Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

for

Synthesis and characterization of heterocyclic disilylchalcogenides

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Theoretical study of model compounds

All calculations were performed on an SGI Altix 450 sever using the Gaussian 03 package. [s1] Geometry optimization was performed by using the DFT (B3LYP) method in conjunction with the relativistic effective core pseudopotential LanL2DZ for Se, Te and the 6-31G(d,p) basis set for the remaining atoms. The corresponding important structural parameters are given in Figures S1-S2. The comparison of calculated and observed structure features are shown in Table S1. Atomic coordinates of optimized structures of the model compounds are given in Tables S2-S7.

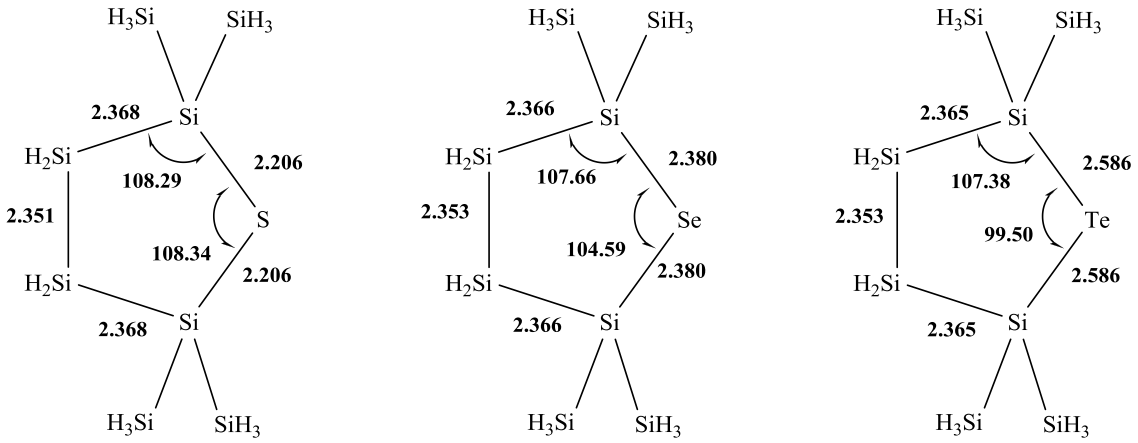

Figure S1. Calculated structures of model compounds **2'**, **3'** and **5'** (bond lengths [Å] and angles [˚])

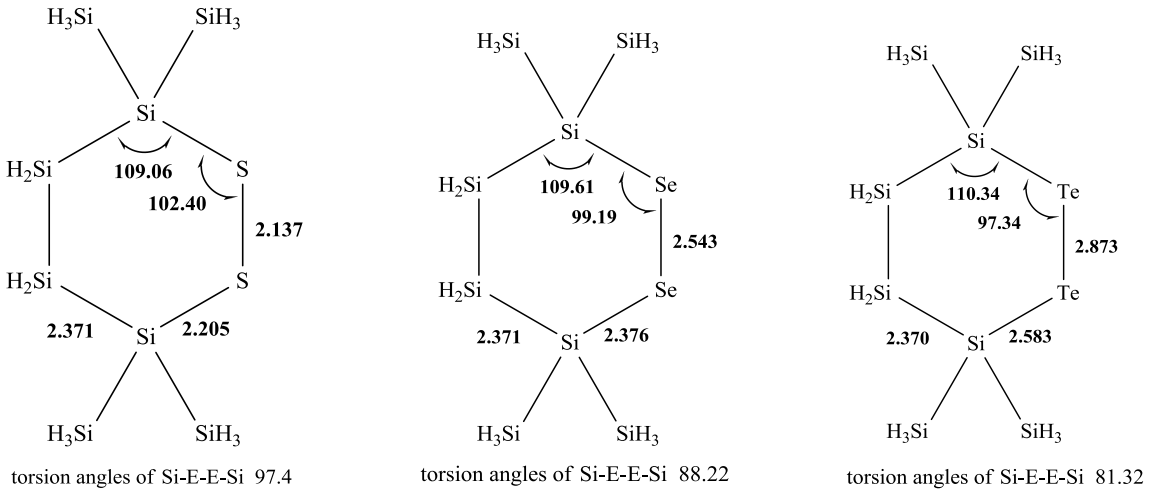

Figure S2. Calculated structures of model compounds **2”**, **3”** and **5”** (bond lengths [Å] and angles [˚])

Table S1. Comparison of calculated and observed structure features.

