A Donor-Acceptor Stabilized Tetra(silanimine)

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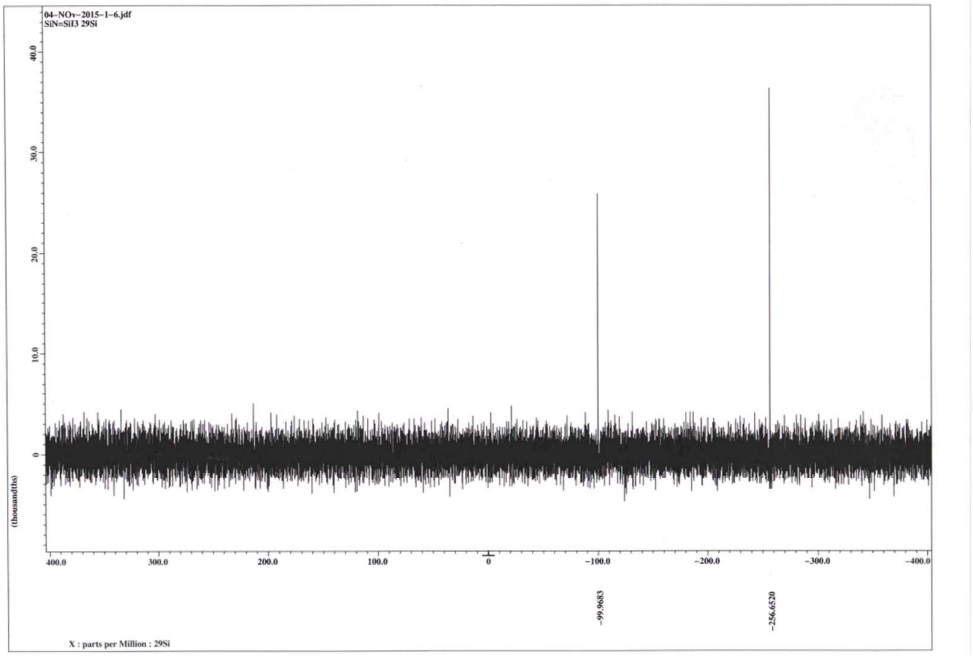
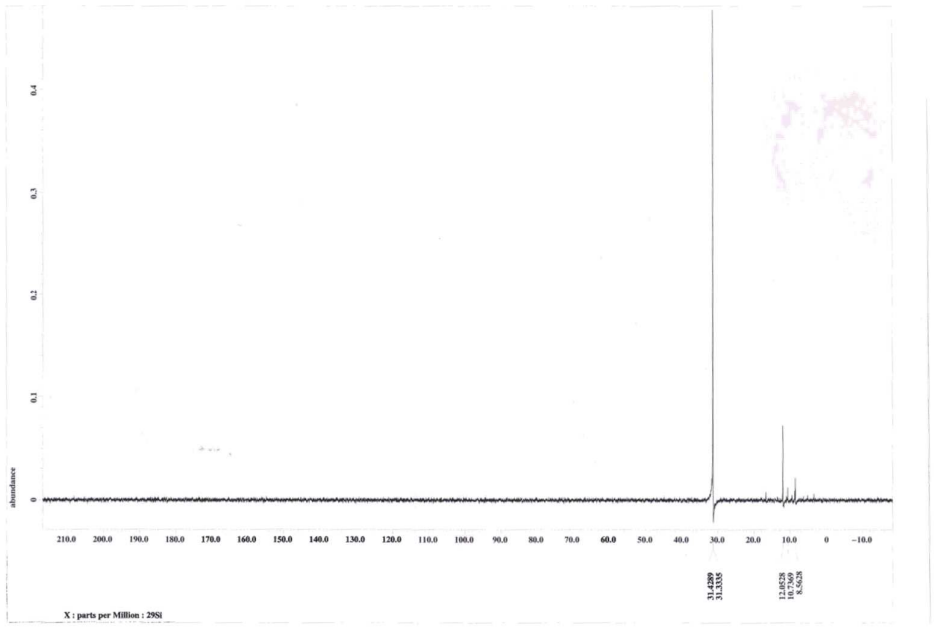
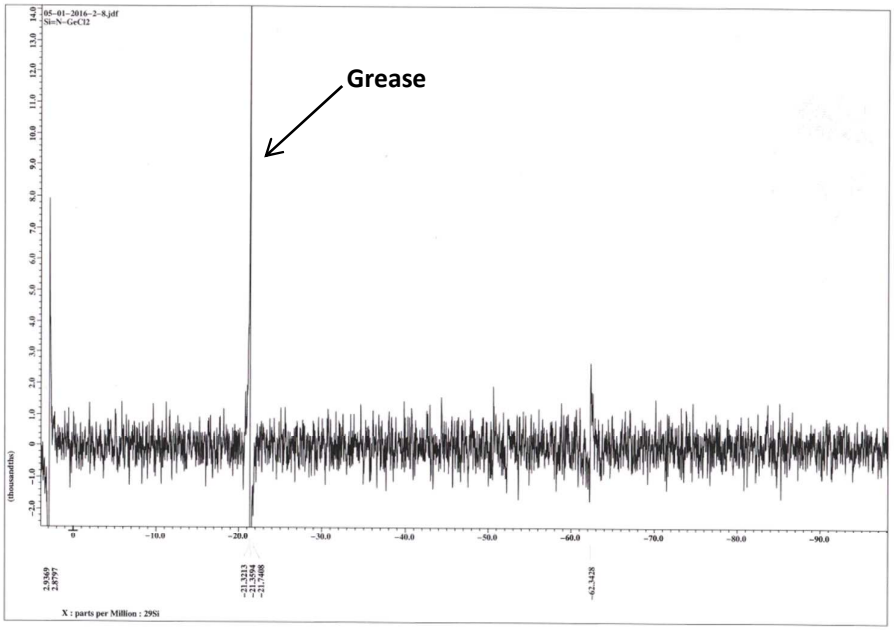
1. Selected NMR spectra of **2 - 3** and **5 – 7**



