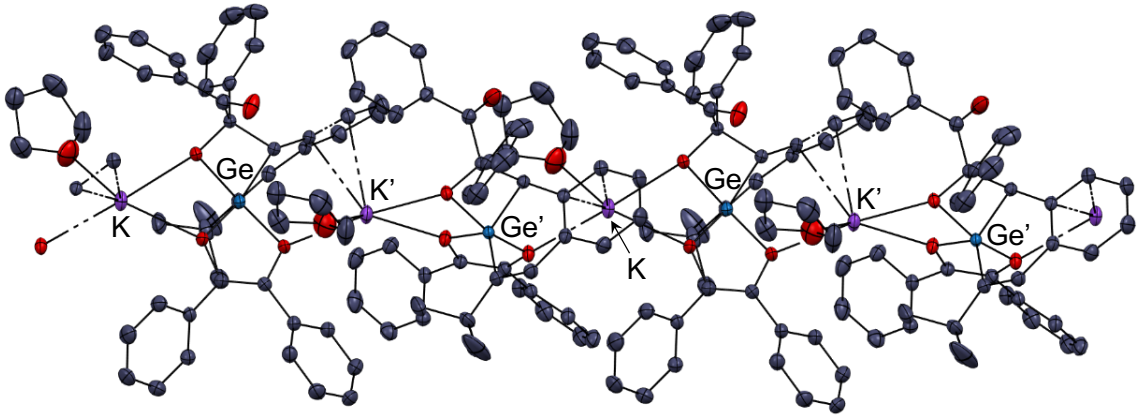


Table S1. Crystallographic data for K^+(benzene)·**5**$^-$ and K^+(crypt-222)·**5**$^-$ and K^+(thf)·**7**$^-$.

	K^+(benzene)·**5**$^-$	K^+(crypt-222)·**5**$^-$	K^+(thf)·**7**$^-$
Empirical formula	$C_{19}H_{21}GeK$	$C_{31}H_{51}GeKN_2O_6$	$C_{45}H_{43}GeKO_5$
Formula weight	361.05	659.42	775.48
Temperature (K)	103(2)	103(2)	90(2)
Crystal color	red	yellow	yellow
Crystal dimensions	0.14 x 0.06 x 0.05	0.31 x 0.10 x 0.10	0.15 x 0.05 x 0.03
Crystal system	Triclinic	monoclinic	Orthorhombic
Space group	*P*-1 (#2)	$P2_1/n$ (#14)	*Pbca* (#61)
a (Å)	11.9817(5)	12.3924(2)	21.666(2)
b (Å)	12.6631(6)	20.5323(3)	14.7024(14)
c (Å)	13.4909(6)	13.1027(2)	24.960(3)
α (°)	66.739(4)	90	90
β (°)	78.875(4)	92.150(2)	90
γ (°)	73.759(4)	90	90
V (Å^3)	1797.57(15)	3331.56(9)	7950.7(14)
Z	4	4	8
D_{calc} (g·cm^{-3})	1.334	1.315	1.296
μ (mm^{-1})	1.927	1.087	0.919
θ range (°)	1.650 to 27.499	1.920 to 25.250	1.862 to 27.525
Reflections collected	15973	41022	140103
R_{int}	n.d.	0.0281	0.0729
Completeness to θ	99.6	99.7	99.9
No. of restrains	0	0	0
No. of parameters	388	386	472
Goodness of fit	1.022	1.032	1.039
R_1 [I>2σ(I)]	0.0640	0.0253	0.0329
wR_2 [I>2σ(I)]	0.1540	0.0648	0.0838
R_1 (all data)	0.0980	0.0275	0.0395
wR_2 (all data)	0.1689	0.0663	0.0888
Largest diff. peak (e·Å^3)	0.931	0.797	0.430
Largest diff. hole (e·Å^3)	−0.689	−0.489	−0.406
CCDC deposition number	2301146	2301147	2301148

3. Theoretical Calculations

DFT calculations were performed using the Gaussian 16 (Rev. B. 01)[6] program package with B3LYP functional[7] along with a combined basis sets: 6-31G(d,p) level in the optimizations; 6-311G(2df,2p) in the GIAO, TD-DFT and NBO (version 7.0)[8] calculations if there is no mentions. The NBO calculations include NPA, WBI and NRT analyses. The frequency calculations were carried out for each optimized structure to confirm the absence of any imaginary frequencies.

3.1. 2-Germanaphthalenyl anion $\mathbf{5}^-$.

Figure S16. Selected bond lengths (Å) and C–Ge–C angles (deg) for (a) K^+(benzene)·$\mathbf{5}^-$ (two independent molecules); (b) K^+(crypt-222)·$\mathbf{5}^-$; (c) optimized structure of $\mathbf{5}^-$.

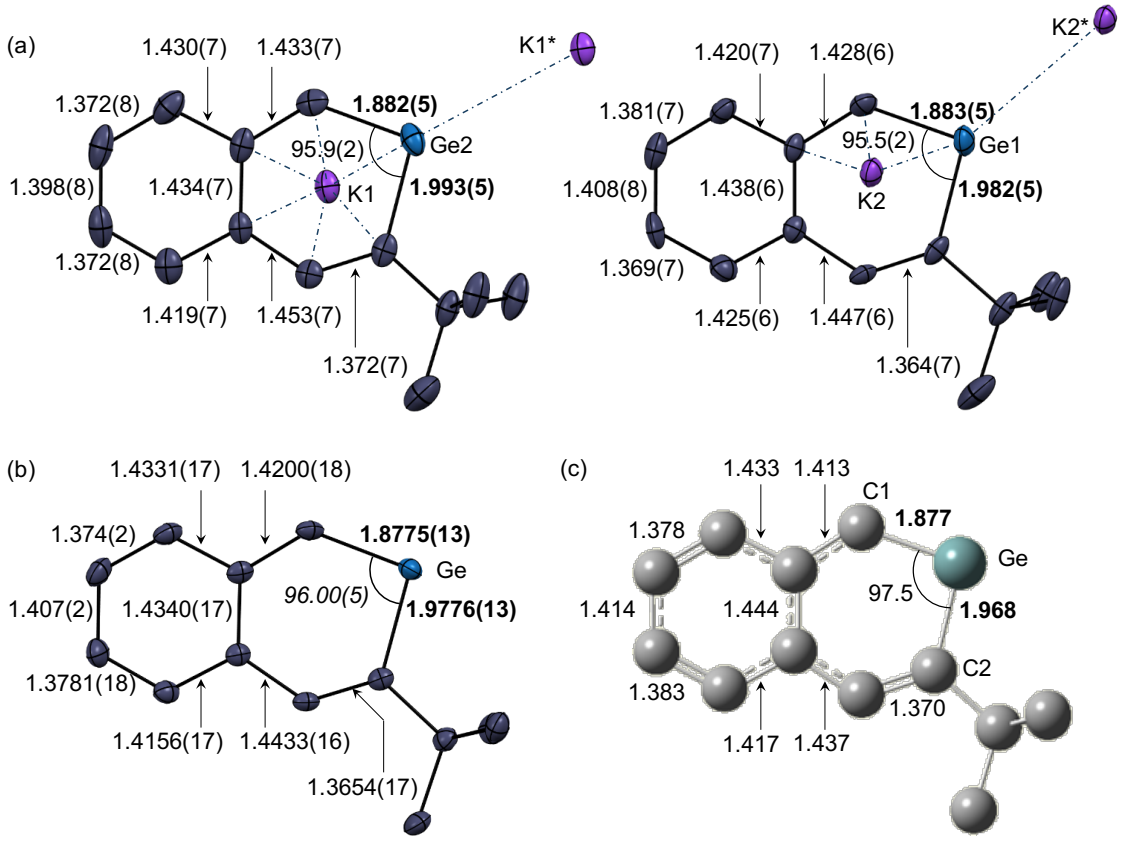
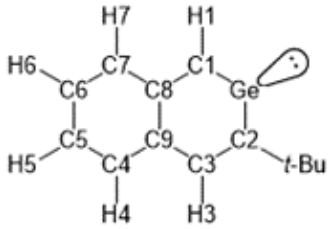


Table S2. Orbital hybridization of the atoms on Ge–C bonds in **5**$^-$ (the numbering of carbon atoms is described in Figure S16c).

Bond	No.	orbital hybridization
Ge–C1	1	C1: s (36.09%), p (63.68%), d (0.20%), f (0.03%); $sp^{1.76}d^{0.01}$ Ge: s (17.46%), p (82.27%), d (0.26%), f (0.01%); $sp^{4.71}d^{0.01}$
	2	**C1: s (0.00%), p (99.94%), d (0.03%), f (0.03%); p only** **Ge: s (0.00%), p (99.78%), d (0.21%), f (0.01%); p only**
Ge–C2	1	C2: s (29.63%), p (70.20%), d (0.15%), f (0.02%); $sp^{2.37}$ Ge: s (13.46%), p (86.25%), d (0.27%), f (0.02%); $sp^{6.41}d^{0.02}$

Table S3. Experimental (in THF-d_8) and theoretically calculated ^{1}H and ^{13}C NMR chemical shifts (ppm) for K^+·**5**$^-$ and K^+(crypt-222)·**5**$^-$.



