Synthesis and Characterizations of The Germathioacid chloride Coordinated by an *N*-Heterocyclic carbene ‡

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‡ Dedicated to Prof. Dr. Robert West in honors of his 90th birthday.

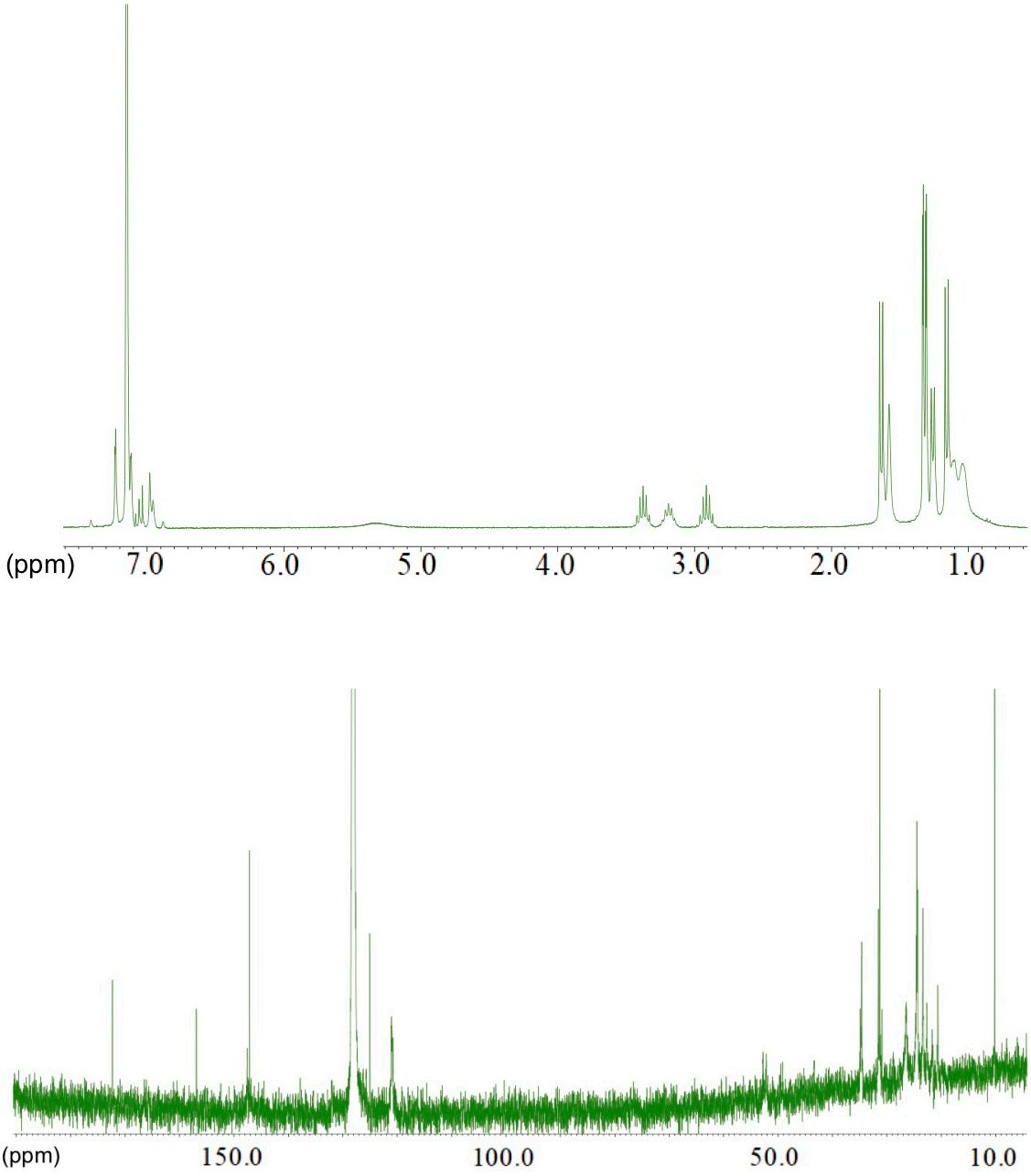

Figure S1. ^{1}H-NMR (top) and ^{13}C{^{1}H}-NMR (bottom) spectra of **2** in C_6D_6