	Calculation		Observed [a]		Δ[d]	
	Si-E [b]	Si-E-R [c]	Si-E	Si-E-R	Si-E	Si-E-R
5-membered ring E = S	2.206	108.34	2.177	109.37	1.33%	0.94%
5-membered ring E = Se	2.380	104.59	2.316	105.72	2.76%	1.07%
5-membered ring E = Te	2.586	99.50	2.539	101.78	1.85%	2.24%
6-membered ring E = Te	2.583	97.34	2.533	99.20	1.97%	1.88%

[a] X-ray data; [b] bond lengths (Å); [c] bond angles (˚), for 5-membered rings, Si-E-Si bond angles, for 6-membered ring, Si-E-E bond angle; [d] $|d_{calc}-d_{obsv}|/d_{obsv}$

Table S2. Atomic Coordinates of model compound **2’**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000000	1.422038
2	14	0	-1.788340	-0.008245	0.130700
3	14	0	-1.095848	-0.425248	-2.095232
4	14	0	-2.788043	2.125613	0.276461

5	14	0	-3.210459	-1.699449	0.958090
6	14	0	1.788340	0.008244	0.130700
7	14	0	1.095848	0.425247	-2.095232
8	14	0	2.788044	-2.125613	0.276462
9	14	0	3.210458	1.699450	0.958089
10	1	0	3.067634	-2.475750	1.694070
11	1	0	1.879708	-3.152727	-0.301454
12	1	0	4.070035	-2.147743	-0.482204
13	1	0	4.475856	1.710248	0.172485
14	1	0	3.542145	1.459319	2.387450
15	1	0	2.553631	3.026462	0.826941
16	1	0	-2.553633	-3.026462	0.826942
17	1	0	-4.475857	-1.710247	0.172486
18	1	0	-3.542146	-1.459318	2.387450
19	1	0	-4.070034	2.147744	-0.482205
20	1	0	-3.067633	2.475751	1.694068
21	1	0	-1.879707	3.152726	-0.301455
22	1	0	1.087543	1.886622	-2.382207
23	1	0	1.999119	-0.244279	-3.071656
24	1	0	-1.087544	-1.886623	-2.382206
25	1	0	-1.999119	0.244277	-3.071656

Table S3. Atomic Coordinates of model compound **3'**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.882854	-0.003503	-0.055166
2	14	0	-1.095705	-0.428270	-2.245896
3	14	0	-2.870939	2.134105	0.075454
4	14	0	-3.314250	-1.706919	0.725793
5	14	0	1.882854	0.003503	-0.055166
6	14	0	1.095705	0.428269	-2.245896
7	14	0	2.870939	-2.134105	0.075455
8	14	0	3.314250	1.706919	0.725793
9	1	0	3.189063	-2.471100	1.488127
10	1	0	1.936340	-3.156850	-0.466677
11	1	0	4.130437	-2.172953	-0.720191
12	1	0	4.564509	1.719324	-0.084310
13	1	0	3.673935	1.477477	2.150243
14	1	0	2.644949	3.027780	0.596389
15	1	0	-2.644949	-3.027779	0.596390

16	1	0	-4.564509	-1.719324	-0.084309
17	1	0	-3.673935	-1.477476	2.150244
18	1	0	-4.130437	2.172953	-0.720192
19	1	0	-3.189063	2.471100	1.488126
20	1	0	-1.936340	3.156850	-0.466679
21	1	0	1.073999	1.893746	-2.513190
22	1	0	1.973976	-0.220618	-3.259776
23	1	0	-1.073999	-1.893747	-2.513189
24	1	0	-1.973976	0.220617	-3.259776
25	34	0	0.000000	0.000000	1.400399