	H1		H3	H4	H5	H6	H7
K^+·**5**$^-$	9.22		7.89	7.38	6.62	6.85	7.11
K^+(crypt-222)·**5**$^-$	9.13		7.78	7.27	6.44	6.71	7.02
calcd.	*9.62*		*7.91*	*7.36*	*6.40*	*6.77*	*7.08*
	C1	C2	C3	C4	C5	C6	C7
K^+·**5**$^-$	169.37	195.53	128.20	132.73	115.73	122.83	124.67
K^+(crypt-222)·**5**$^-$	168.59	194.63	127.74	132.53	113.86	121.57	124.92
calcd.	*176.50*	*201.53*	*130.81*	*136.44*	*114.48*	*123.83*	*128.40*
	C8	C9					
K^+·**5**$^-$	139.81	130.51					
K^+(crypt-222)·**5**$^-$	140.31	131.03					
calcd.	*144.62*	*135.11*					

Figure S17. $NICS_{total}(r)$ plots of $\mathbf{5}^-$ and $\mathbf{1}^-$. The parameter "r" denominates the distance (Å) from the geometrical center of the ring along the z-axis, which is oriented in perpendicular direction with respect to the plane of the ring.

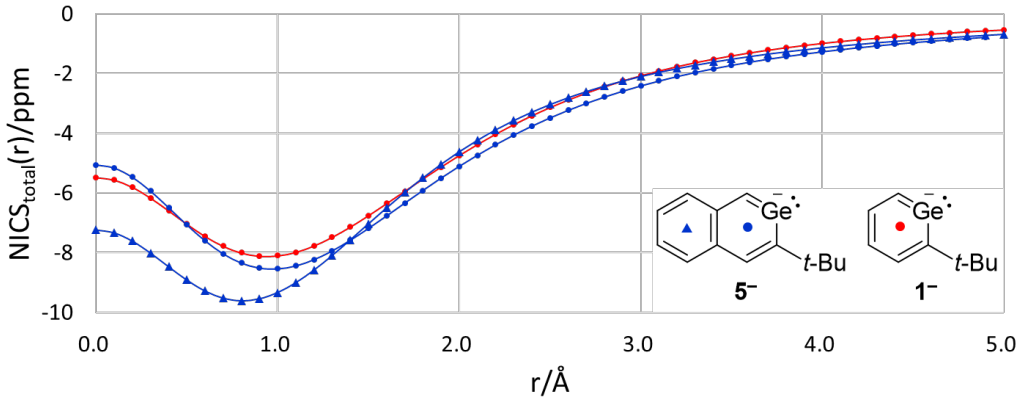


Figure S18. Detailed $NICS_{zz}(r)$ plots for $\mathbf{1}^-$ and $\mathbf{5}^-$ (a), and $\mathbf{5}^-$, **6**, 2-naphthyl anion and naphthalene (b). Determination of the parameter "r" is same as in Figure S17.

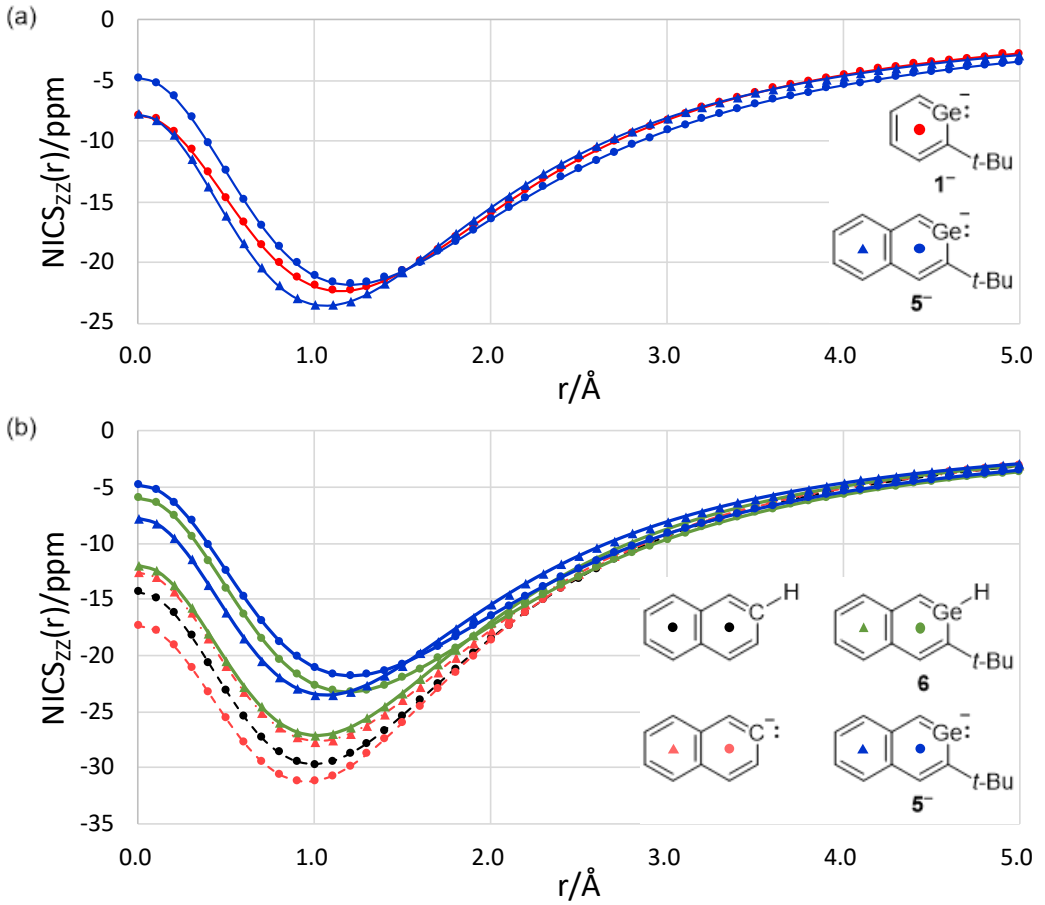
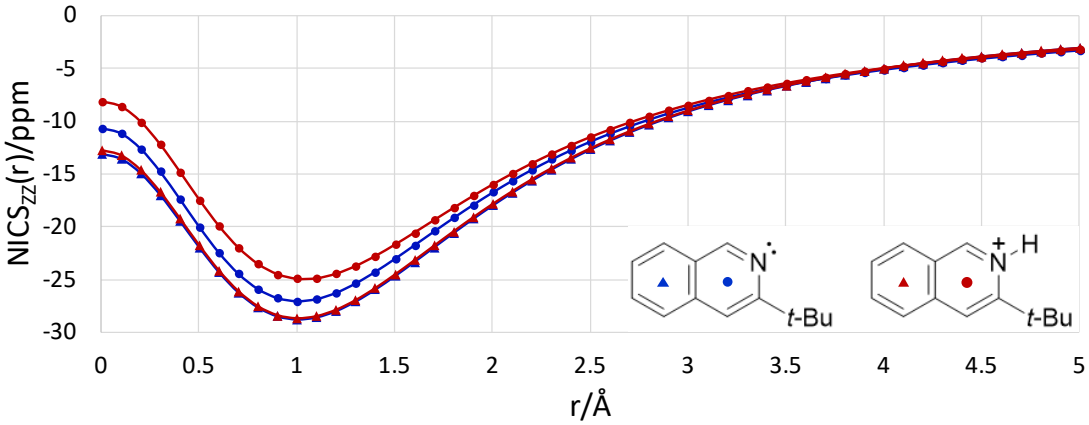


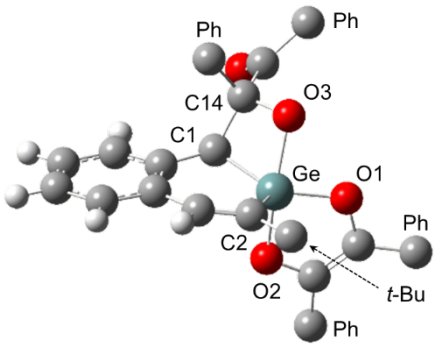
Figure S19. $NICS_{zz}(r)$ plots for isoquinoline and isoquinolinium. Determination of the parameter "r" is same as in Figure S17.

The plots suggest that after protonation of isoquinolinium, aromaticity gets greater in the NC_5 ring, while showing negligible change in the C_6 ring. This enhancement of aromaticity only in NC_5 ring is most likely caused by appearance of the sp^2-lonepair on the nitrogen atom, suggesting considerable effect of sp^2-lonepair on aromaticity of involving aromatic ring.



3.2. Benzil adduct 7^-.

Figure S20. Selected bond lengths (Å) and angles (deg.) for optimized structure of 7^- (*t*-Bu and phenyl groups are omitted for clarity).



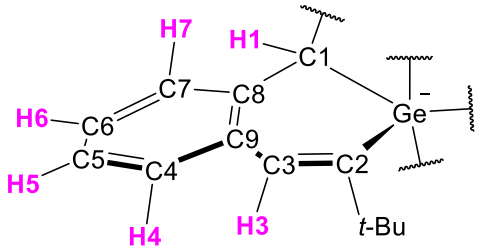
Ge−C1	1.9588	C1-Ge-C2	105.17
Ge−C2	1.9449	C1-Ge-O1	133.26
Ge−O1	1.8515	C2-Ge-O1	120.44
Ge−O2	1.9375	O2-Ge-O3	161.56
Ge−O3	1.9522		
C1−C14	1.5833		
O3−C14	1.4130		

Table S4. Selected results of NBO analysis of 7^-.

	O1	O2	O3	C1	C2	Ge
WBI[a] with Ge	0.544	0.435	0.397	0.681	0.715	-
NPA charge	–0.822	–0.819	–0.901	–0.649	–0.381	+1.944

[a]Wiberg bond index.

Table S5. Experimental ^{1}H and ^{13}C NMR chemical shifts (ppm) along with calculated values for selected atoms.