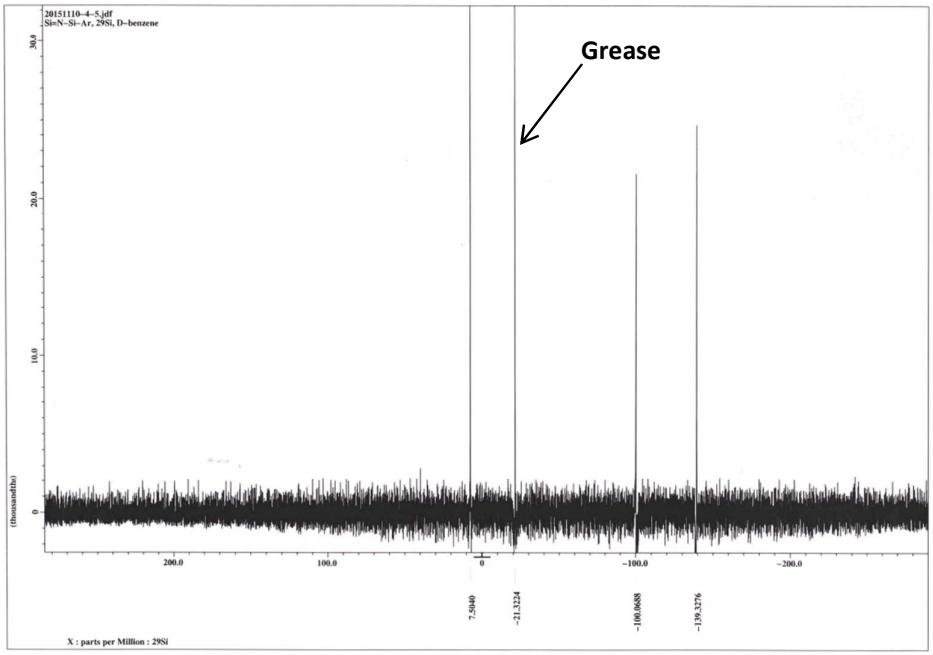
(a) ^{29}Si NMR spectrum of compound **2**



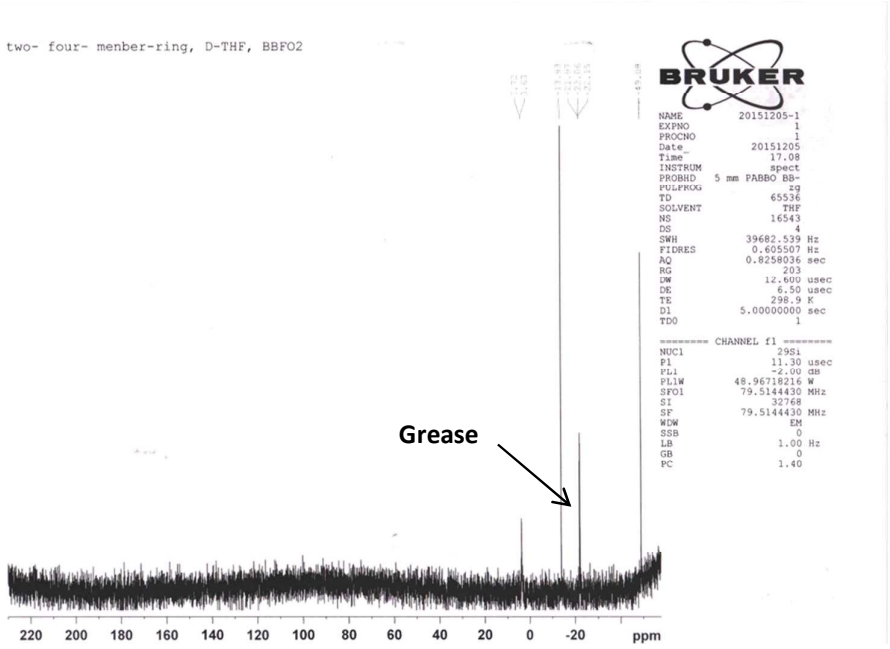
(b) ^{29}Si NMR spectrum of compound **3**