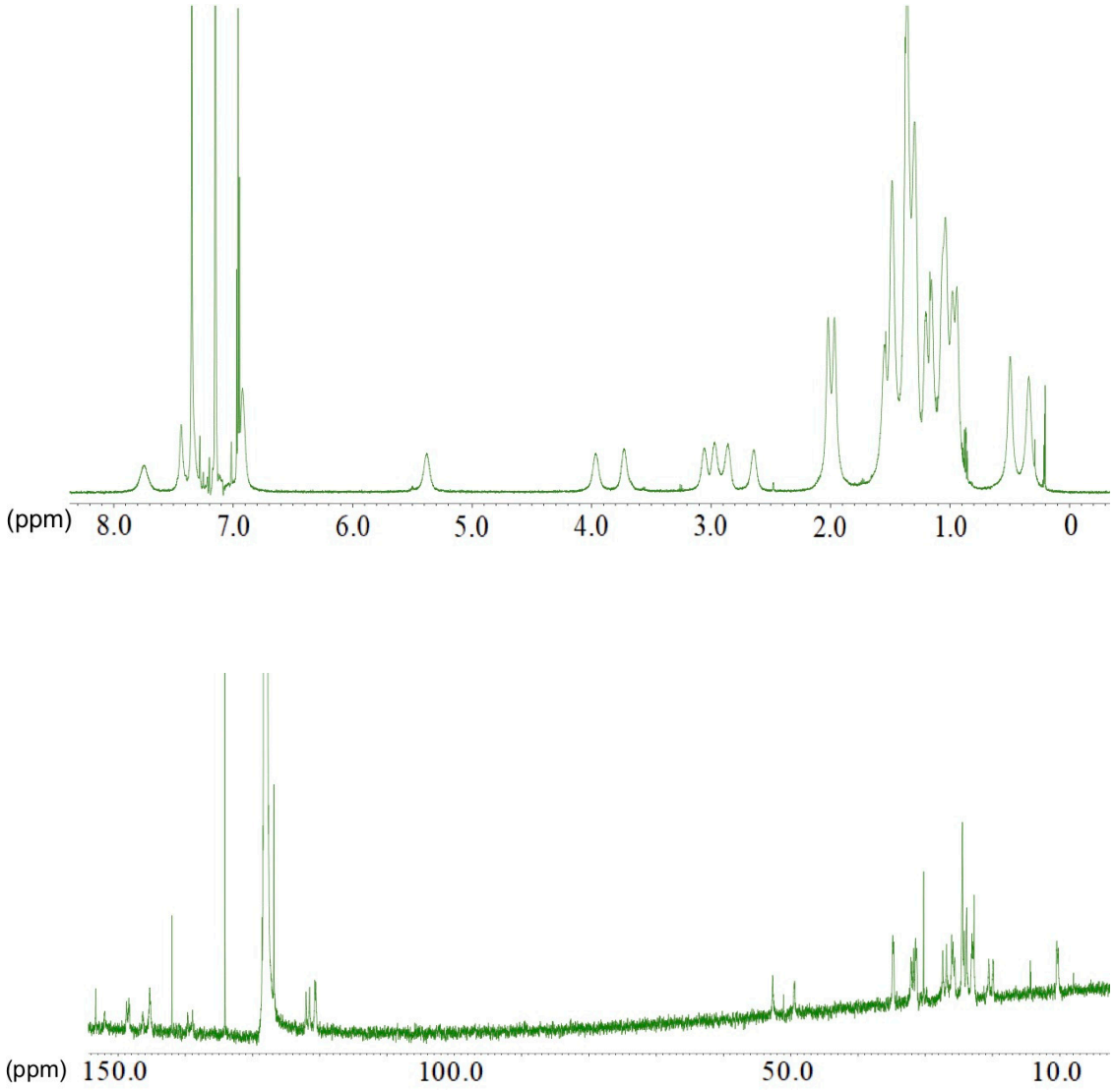

Figure S2. ^{1}H-NMR (top) and ^{13}C{^{1}H}-NMR (bottom) spectra of **3** in C_6D_6