	H1	H3	H4	H5	H6	H7
K^{+}(thf)·***7***$^{-}$	5.29	6.32	6.50	6.74	6.88	7.18
K^{+}(crypt-222)·***7***$^{-}$	5.29	6.19	6.43	6.63	6.78	7.12
A*/*X	*5.06*	*6.69*	*7.00*	*6.78*	*6.71*	*7.00*
B*/*X	*5.43*	*6.67*	*6.82*	*6.66*	*6.55*	*6.78*
C*/*X	*5.31*	*7.23*	*7.40*	*7.23*	*7.12*	*7.39*

	C1	C3	C4	C5	C6	C7
K^{+}(thf)·***7***$^{-}$	66.67	136.77	131.75	125.62	125.72	132.85
K^{+}(crypt-222)·***7***$^{-}$	67.06	134.75	131.28	124.77	124.84	127.96
A*/*X	*51.12*	*136.72*	*137.10*	*129.10*	*130.56*	*142.66*
B*/*X	*66.86*	*137.54*	*135.96*	*127.32*	*128.16*	*140.76*
C*/*X	*63.34*	*154.30*	*152.27*	*142.83*	*144.51*	*158.17*

	C2	C8	C9
K^{+}(thf)·***7***$^{-}$	155.63	137.55	137.92
K^{+}(crypt-222)·***7***$^{-}$	158.61	138.91	140.14
A*/*X	*165.23*	*150.58*	*147.70*
B*/*X	*166.31*	*149.61*	*146.20*
C*/*X	*186.74*	*166.80*	*162.71*

A: HF, ***B***: B3LYP, ***C***: M06-2X, ***X***: 6-311G(2df,2p).

Figure S21. Selected NBOs for lone pairs on the O1 – O3 atoms and vacant orbital on the Ge atom of **7**$^-$.

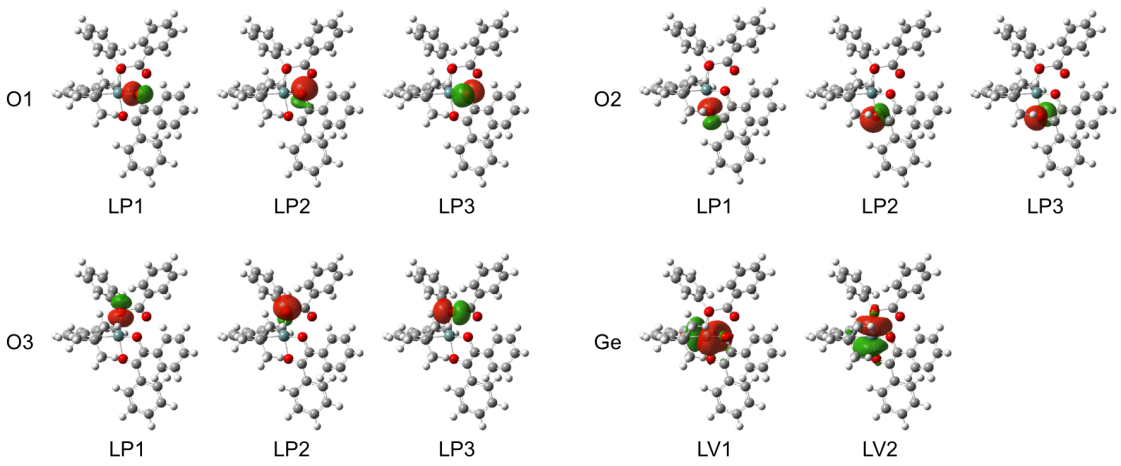
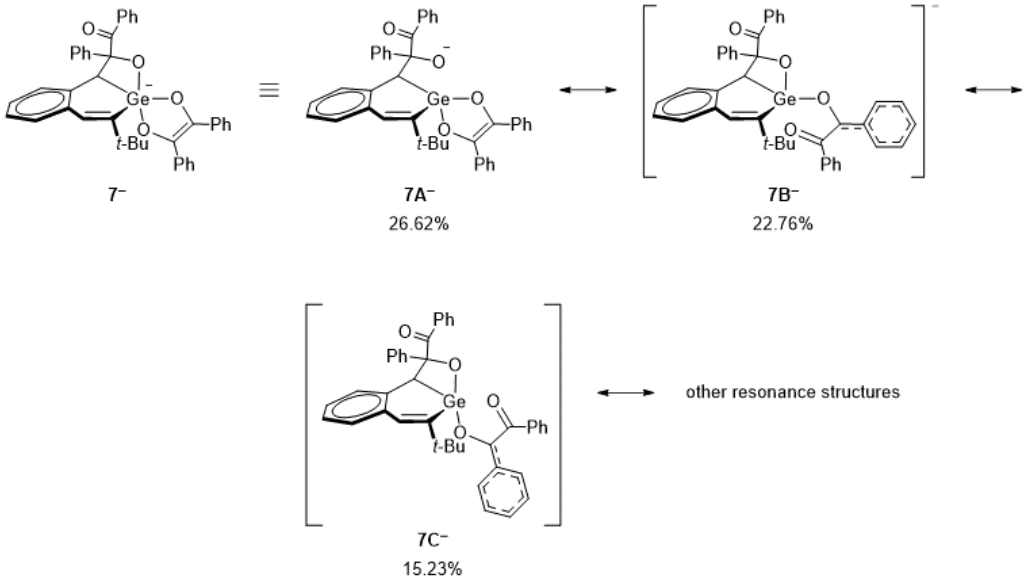


Table S6. Second order perturbation energies between the NBOs (kcal/mol).

		O1			O2			O3		
		LP1	LP2	LP3	LP1	LP2	LP3	LP1	LP2	LP3
Ge	LV1	169.23	13.78	0.15	36.31	14.92	-	2.58	-	5.48
	LV2	5.49	6.00	0.29	84.44	-	2.22	102.95	9.65	0.96
total		194.94			137.89			121.62		

Scheme S1. Summary of natural resonance theory (NRT) analysis calculated at the B3LYP/6-31G(d,p) level of theory.



4. Investigation of UV-vis Absorption Spectra of New Compounds.

Compound K^+(benzene)·**5**$^-$ shows a red color in the solid state and a yellow color in solution. In addition, K^+(thf)·**7**$^-$ shows a green color, while K^+(crypt-222)·**7**$^-$ shows a yellow color both in the solid state and in solution. These color changes seemed to be induced by situations of the coordination around the potassium atom and accordingly interactions with counter anions (**5**$^-$ or **7**$^-$).

TD-DFT calculations for models with $[K_2(benzene)_2\cdot\mathbf{5}_4]^{2-}$ and $[K(thf)\cdot\mathbf{7}_2]^-$, along with for free anions **5**$^-$ and **7**$^-$, were carried out in order to investigate the cause of the color changes. The models were derived from the infinite structure of K^+(benzene)·**5**$^-$ and K^+(thf)·**7**$^-$ determined by X-ray crystallographic analyses respectively.

The structural optimization of $[K_2(benzene)_2\cdot\mathbf{5}_4]^{2-}$ and $[K(thf)\cdot\mathbf{7}_2]^-$ was performed using the atom-coordinates of X-ray crystallographic data with Opt=ReadFreeze (with "noatoms atoms=H") keyword to fix the geometry of all atoms except for H atoms. In other words, only the positions of H atom were optimized (in the X-ray crystallographic analysis, the positions of H atoms were determined by the calculations). TD-DFT calculations were performed based on the optimized structures.

Figure S22. Experimental UV-vis absorption spectrum of K^+·**5**$^-$ in THF at 298 K, along with simulated spectrum of free anion **5**$^-$ and responsible frontier orbitals (isovalues = 0.03) for four longest absorptions calculated at the B3LYP/6-311G(2df,2p)//B3LYP/6-31G(d,p) level of theory. In the transition at 337.1 nm, HOMO → LUMO+1 transition (c) has the largest contribution.

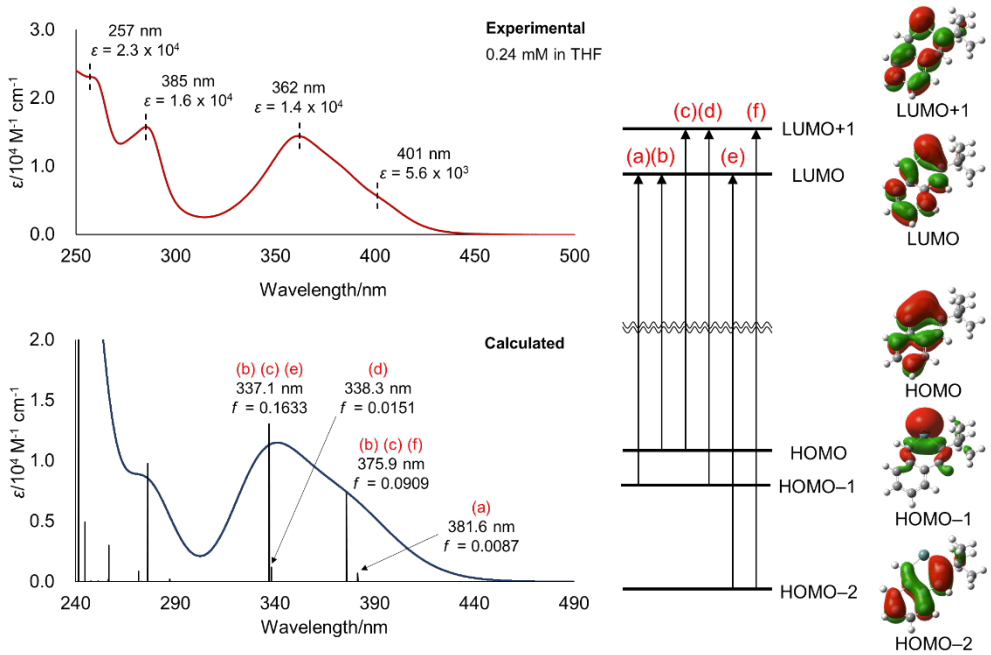


Figure S23. Experimental UV-vis absorption spectrum of K^+(benzene)·**5**$^-$ in the solid state obtained from Kubelka-Munk transformation[9] of its refraction spectrum. Simulated spectrum of $[K_2(benzene)_2\cdot\mathbf{5}_4]^{2-}$ calculated at the B3LYP/6-311G(2df,2p)//B3LYP/6-31G(d,p) level of theory is also shown, along with responsible frontier orbitals (isovalues = 0.02) for the absorptions at 501.09 and 489.12 nm. In the absorption at 489.12 nm, HOMO → LUMO+1 transition (d) has the largest contribution.