(c) ^{29}Si NMR spectrum of compound **5**



(d) ^{29}Si NMR spectrum of compound **6**



(e) ^{29}Si NMR spectrum of compound **7**

2. X-ray crystal structures of Si_2I_6

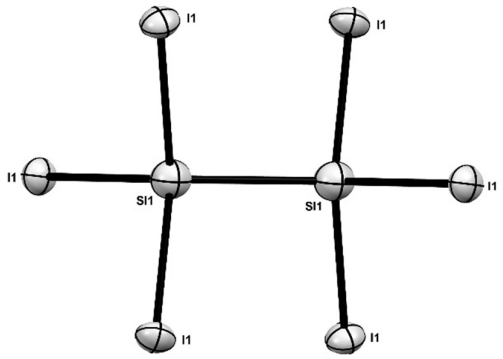
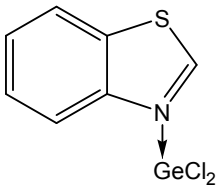


Figure S1. Molecular structure of Si_2I_6 (ellipsoids set at 50% probability). Selected bond lengths (Å) and angles (°): Si1-I1 2.430(9), Si1-Si1 2.328(5), I1-Si1-Si1 107.63(5), I1-Si1-I1 111.25(5).

3. Dichlorogermylene-benzothiazole adduct



Scheme S1. The dichlorogermylene-benzothiazole adduct

4. Table S1. Selected X-ray crystallography data of **2 - 3** and **5 – 7**

	2	**3**	**5**	**6**	**7**	
Formula	$C_{18.50}$ H_{27} I_4 N_3 Si_2	C_{21} H_{41} Cl_4 Ge N_3 Si_3	C_{18} H_{32} Cl_3 Ge N_3 Si_2	$C_{33.50}$ H_{53} I_3 N_4 Si_3	C_{74} H_{114} N_8 Si_6	Si_2I_6
M	855.21	634.23	525.58	976.77	1284.27	817.58
Color	colorless	colorless	colorless	colorless	red	colorless
Crystal System	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	trigonal
Space group	P 1 21/c 1	P 1 21/c 1	P 1 21/c 1	P -1	P 1 21/c 1	R -3
a/Å	22.2720(16	18.7105(7)	16.9206(8)	9.8334(3)	19.722(4)	7.1295(14)
b/Å	13.6343(9)	21.6514(7))	8.2680(4)	12.8781(4)	13.144(3)	7.1295(14)
c/Å	19.8421(15)	16.3484(6)	18.3628(9)	17.7755(5)	30.205(6)	22.100(5)
α/deg	90	90	90	107.4942(17)	90	90
β/deg	111.712(3)	108.8162(16)	106.236(3)	103.8934(18)	100.459(4)	90
γ/deg	90	90	90	97.4496(18)	90	120
$V/Å^3$	5597.8(7)	6268.9(4)	2466.5(2)	2033.96(11)	7700.(3)	972.8(4)
Z	8	8	4	2	4	3
d_{calcd}/g cm^{-3}	2.030	1.344	1.415	1.595	1.108	4.187
μ/ mm^{-1}	4.549	1.448	1.674	2.421	0.153	14.308
F(000)	3192	2640	1088	966	2972	1038
Crystal size/ mm	0.120 x 0.220 x 0.320	0.200 x 0.300 x 0.320	0.160 x 0.220 x 0.420	0.390 x 0.400 x 0.420	0.180 x 0.200 x 0.280	0.160 x 0.180 x 0.210
Index range	$0 \le h \le 30$ $-20 \le k \le 0$ $-29 \le l \le 27$	$-22 \le h \le 22$ $-26 \le k \le 22$ $-19 \le l \le 19$	$-25 \le h \le 25$ $-12 \le k \le 12$ $-27 \le l \le 19$	$-12 \le h \le 11$ $-15 \le k \le 15$ $-21 \le l \le 21$	$-24 \le h \le 24$ $-16 \le k \le 16$ $-35 \le l \le 37$	$-8 \le h \le 10$ $-10 \le k \le 10$ $-31 \le l \le 31$
No.of reflections collected	19224	76084	39499	74954	44318	6201
R1, wR2 [I > 2σ(I)]	0.0733,0.1215	0.0531,0.1178	0.0508,0.1041	0.0208,0.0422	0.1055,0.2143	0.0324, 0.0731
R1, wR2 (all data)	0.1616,0.1463	0.0927,0.1382	0.0958,0.1198	0.0251,0.0437	0.1420,0.2295	0.0475, 0.0796
GOF, F^2	1.015	1.020	1.016	1.088	1.163	1.054
no. of data/ restraints/ param	19224/99/ 498	11555/ 0/ 601	9056/ 0/ 253	7733/129/ 426	7613/258/ 483	691/0/13
largest diff peak, hole/ eÅ^{-3}	1.965, -1.440	0.805, -0.718	0.855, -0.688	0.588, -0.598	0.458, -0.471	1.094, -2.501