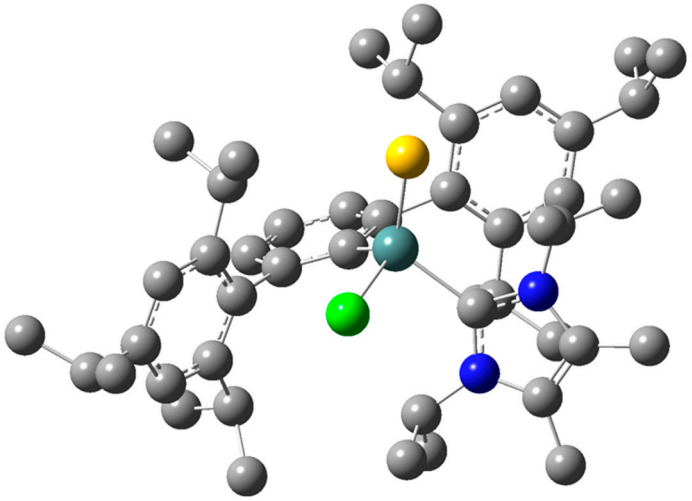

Figure S3. Optimized geometries of germathioacid chloride **3**. The geometries were given by ball and stick model (atom color: C: Silver, S: Dark yellow, N: Blue, Cl: Light green, Ge: Green). Hydrogen atoms were omitted for clarify. Selected bond lengths (Å), angles (deg), and Wiberg bond index (WBI): Ge–S = 2.107, Ge–Cl = 2.297, Ge–(NHC) = 2.078, Ge–C(Ar_{Tip}) = 1.984, S–Ge–Cl = 105.6, S–Ge–C(NHC) = 116.4, S–Ge–C(Ar_{Tip}) = 116.9, C(Ar_{Tip})–Ge–Cl = 113.1, C(Ar_{Tip}) –Ge–C(NHC) = 110.8, C(NHC)–Ge–Cl = 90.9. WBI_{Ge-S} = 1.367, $WBI_{Ge–Cl}$ = 0.664, $WBI_{Ge–C(NHC)}$ = 0.603, $WBI_{Ge–C(ArTip)}$ = 0.709. NPA charges of germathioacid chloride **3**: Ge = +1.240, S = –0.762, Cl = –0.456, C(NHC) = +0.114, C(Ar_{Tip}) = –0.442.

Cartesian Coordinates (in Å) and Energies

Germathioacid chloride

Energy (RB3LYP) = -4875.7021922 A.U.

Free Energy = -4874.731276 A.U.

Ge	-0.09577900	0.04161200	-1.00136500
S	0.52572100	-1.22663400	-2.56447000
Cl	-1.91167900	1.18689500	-1.81946100
C	-0.43805400	-0.80653800	0.75949200
C	-1.73410700	-1.12769900	1.25808900
C	-1.84087800	-1.93139700	2.40633600
H	-2.83166800	-2.21916700	2.73828200
C	-0.72747600	-2.37837400	3.10166400
H	-0.84080000	-2.98969600	3.99227900
C	0.53387300	-2.06209000	2.61797500
H	1.41658300	-2.43197800	3.12891900
C	0.70522300	-1.31354100	1.44194100
C	-3.07071800	-0.75580600	0.65421000
C	-3.55143700	-1.45009800	-0.48536900
C	-4.84630500	-1.19313500	-0.94349300
H	-5.20069600	-1.72879800	-1.81828200
C	-5.69885900	-0.28569400	-0.31424200
C	-5.22471600	0.35459600	0.82834000
H	-5.88763400	1.04295500	1.34541900
C	-3.93956900	0.13258700	1.33896100
C	-2.74555300	-2.54696900	-1.18042600
H	-1.69514000	-2.43616200	-0.90379500
C	-2.79846500	-2.46177400	-2.71401800
H	-3.80367500	-2.65037800	-3.10736800
H	-2.12758400	-3.20988800	-3.14642000
H	-2.45615400	-1.48232200	-3.05157500
C	-3.20271100	-3.93407600	-0.68425800
H	-3.10172700	-4.02610300	0.40216100
H	-2.60156300	-4.72371400	-1.14852600
H	-4.25316800	-4.11615400	-0.93871400
C	-7.10206100	-0.01145600	-0.83805800
H	-7.55946700	0.72331700	-0.16160200
C	-7.07320700	0.61212100	-2.24594100
H	-6.63731200	-0.07825000	-2.97581700
H	-6.47480000	1.52799700	-2.26000400
H	-8.08674300	0.85809400	-2.58232400
C	-7.98454400	-1.27336000	-0.81057900
H	-9.00455400	-1.04044000	-1.13609600
H	-8.03643000	-1.69868000	0.19657900
H	-7.59191000	-2.04726000	-1.47886500
C	-3.56976900	0.83573600	2.65032000
H	-2.48171600	0.78789600	2.76779700
C	-3.98292000	2.32021600	2.67330000
H	-3.66057100	2.84706200	1.77316000
H	-3.55262000	2.82207700	3.54736500
H	-5.06875900	2.43692800	2.74650900
C	-4.20542000	0.14083700	3.87441400
H	-5.29744700	0.13937100	3.78860000