In the LUMO+1 of model molecule $[K_2(benzene)_2\cdot\mathbf{5}_4]^{2-}$, the lobes on the Ge···Ge moiety were found. This type of thorough-space interaction can be considered as an important factor for the color change of $K^+\cdot$**5**$^-$ in the solid state.

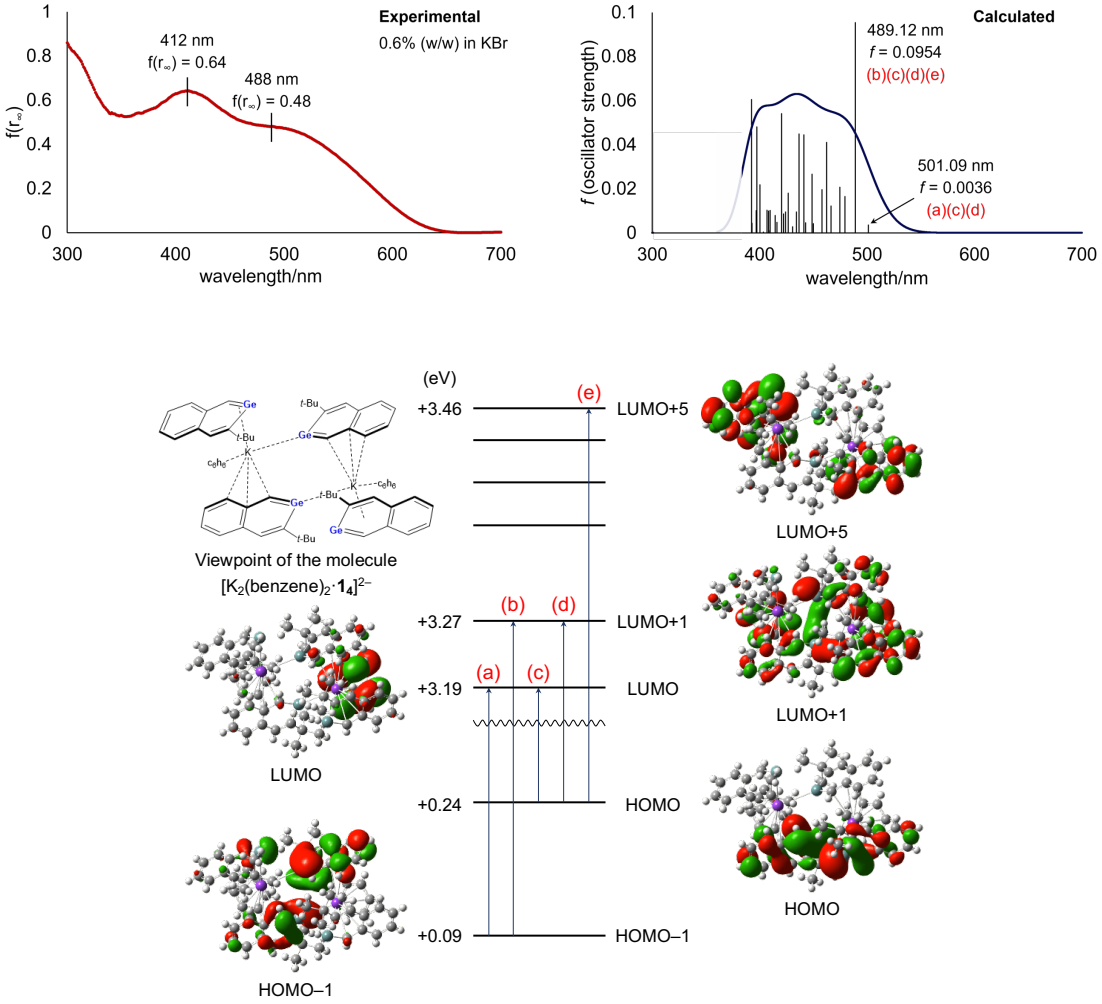


Figure S24. Observed UV-vis absorption spectrum of $K^+ \cdot \mathbf{7}^-$ in THF at 298 K, along with simulated spectrum of $[K(thf) \cdot \mathbf{7}_2]^-$ and responsible frontier orbitals (isovalues = 0.03) for the absorption at 340.66 nm calculated at the CAM-B3LYP/6-311G(2df,2p)//B3LYP/6-31G(d) level of theory. HOMO → LUMO+3 transition has the largest contribution. HOMO−2, π(2-GeNp skeleton) orbital was not involved in the transition (GeNp = GermaNaphthalene).

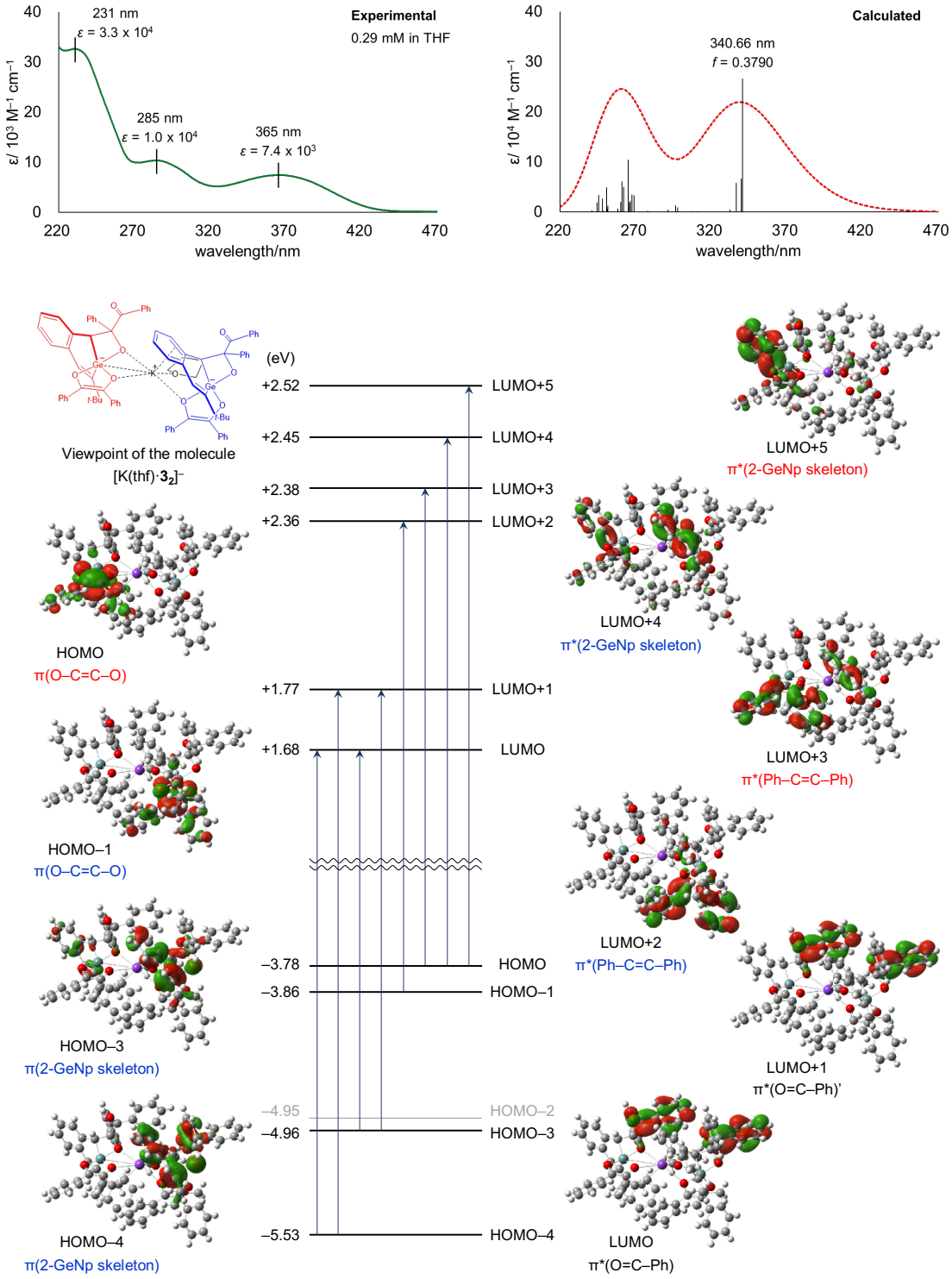
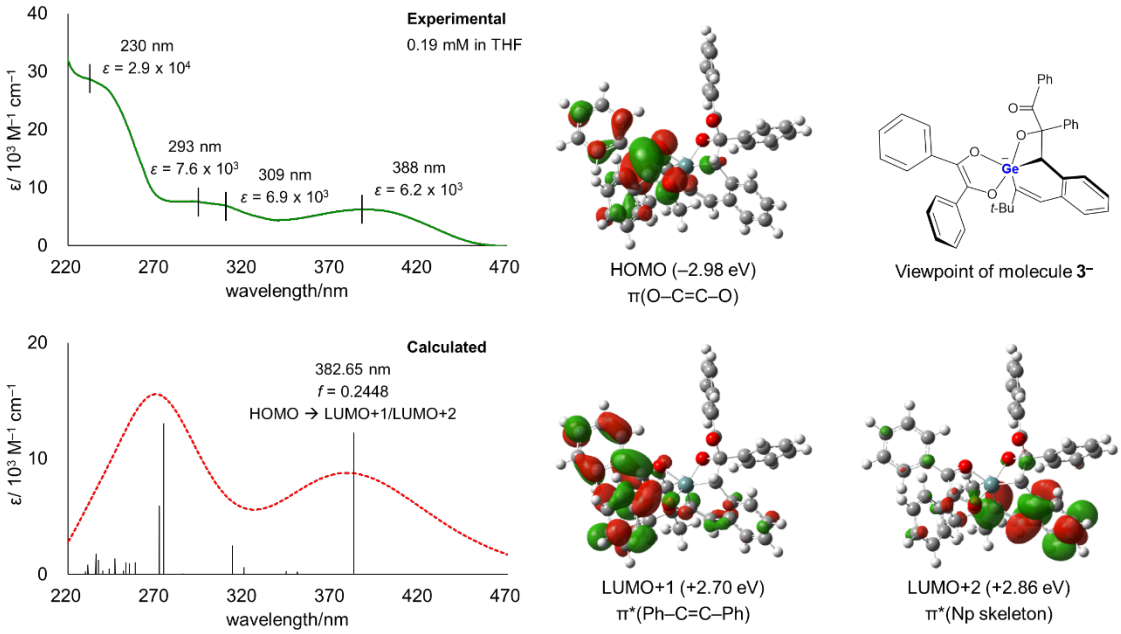


Figure S25. Observed UV-vis absorption spectrum of K^+(crypt-222)·**7**$^-$ in THF at 298 K, along with simulated spectrum of free anion **7**$^-$ and responsible frontier orbitals (isovalues = 0.03) calculated at the CAM-B3LYP/6-311G(2df,2p)//B3LYP/6-31G(d,p) level of theory.



5. Atomic Coordinates (xyz) for the Calculated Structures

3-*tert*-Butyl-2-germanaphthalenide **5**$^-$

Electronic Energy = −2579.459887 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	−2.268455	−3.432559	0.000000	C	1.473762	−1.361068	0.000000	H	−0.193616	2.759542	2.167135
C	−2.239288	−2.050332	0.000000	H	1.088148	−4.002491	0.000000	C	0.224314	3.202943	−1.256270
C	−1.032043	−1.308260	0.000000	H	−1.045980	−5.229269	0.000000	H	0.030656	4.285170	−1.279070
C	0.224314	−2.020247	0.000000	C	−0.090227	1.038999	0.000000	H	1.306576	3.044301	−1.279424
C	0.148612	−3.451438	0.000000	H	2.330735	−2.041199	0.000000	H	−0.193616	2.759542	−2.167135
C	−1.044568	−4.140047	0.000000	Ge	1.799327	0.486756	0.000000	C	−1.908467	2.894554	0.000000
H	−2.146005	0.484590	0.000000	C	−0.403490	2.551175	0.000000	H	−2.416426	2.495551	−0.884639
H	−3.216095	−3.966611	0.000000	C	0.224314	3.202943	1.256270	H	−2.416426	2.495551	0.884639
H	−3.175367	−1.491827	0.000000	H	1.306576	3.044301	1.279424	H	−2.046443	3.983424	0.000000
C	−1.112421	0.126344	0.000000	H	0.030656	4.285170	1.279070				

3-*tert*-Butyl-2-germanaphthalene **7**

Electronic Energy = −2580.017822 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	3.702349	1.653626	0.000000	C	1.143497	−1.751509	0.000000	H	−4.557374	0.094003	0.000000
C	2.338947	1.838212	0.000000	H	3.784490	−1.748797	0.000000	H	−3.443443	−0.952699	−0.885433
C	1.423390	0.748616	0.000000	H	5.303510	0.188397	0.000000	C	−2.716088	1.680829	−1.265154
C	1.959270	−0.592474	0.000000	C	−1.078798	0.245555	0.000000	H	−3.734711	2.084360	−1.287900
C	3.379723	−0.740182	0.000000	H	1.641144	−2.715721	0.000000	H	−2.021728	2.525384	−1.301734
C	4.227952	0.341050	0.000000	H	−1.618684	−2.737360	0.000000	H	−2.563124	1.084476	−2.170402
H	−0.168738	2.142814	0.000000	Ge	−0.657616	−1.566526	0.000000	C	−2.716088	1.680829	1.265154
H	4.370849	2.509086	0.000000	C	−2.501563	0.819478	0.000000	H	−2.021728	2.525384	1.301734
H	1.930504	2.845807	0.000000	C	−3.542126	−0.315410	0.000000	H	−3.734711	2.084360	1.287900
C	0.026873	1.069307	0.000000	H	−3.443443	−0.952699	0.885433	H	−2.563124	1.084476	2.170402

Naphthalene

Electronic Energy = −385.905364 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	2.433240	-0.708341	0.000000	H	-1.242200	-2.489442	0.000000	H	3.377441	1.245042	0.000000
C	1.244744	-1.402398	0.000000	H	3.377441	-1.245042	0.000000	C	-2.433240	0.708341	0.000000
C	0.000000	-0.716837	0.000000	H	1.242200	-2.489442	0.000000	C	-2.433240	-0.708341	0.000000
C	0.000000	0.716837	0.000000	C	-1.244744	-1.402398	0.000000	H	-1.242200	2.489442	0.000000
C	1.244744	1.402398	0.000000	C	-1.244744	1.402398	0.000000	H	-3.377441	1.245042	0.000000
C	2.433240	0.708341	0.000000	H	1.242200	2.489442	0.000000	H	-3.377441	-1.245042	0.000000

2-Naphthyl anion

Electronic Energy = −385.237244 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	−2.431323	−0.770404	0.000000	H	1.334458	−2.417824	0.000000	C	2.358653	0.837411	0.000000
C	−1.220992	−1.441891	0.000000	H	−3.326272	−1.410907	0.000000	C	2.439581	−0.577985	0.000000
C	0.000000	−0.716883	0.000000	H	−1.173631	−2.535577	0.000000	H	1.063378	2.547354	0.000000
C	−0.090417	0.720056	0.000000	C	1.280284	−1.328704	0.000000	H	3.272864	1.429937	0.000000
C	−1.382071	1.326254	0.000000	C	1.126561	1.458890	0.000000	H	3.412197	−1.067007	0.000000
C	−2.617735	0.664200	0.000000	H	−1.358232	2.428359	0.000000				

2-*tert*-Butylgermabenzenide **1**$^-$

Electronic Energy = −2425.802934 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	−1.511712	2.055551	0.000000	H	−3.603823	1.670038	0.000000	H	3.330907	−1.461183	0.000000
C	−0.177847	1.623572	0.000000	C	1.830397	0.123742	0.000000	H	1.840047	−1.883820	0.878188
C	0.294111	0.307890	0.000000	C	2.449813	0.772111	1.262033	C	2.449813	0.772111	−1.262033
C	−2.528178	−0.194554	0.000000	H	3.542556	0.646254	1.285333	H	2.032137	0.311336	−2.163802
C	−2.616365	1.191033	0.000000	H	2.235133	1.844396	1.311256	H	2.235133	1.844396	−1.311256
H	−1.694758	3.130575	0.000000	H	2.032137	0.311336	2.163802	H	3.542556	0.646254	−1.285333
H	0.558337	2.438246	0.000000	C	2.235618	−1.363068	0.000000	Ge	−0.904981	−1.206819	0.000000
H	−3.484913	−0.726132	0.000000	H	1.840047	−1.883820	−0.878188				

3-*tert*-Butyl-2-naphthyl anion

Electronic Energy = −542.513894 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	1.091003	0.151636	0.000177	H	-0.959978	2.858952	0.000175	H	2.518447	-2.189069	-0.886002
C	0.141811	-0.855487	0.000295	C	-3.983805	0.153707	-0.000217	C	3.230891	0.469574	-1.253053
C	-1.248401	-0.550212	0.000205	C	-3.600744	-1.209675	-0.000074	H	2.907560	1.514939	-1.279687
C	-1.631250	0.833211	0.000091	H	-3.310894	2.191839	-0.000274	H	4.328920	0.410981	-1.235475
C	-0.598216	1.819309	0.000228	H	-5.040418	0.417916	-0.000382	H	2.877281	-0.023863	-2.167673
C	0.769859	1.566606	0.000232	H	-4.361404	-1.988203	-0.000134	C	3.231434	0.469526	1.252685
H	-1.958355	-2.591833	0.000219	C	2.606607	-0.183384	-0.000089	H	4.329476	0.411117	1.234488
H	0.412740	-1.912331	0.000424	C	2.926378	-1.687827	-0.000158	H	2.907927	1.514813	1.279644
C	-2.260078	-1.544274	0.000127	H	4.012750	-1.847991	-0.000463	H	2.878449	-0.024147	2.167398
C	-3.019070	1.141604	-0.000157	H	2.518991	-2.189000	0.885984				

3-*tert*-Butylisoquinoline

Electronic Energy = −559.211532 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-3.620201	-1.160219	0.000000	C	-0.546537	1.732665	0.000000	H	2.534521	-2.182878	-0.888298
C	-2.300598	-1.554711	0.000000	H	-3.235633	2.232560	0.000000	C	3.194956	0.481344	-1.260383
C	-1.262458	-0.585417	0.000000	H	-5.013646	0.502989	0.000000	H	2.954114	1.546302	-1.292052
C	-1.615698	0.795574	0.000000	C	1.074754	0.082048	0.000000	H	4.284791	0.367990	-1.259675
C	-2.981404	1.175717	0.000000	H	-0.780847	2.798627	0.000000	H	2.806529	0.015915	-2.173000
C	-3.966939	0.214309	0.000000	N	0.725491	1.408511	0.000000	C	3.194956	0.481344	1.260383
H	0.403638	-1.959387	0.000000	C	2.586428	-0.175593	0.000000	H	4.284791	0.367990	1.259675
H	-4.408174	-1.907871	0.000000	C	2.926693	-1.675393	0.000000	H	2.954114	1.546302	1.292052
H	-2.038838	-2.609383	0.000000	H	4.013407	-1.807296	0.000000	H	2.806529	0.015915	2.173000
C	0.118967	-0.913339	0.000000	H	2.534521	-2.182878	0.888298				