H	-3.94169800	0.67086500	4.79705100
H	-3.87926300	-0.89516000	3.98074400
C	2.15474600	-1.20143900	1.00568100
C	2.73704400	-2.25622400	0.24906400
C	4.11966000	-2.25528500	0.03865400
H	4.55432600	-3.06904400	-0.53186400
C	4.96052400	-1.26836900	0.55800000
C	4.37252500	-0.24875100	1.30580500
H	5.01590400	0.51321500	1.73660300
C	2.99333700	-0.19927000	1.55184100
C	1.92036800	-3.44769200	-0.25526200
H	0.89831800	-3.09063000	-0.40017300
C	2.40227300	-3.99401400	-1.61047400
H	2.50836400	-3.19351800	-2.34381500
H	1.66733100	-4.70707600	-1.99731300
H	3.35444700	-4.53054000	-1.52167400
C	1.91535300	-4.59878600	0.77357200
H	2.93454100	-4.95892200	0.95652000
H	1.32764100	-5.44072900	0.39116200
H	1.48582700	-4.30141600	1.73203100
C	6.47437700	-1.33570600	0.39376300
H	6.87870200	-0.37803500	0.74913600
C	6.91991600	-1.51094800	-1.06824900
H	6.57358400	-2.46320600	-1.48323600
H	8.01299400	-1.50064900	-1.13902200
H	6.53134500	-0.71007300	-1.70392800
C	7.07263000	-2.44482900	1.28225900
H	6.70769400	-3.43101400	0.97538300
H	6.79949000	-2.30108000	2.33216000
H	8.16602100	-2.45395500	1.21102700
C	2.45266500	0.87917600	2.49092500
H	1.39785500	1.01829800	2.23220000
C	3.16560100	2.23517300	2.34557500
H	4.18299700	2.19941900	2.74860000
H	2.63122600	3.00422400	2.91373200
H	3.22868400	2.55849200	1.30414600
C	2.52520100	0.43681200	3.96799700
H	1.93604200	-0.46209100	4.15522000
H	2.14774500	1.22888400	4.62538100
H	3.56234300	0.22958600	4.25392700
C	0.96157800	1.81648000	-0.77424000
N	2.08017900	2.16054100	-1.45909200
C	2.41749400	3.48488100	-1.19541900
C	1.50179200	3.95580300	-0.29458200
N	0.60825200	2.91303900	-0.04780200
C	2.72011200	1.27785100	-2.48047700
H	2.38930200	0.27316600	-2.21637600
C	4.24832900	1.27085600	-2.42989100
H	4.71405600	2.14080000	-2.89678300
H	4.58551800	0.38849100	-2.98143200
H	4.60965000	1.17151300	-1.40273200
C	2.12470200	1.60442900	-3.85136500
H	1.03744400	1.50686200	-3.80612800
H	2.49023300	0.88251500	-4.58671300

H	2.39266600	2.61084700	-4.19296600
C	3.56852100	4.22170400	-1.80373900
H	3.48103300	5.28603200	-1.57959600
H	3.58694000	4.11899200	-2.89123800
H	4.53342600	3.88102900	-1.41743600
C	1.49960900	5.29278200	0.37806200
H	1.82698300	5.21978300	1.42030700
H	0.52276500	5.77732100	0.36567100
H	2.19733500	5.95821100	-0.13291000
C	-0.66628700	3.04480100	0.71847300
H	-1.11687600	2.05293200	0.68125400
C	-0.44181600	3.40009600	2.19147300
H	0.23095000	2.69169000	2.67731200
H	-1.40439100	3.35598000	2.70525100
H	-0.04703100	4.40861400	2.32749700
C	-1.61300800	4.02075800	0.00533700
H	-1.31601600	5.06323100	0.14237800
H	-2.61816800	3.91289800	0.41733500
H	-1.66724100	3.79259200	-1.05873300