3-*tert*-Butylisoquinolinium

Electronic Energy = −559.604921 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-3.623089	1.180643	0.000000	C	-0.621905	-1.738382	0.000000	H	2.531234	2.197447	0.890010
C	-2.300588	1.570443	0.000000	H	-3.291846	-2.220014	0.000000	C	3.209938	-0.455207	1.269293
C	-1.275931	0.594084	0.000000	H	-5.039056	-0.463230	0.000000	H	3.061755	-1.540639	1.310065
C	-1.650979	-0.793391	0.000000	C	1.086330	-0.034021	0.000000	H	4.289544	-0.283829	1.279076
C	-3.023480	-1.168225	0.000000	H	-0.807350	-2.806866	0.000000	H	2.789019	-0.021279	2.180772
C	-3.989048	-0.191483	0.000000	N	0.655909	-1.348006	0.000000	C	3.209938	-0.455207	-1.269293
H	0.388624	1.972186	0.000000	C	2.598071	0.190319	0.000000	H	4.289544	-0.283829	-1.279076
H	-4.403939	1.934443	0.000000	C	2.922190	1.695075	0.000000	H	3.061755	-1.540639	-1.310065
H	-2.034082	2.622342	0.000000	H	4.006717	1.828075	0.000000	H	2.789019	-0.021279	-2.180772
C	0.104497	0.927865	0.000000	H	2.531234	2.197447	-0.890010	H	1.370185	-2.068893	0.000000

9-Germaanthlacenide **2**$^-$

Electronic Energy = −2575.848264 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	3.704772	-1.339512	0.000013	C	-1.260974	-1.051863	-0.000036	H	2.312106	-2.956822	-0.000146
C	2.439214	-1.874338	-0.000054	C	-2.439208	-1.874345	-0.000029	H	2.903759	1.963546	0.000174
C	1.260983	-1.051856	-0.000013	H	-2.312097	-2.956829	-0.000123	H	4.889609	0.488318	0.000257
C	1.442918	0.381829	0.000021	C	-3.704765	-1.339520	0.000052	H	-4.572159	-1.998657	0.000077
C	2.770740	0.880919	0.000127	C	-3.886582	0.066395	0.000116	H	-4.889616	0.488303	0.000238
C	3.886579	0.066399	0.000138	C	-2.770747	0.880922	0.000100	H	-2.903792	1.963548	0.000084
C	-0.000003	-1.680329	-0.000054	H	0.000018	-2.770905	-0.000092	Ge	-0.000001	1.659341	-0.000081
C	-1.442919	0.381838	-0.000019	H	4.572169	-1.998645	-0.000051				

3-*tert*-Butyl-2-(2,4,6-trimethylphenyl)-2-germanaphthalene **4'**

Electronic Energy = −2929.056567 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	4.935666	-2.359453	-0.000106	C	-3.900378	-0.761753	-1.199019	Ge	0.113108	-0.289107	0.000050
C	3.570364	-2.528395	-0.000062	C	-3.900464	-0.761755	1.198852	H	0.953304	-2.708686	0.000016
C	2.668614	-1.423538	-0.000032	C	-4.616383	-0.823195	-0.000091	C	0.445758	2.693261	0.000143
C	3.231274	-0.097489	-0.000044	H	-4.436412	-0.837553	-2.142400	C	-0.450751	2.830863	1.251996
C	4.646384	0.031913	-0.000088	H	-4.436556	-0.837533	2.142197	H	-1.268171	2.103391	1.224130
C	5.487274	-1.059278	-0.000119	C	-1.777973	-0.631430	2.542820	H	0.126379	2.673552	2.169002
H	5.590561	-3.226480	-0.000129	H	-1.059412	0.190530	2.628557	H	-0.901814	3.828672	1.300682
H	3.146893	-3.529546	-0.000052	H	-2.472622	-0.562574	3.384330	C	1.469868	3.843494	0.000219
C	1.270486	-1.669809	0.000001	H	-1.203472	-1.558470	2.654621	H	2.111394	3.818478	-0.886633
C	2.463954	1.117408	-0.000004	C	-6.121616	-0.939456	-0.000218	H	0.943718	4.803481	0.000279
H	5.066258	1.035135	-0.000096	H	-6.482796	-1.467374	0.887263	H	2.111390	3.818362	0.887071
H	6.564279	-0.921770	-0.000153	H	-6.593014	0.051330	-0.003549	C	-0.450793	2.831070	-1.251656
C	1.101579	1.306250	0.000034	H	-6.482207	-1.472936	-0.884632	H	0.126295	2.673865	-2.168708
H	3.085469	2.011291	0.000003	C	-1.777812	-0.631452	-2.542842	H	-1.268242	2.103631	-1.223859
C	-1.808913	-0.509017	-0.000006	H	-2.472397	-0.562661	-3.384410	H	-0.901816	3.828905	-1.300186
C	-2.510033	-0.615422	-1.219248	H	-1.059275	0.190531	-2.628558				
C	-2.510089	-0.615427	1.219167	H	-1.203265	-1.558475	-2.654557				

Benzil adduct **7**$^-$

Electronic Energy = −3959.521709 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	3.211400	−4.541704	1.240241	C	−2.673976	−0.675333	0.552664	H	1.047562	−0.392122	2.133232
C	2.605427	−4.106718	0.065260	C	−2.640823	0.491900	−0.171328	C	2.116700	0.580236	0.456626
C	1.954545	−2.862424	−0.033283	O	−1.495342	−1.321979	0.666970	C	2.363700	1.671087	1.534995
C	1.947856	−2.015689	1.110052	O	−1.395632	0.867996	−0.602257	C	2.163834	3.138419	1.248831
C	2.558475	−2.476719	2.284293	Ge	−0.068392	−0.393159	−0.232105	C	1.231726	3.658830	0.333682
C	3.180887	−3.721251	2.366687	C	−3.789848	−1.319815	1.268837	C	2.946538	4.029012	2.005444
H	1.595007	−3.293608	−2.094642	C	−3.760916	−2.719560	1.427532	C	1.107249	5.041437	0.181240
H	3.698978	−5.512821	1.273985	C	−4.838404	−0.610739	1.885185	H	0.620161	2.967223	−0.229930
H	2.617449	−4.751676	−0.810810	C	−4.764735	−3.384152	2.127850	C	2.829051	5.404593	1.835242
C	1.298277	−2.574723	−1.329497	H	−2.928179	−3.263915	0.996533	H	3.643765	3.613308	2.725152
C	1.341430	−0.641208	1.113344	C	−5.840709	−1.278213	2.585082	C	1.904994	5.915736	0.919208
H	2.553037	−1.819217	3.149938	H	−4.856796	0.471474	1.823653	H	0.377694	5.434322	−0.521981
H	3.643890	−4.039983	3.297204	C	−5.816270	−2.670332	2.707111	H	3.452349	6.079161	2.416875
C	0.403206	−1.623148	−1.661482	H	−4.722132	−4.466234	2.227725	H	1.805774	6.990488	0.786816
C	−0.217380	−1.501375	−3.052862	H	−6.636946	−0.704804	3.053866	C	3.491468	0.237760	−0.149339
C	−1.736674	−1.778589	−2.949452	H	−6.597014	−3.188262	3.258221	C	3.639652	0.294188	−1.538924
H	−2.235464	−1.056174	−2.299199	C	−3.712754	1.407026	−0.579816	C	4.603560	−0.099707	0.635139
H	−2.203898	−1.717085	−3.940506	C	−5.031538	0.988374	−0.852296	C	4.868960	0.011531	−2.135668
H	−1.920060	−2.779115	−2.543884	C	−3.403890	2.766441	−0.797120	H	2.765339	0.555958	−2.121640
C	−0.002851	−0.057340	−3.571602	C	−6.002829	1.894113	−1.269595	C	5.831926	−0.382256	0.038038
H	−0.518592	0.083734	−4.530144	H	−5.288091	−0.059726	−0.747757	H	4.502226	−0.133739	1.714058
H	−0.386622	0.682455	−2.864112	C	−4.377803	3.668722	−1.217638	C	5.971624	−0.327304	−1.350424
H	1.062071	0.143045	−3.728790	H	−2.384842	3.094808	−0.628142	H	4.965234	0.058655	−3.218017
C	0.382591	−2.480959	−4.079429	C	−5.687465	3.243809	−1.451788	H	6.683154	−0.646353	0.661016
H	1.463873	−2.341981	−4.185742	H	−7.010292	1.538534	−1.473062	H	6.930504	−0.546272	−1.814123
H	0.199963	−3.525321	−3.803139	H	−4.110425	4.712426	−1.366382	O	2.790541	1.340869	2.637152
H	−0.074810	−2.315029	−5.061617	H	−6.446092	3.947746	−1.783860	O	1.218368	1.012795	−0.540572

Five-membered ring intermediate **8**$^-$

Electronic Energy = −3269.512384 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	−6.403372	−0.575074	1.118363	H	−1.831390	3.210250	−1.753792	C	4.960778	2.289670	0.292104
C	−5.590357	−0.132111	0.092629	C	−0.330581	0.314915	−2.960848	H	4.098967	0.596423	−0.706090
C	−4.176545	−0.119460	0.174274	H	0.039600	0.712513	−3.914629	C	4.774888	3.315286	1.223603
C	−3.539208	−0.593806	1.389805	H	0.503298	0.319510	−2.253701	H	3.384977	4.210325	2.609087
C	−4.421698	−1.041576	2.431711	H	−0.628901	−0.728071	−3.107787	H	5.895510	2.218309	−0.259103
C	−5.791241	−1.036184	2.306999	C	−2.543732	1.290627	−3.587129	H	5.564867	4.037519	1.412573
H	−4.118915	0.710908	−1.769031	H	−2.959710	0.317172	−3.869683	C	2.664243	−1.767524	−0.100205
H	−7.485187	−0.568031	1.015326	H	−3.376778	1.948411	−3.318394	C	3.860112	−1.748579	0.644239
H	−6.042382	0.229612	−0.830840	H	−2.059883	1.721765	−4.471628	C	2.470338	−2.834813	−1.000736
C	−3.455579	0.382412	−0.966920	C	1.598180	0.513948	0.488985	C	4.839221	−2.720268	0.453861
C	−2.147534	−0.637483	1.586951	C	1.572958	−0.796983	0.078637	H	4.013298	−0.972992	1.385816
H	−3.965415	−1.399758	3.352716	O	0.375024	1.091107	0.681899	C	3.451366	−3.805404	−1.187476
H	−6.407881	−1.389769	3.132158	O	0.336931	−1.309380	−0.174942	H	1.529472	−2.884294	−1.536553
C	−2.106725	0.513966	−1.180724	Ge	−1.022527	−0.085830	0.252777	C	4.647344	−3.753204	−0.468111
H	−1.787804	−1.020309	2.538223	C	2.722895	1.428304	0.733988	H	5.751524	−2.680598	1.044421
C	−1.519350	1.157698	−2.442490	C	2.538167	2.487531	1.646472	H	3.277834	−4.612152	−1.895843
C	−1.002318	2.572917	−2.081074	C	3.948583	1.366802	0.041705	H	5.411263	−4.513130	−0.610834
H	−0.276500	2.524135	−1.264516	C	3.552473	3.409317	1.892778				
H	−0.523759	3.051998	−2.946479	H	1.579282	2.567460	2.145730				

Four-membered ring imaginary intermediate **10**$^-$

Electronic Energy = −3269.463954 Hartree, ΔE(**10**$^-$−**8**$^-$) = +0.048430 Hartree = +30.4 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	−3.347786	3.558402	−0.712857	H	−4.287251	−2.852502	−0.996809	C	0.336357	2.030287	3.594711
C	−3.476554	2.290610	−0.148504	C	−1.612116	−3.342166	1.171936	H	0.585899	3.921200	2.585990
C	−2.530829	1.272206	−0.363261	H	−1.957099	−4.316170	1.545054	H	0.122530	0.003254	4.299024
C	−1.385703	1.560830	−1.153537	H	−0.826038	−3.519053	0.431068	H	0.231458	2.474917	4.581719
C	−1.283208	2.840976	−1.719719	H	−1.160068	−2.798574	2.007631	O	2.285743	1.746338	−1.427914
C	−2.242375	3.834061	−1.515918	C	−3.834472	−2.326264	1.684951	C	3.441750	−0.077002	−0.488617
H	−3.666157	−0.006365	0.912888	H	−3.436502	−1.699804	2.490593	C	4.640178	0.657966	−0.521775
H	−4.105445	4.317116	−0.530057	H	−4.744935	−1.848914	1.306414	C	3.495077	−1.447562	−0.183538
H	−4.345973	2.063219	0.465872	H	−4.125410	−3.290748	2.119713	C	5.859211	0.051314	−0.236341
C	−2.824220	−0.053537	0.215763	C	0.777146	0.206979	−0.337357	H	4.584326	1.710824	−0.777098
C	−0.314840	0.556431	−1.429016	O	0.710029	−1.197843	−0.229532	C	4.722965	−2.053668	0.090775
H	−0.402566	3.060516	−2.318995	C	2.178307	0.685514	−0.820328	H	2.564015	−1.999901	−0.182290
H	−2.120092	4.813770	−1.972585	C	0.598716	0.881689	1.038809	C	5.904061	−1.311751	0.071477
C	−2.255341	−1.243925	−0.058239	C	0.671151	2.272224	1.208213	H	6.775085	0.637156	−0.254768
Ge	−0.783585	−1.431617	−1.454299	C	0.407066	0.076924	2.166366	H	4.753355	−3.116250	0.318730
C	−2.790634	−2.539958	0.569412	C	0.535276	2.840555	2.474547	H	6.855496	−1.790662	0.291363
C	−3.448477	−3.392915	−0.543873	H	0.837124	2.905096	0.343658	H	0.204026	0.870901	−2.335890
H	−2.732507	−3.622573	−1.338510	C	0.274652	0.645213	3.433967				
H	−3.828610	−4.339090	−0.135177	H	0.361745	−0.994157	2.011332				

K-bridged tetramer $[K_2(benzene)_2\cdot \mathbf{5}_4]^{2-}$

Electronic Energy = −11989.7562422 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	0.941777	1.885570	1.030705	H	2.854188	−4.248855	3.434180	H	3.154452	−2.396613	−4.353272
H	0.915294	1.054781	1.449581	H	2.411949	−3.772938	4.860861	H	2.776700	−1.950248	−2.898726
Ge	−0.370099	2.184584	−0.278926	H	3.919181	−3.687304	4.438071	C	0.857329	−3.421053	−5.188185
C	0.114079	4.082334	−0.597707	C	1.306679	−2.054424	3.161616	H	−0.059578	−3.357874	−5.462456
C	1.104549	4.704312	0.094674	H	1.143163	−1.162274	2.844940	H	1.429158	−3.195815	−5.926046
H	1.204230	5.613640	−0.073553	H	0.739160	−2.235274	3.914060	H	1.045164	−4.318024	−4.900850
C	3.069195	4.962544	1.542290	H	1.116985	−2.681585	2.459557	C	−4.967052	1.215470	−2.774329
H	3.080874	5.862517	1.306139	C	3.036337	−1.210826	4.749103	H	−5.595472	1.857487	−2.534891
C	4.075298	4.477497	2.354279	H	3.953263	−1.273959	5.023287	C	−5.251884	−0.129771	−2.599221
H	4.753266	5.039724	2.652192	H	2.464527	−1.436018	5.486877	H	−6.073003	−0.388827	−2.248109
C	4.056774	3.131323	2.719627	H	2.848503	−0.313855	4.461768	C	−4.309640	−1.091293	−2.950329
H	4.738085	2.788556	3.250419	C	4.606890	2.723454	−1.259515	H	−4.493579	−1.995621	−2.833821
C	3.034674	2.308229	2.298449	H	4.750827	3.302306	−0.545912	C	−3.083247	−0.681055	−3.479577
H	3.038005	1.417785	2.568424	C	3.413726	2.764549	−1.962728	H	−2.446648	−1.318679	−3.710419
C	1.976242	2.769194	1.467179	H	2.749479	3.367310	−1.718823	C	−2.802248	0.657894	−3.663135
C	2.016860	4.141250	1.052729	C	3.213142	1.906854	−3.028243	H	−1.987725	0.924084	−4.024750
C	−0.651087	4.826655	−1.728051	H	2.410344	1.936862	−3.496496	C	−3.756309	1.605137	−3.300388
C	−2.150883	4.825810	−1.429913	C	4.198796	0.997096	−3.410694	H	−3.573922	2.510087	−3.415059
H	−2.319003	5.338782	−0.636023	H	4.064225	0.429847	−4.134751	C	−4.989037	1.993028	1.319913
H	−2.450136	3.923707	−1.297895	C	5.391155	0.954234	−2.683785	C	−6.023520	1.109358	0.883526
H	−2.623512	5.215632	−2.168835	H	6.052996	0.343688	−2.917229	H	−4.962571	2.823772	0.901125
C	−0.197541	6.278695	−1.931070	C	5.592691	1.804819	−1.631200	C	−4.161356	−0.203781	2.948412
H	−0.685887	6.667304	−2.660829	H	6.393356	1.771485	−1.158015	C	−5.151881	−0.825768	2.255901
H	0.741427	6.295685	−2.129454	Ge	0.530667	−1.508140	−1.216572	H	−5.251514	−1.735212	2.424192
H	−0.364948	6.781442	−1.130557	K	−3.070801	0.071862	−0.352146	C	−7.116388	−1.084017	0.808305
C	−0.414123	4.060810	−3.043372	Ge	−3.677179	1.693968	2.629631	H	−7.128152	−1.983964	1.044567
H	−0.725552	3.157330	−2.948244	C	−0.952316	−2.118541	−0.244592	C	−8.122492	−0.598970	−0.003684
H	0.525057	4.054831	−3.244883	H	−1.021108	−1.809658	0.629988	H	−8.800477	−1.161243	−0.301510
H	−0.891567	4.490897	−3.755364	C	0.200904	−2.630012	−2.822122	C	−8.104034	0.747275	−0.369009
K	3.253522	0.194408	−0.160685	C	−0.859985	−3.506012	−2.883830	H	−8.785363	1.089997	−0.899713
C	4.846000	−2.513292	−0.194577	H	−0.894514	−4.043330	−3.642254	C	−7.081952	1.570323	0.052257
H	4.914793	−2.822174	−1.069157	C	−2.979787	−4.583190	−2.277843	H	−7.085264	2.460813	−0.217806
Ge	3.363018	−3.123693	0.777403	H	−2.921147	−5.066456	−3.070246	C	−6.064137	−0.262698	1.297976
C	3.692690	−2.001919	2.382997	C	−4.082034	−4.741449	−1.479136	C	−3.396191	−0.948102	4.078757
C	4.753736	−1.125892	2.444638	H	−4.773028	−5.304964	−1.744983	C	−1.896376	−0.947212	3.780531
H	4.788199	−0.588502	3.203085	C	−4.166177	−4.061251	−0.280168	H	−1.728190	−1.460255	2.986618
C	6.873471	−0.048643	1.838674	H	−4.915184	−4.170917	0.259828	H	−1.597148	−0.045279	3.648534
H	6.814813	0.434578	2.631164	C	−3.157393	−3.229645	0.121332	H	−1.423766	−1.337080	4.519540
C	7.975701	0.109571	1.040054	H	−3.230390	−2.797614	0.941214	C	−3.849736	−2.400143	4.281775
H	8.666779	0.673061	1.305791	C	−1.991123	−3.001770	−0.680045	H	−3.361373	−2.788706	5.011447
C	8.059844	−0.570628	−0.158914	C	−1.925369	−3.704926	−1.928254	H	−4.788639	−2.417204	4.480136
H	8.808868	−0.460916	−0.698997	C	1.114767	−2.444477	−4.023159	H	−3.682330	−2.902890	3.481262
C	7.051060	−1.402233	−0.560414	C	0.880831	−1.024247	−4.569758	C	−3.633155	−0.182258	5.394077

H	7.124056	−1.834264	−1.380296	H	1.039479	−0.383023	−3.873261	H	−3.321708	0.721268	5.298863
C	5.884808	−1.630062	0.240876	H	1.481645	−0.858994	−5.299986	H	−4.572389	−0.176287	5.595458
C	5.819053	−0.926906	1.489085	H	−0.025569	−0.944583	−4.877283	H	−3.155765	−0.612353	6.105939
C	2.778899	−2.187401	3.584077	C	2.587005	−2.577408	−3.600785				
C	3.012902	−3.607703	4.130653	H	2.750448	−3.469613	−3.284152				

K-bridged dimer $[K(thf)\cdot\mathbf{7}_2]^-$

Electronic Energy = −8751.320178 Hartree

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	2.885722	−0.830902	−0.794328	C	4.040963	2.969029	3.273618	C	−4.430853	−5.145515	3.213365
H	2.363169	−1.443090	−0.057421	C	4.916770	2.286881	4.125982	H	−4.704443	−5.781207	4.052526
Ge	3.549192	0.892474	−0.157149	H	5.109008	1.234445	3.939168	C	−4.656192	−5.561745	1.917517
C	3.773675	1.966622	−1.763174	C	5.554312	2.940455	5.160563	H	−5.112282	−6.531126	1.726871
C	3.120545	1.489440	−2.836154	H	6.233397	2.382839	5.803145	C	−4.306808	−4.752881	0.852095
H	3.197691	2.039778	−3.775172	C	5.339447	4.272520	5.380288	H	−4.502660	−5.089668	−0.163232
C	1.402607	0.341136	−4.106148	H	5.846749	4.786430	6.194396	C	−2.675159	−3.403991	−1.224728
H	1.547490	1.130155	−4.841676	C	4.479135	4.970815	4.549296	O	−3.149940	−3.518700	−2.327861
C	0.427820	−0.610929	−4.320790	H	4.313029	6.034628	4.705992	C	−1.332070	−3.999858	−0.938858
H	−0.185402	−0.563201	−5.218134	C	1.001267	3.088261	2.218209	C	−0.734523	−4.734672	−1.952748
C	0.213518	−1.583889	−3.386212	C	0.808961	3.277527	3.588288	H	−1.270734	−4.843533	−2.890314
H	−0.575030	−2.319283	−3.518557	H	1.510151	2.838784	4.290692	C	0.511113	−5.308845	−1.777314
C	1.029593	−1.641088	−2.259959	C	−0.241620	4.035747	4.053403	H	0.964123	−5.876609	−2.586700
H	0.900963	−2.445620	−1.543635	H	−0.367288	4.188501	5.123253	C	1.166375	−5.159344	−0.577113
C	2.031896	−0.701692	−2.036109	C	−1.165274	4.570361	3.157774	H	2.153067	−5.592718	−0.432998
C	2.199490	0.340370	−2.967834	H	−2.002242	5.158296	3.529413	C	0.593917	−4.434643	0.427470
C	4.551313	3.278008	−1.775727	C	−1.012451	4.355757	1.810595	H	1.131812	−4.294950	1.359593
C	5.938673	3.043760	−1.180116	H	−1.728597	4.758134	1.101325	C	−0.652573	−3.858964	0.270560
H	6.501558	3.986822	−1.141366	C	0.058777	3.613760	1.343051	H	−1.086234	−3.268650	1.066256
H	6.516393	2.334915	−1.784835	H	0.184055	3.460377	0.276595	O	−2.659277	0.893957	−0.884712
H	5.885862	2.643479	−0.162484	C	3.838972	4.328085	3.509539	C	−3.167678	2.019319	−1.537551
C	3.811133	4.309913	−0.928795	H	3.182336	4.888193	2.850696	C	−4.506004	2.010130	−1.752450
H	4.355030	5.264660	−0.929118	K	−0.317639	0.032998	0.127799	O	−5.184457	0.930153	−1.249927
H	3.713879	3.986213	0.111644	C	−4.703119	−1.928470	−0.707957	C	−2.158003	3.026094	−1.846799
H	2.801636	4.493051	−1.313762	H	−4.749726	−2.085577	−1.784119	C	−0.915371	2.648682	−2.368639
H	4.732786	3.823539	−3.182741	Ge	−4.002527	−0.174246	−0.209849	H	−0.730185	1.601874	−2.591664
H	5.351553	4.729844	−3.156682	C	−4.685344	0.146164	1.583082	C	0.064986	3.587049	−2.618324
H	3.781082	4.100447	−3.652374	C	−5.716243	−0.644850	1.925305	H	1.022595	3.256583	−3.009056
H	5.233590	3.100931	−3.837796	H	−6.163378	−0.510064	2.911143	C	−0.158604	4.911865	−2.365912
C	4.353175	−1.352174	−0.916946	C	−7.699476	−2.013547	1.649168	H	0.618538	5.648243	−2.558518
O	5.120619	−0.279327	−0.327470	H	−8.008795	−1.596611	2.605937	C	−1.379233	5.310829	−1.847074
C	4.749246	−1.675284	−2.351546	C	−8.551953	−2.864004	0.976331	H	−1.562817	6.361187	−1.630533
C	5.502244	−0.815393	−3.103254	H	−9.518032	−3.113889	1.411115	C	−5.326563	3.038272	−2.419451
H	5.858177	0.092483	−2.628017	C	−8.190878	−3.358973	−0.244588	C	−4.861582	3.773575	−3.511716
C	5.800962	−1.088705	−4.422284	H	−8.859602	−4.013435	−0.800193	H	−3.871328	3.571333	−3.906659
H	6.405416	−0.386345	−4.993245	C	−6.935914	−3.051574	−0.762537	C	−5.637034	4.760358	−4.077301
C	5.331744	−2.242113	−5.016386	H	−6.627158	−3.466603	−1.719393	H	−5.255844	5.333577	−4.919568

H	5.560142	−2.461737	−6.057097	C	−6.053692	−2.211925	−0.088815	C	−6.926452	4.991115	−3.602694
C	4.561591	−3.110944	−4.271239	C	−6.461473	−1.647857	1.134960	H	−7.542899	5.761062	−4.062816
H	4.175964	−4.022902	−4.722990	C	−4.151163	1.255297	2.482567	C	−7.412304	4.245935	−2.557250
C	4.273410	−2.831735	−2.948195	C	−2.631706	1.130773	2.583338	H	−8.421317	4.412919	−2.185599
H	3.652501	−3.520365	−2.379244	H	−2.214075	1.889021	3.254166	H	−6.621705	3.270808	−1.973499
C	4.565419	−2.595743	−0.006424	H	−2.341136	0.145500	2.958352	H	−6.998365	2.668342	−1.152719
O	3.637517	−3.086879	0.587934	H	−2.174105	1.285671	1.604238	O	0.620544	−0.895333	2.463708
C	5.936853	−3.168062	0.173258	C	−4.502679	2.610080	1.873479	C	−0.144052	−1.493337	3.494904
C	6.052934	−4.302851	0.963047	H	−4.110210	3.424569	2.496109	H	−0.314995	−0.753791	4.296068
H	5.151460	−4.712423	1.408130	H	−4.081279	2.726792	0.870732	H	−1.113883	−1.763176	3.074334
C	7.284397	−4.888798	1.191575	H	−5.589286	2.732916	1.792146	C	0.664518	−2.641235	3.974011
H	7.354550	−5.776328	1.816601	C	−4.720837	1.176820	3.889527	H	0.584315	−2.779606	5.058259
C	8.412399	−4.346571	0.620785	H	−4.274748	1.957029	4.519334	H	0.349493	−3.582453	3.511110
H	9.384340	−4.803858	0.797815	H	−5.806469	1.329044	3.909243	C	2.096847	−2.261028	3.530982
C	8.314850	−3.227343	−0.153747	H	−4.508246	0.209686	4.361196	H	2.460415	−2.944233	2.758563
H	9.209560	−2.790533	−0.592687	C	−3.425658	−2.607578	−0.118816	H	2.814502	−2.307346	4.358806
C	7.091309	−2.632599	−0.396628	O	−2.588313	−1.476653	0.208776	C	1.954662	−0.905407	2.982514
H	7.029250	−1.720044	−0.974873	C	−3.729392	−3.512044	1.068207	H	2.643048	−0.661397	2.175951
O	4.287157	1.457840	1.435520	C	−3.521208	−3.104754	2.357493	H	2.041912	−0.120930	3.751138
C	3.413442	2.279730	2.151227	H	−3.109621	−2.115457	2.515615	C	−2.365491	4.380583	−1.590282
C	2.143910	2.327694	1.678599	C	−3.860107	−3.907762	3.427118	H	−3.313777	4.699854	−1.168375
O	1.905317	1.613121	0.533329	H	−3.684495	−3.554774	4.441693				

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