Table S4. Atomic Coordinates of model compound **5'**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.973386	-0.234718	-0.000502
2	14	0	1.084473	-2.378106	-0.456174
3	14	0	2.961732	-0.182822	2.139945
4	14	0	3.467038	0.465609	-1.685942
5	14	0	-1.973386	-0.234718	0.000502
6	14	0	-1.084473	-2.378106	0.456172
7	14	0	-2.961733	-0.182820	-2.139945
8	14	0	-3.467038	0.465608	1.685943
9	1	0	-3.353275	1.208107	-2.491646
10	1	0	-1.995477	-0.682402	-3.154540
11	1	0	-4.177928	-1.043234	-2.176481
12	1	0	-4.682309	-0.395853	1.674415
13	1	0	-3.884919	1.875260	1.459917
14	1	0	-2.813943	0.359397	3.016858
15	1	0	2.813944	0.359400	-3.016857
16	1	0	4.682310	-0.395852	-1.674415
17	1	0	3.884919	1.875261	-1.459915
18	1	0	4.177927	-1.043236	2.176481
19	1	0	3.353274	1.208105	2.491648
20	1	0	1.995476	-0.682405	3.154539
21	1	0	-1.015480	-2.596444	1.928367
22	1	0	-1.951072	-3.438825	-0.132149
23	1	0	1.015480	-2.596443	-1.928369
24	1	0	1.951072	-3.438825	0.132146
25	52	0	0.000000	1.435943	0.000000

Table S5. Atomic Coordinates of model compound **2”**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.197518	0.040825	-0.005661
2	14	0	-1.040689	0.551171	2.000695
3	14	0	1.040948	-0.553733	1.999830
4	14	0	2.197828	-0.040795	-0.005818
5	14	0	-3.323458	1.923134	-0.879319
6	14	0	-3.690535	-1.760810	0.338324
7	14	0	3.324235	-1.922260	-0.880669
8	14	0	3.689314	1.761753	0.339964
9	1	0	1.866563	-0.131586	3.167875
10	1	0	0.827570	-2.023317	2.111742
11	1	0	-1.866334	0.127043	3.168006
12	1	0	-0.827597	2.020616	2.114905
13	1	0	-3.013157	-2.876161	1.050123
14	1	0	-4.825567	-1.279096	1.171414
15	1	0	-4.224084	-2.262883	-0.955010
16	1	0	-4.223689	2.483105	0.166838
17	1	0	-2.350439	2.970121	-1.283312
18	1	0	-4.144080	1.534337	-2.056999
19	1	0	2.351275	-2.969111	-1.285161
20	1	0	4.224524	-2.482739	0.165159
21	1	0	4.144699	-1.532704	-2.058203
22	1	0	4.221762	2.266205	-0.952893
23	1	0	4.825231	1.280307	1.171991
24	1	0	3.010820	2.875337	1.053464
25	16	0	-0.763395	-0.747125	-1.483082
26	16	0	0.763441	0.747783	-1.482717

Table S6. Atomic Coordinates of model compound **3”**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.318654	0.324454	0.123601
2	14	0	1.000803	2.231477	0.621837

3	14	0	-1.000805	2.231444	-0.621946
4	14	0	-2.318656	0.324447	-0.123614
5	14	0	3.407084	-0.538016	2.029941
6	14	0	3.855323	0.827200	-1.601734
7	14	0	-3.407099	-0.538104	-2.029911
8	14	0	-3.855308	0.827276	1.601712
9	1	0	-1.797076	3.453097	-0.304516
10	1	0	-0.686403	2.273016	-2.076906
11	1	0	1.797072	3.453114	0.304346
12	1	0	0.686402	2.273122	2.076795
13	1	0	3.170401	1.525812	-2.720880
14	1	0	4.914635	1.718102	-1.054121
15	1	0	4.490890	-0.413372	-2.118778
16	1	0	4.204720	0.540683	2.678075
17	1	0	2.409133	-1.050185	3.003390
18	1	0	4.325155	-1.640011	1.636645
19	1	0	-2.409154	-1.050317	-3.003343
20	1	0	-4.204737	0.540568	-2.678087
21	1	0	-4.325170	-1.640081	-1.636563
22	1	0	-4.490863	-0.413272	2.118829
23	1	0	-4.914631	1.718144	1.054065
24	1	0	-3.170375	1.525949	2.720811
25	34	0	-0.950334	-1.359937	0.844685
26	34	0	0.950336	-1.359971	-0.844631

Table S7. Atomic Coordinates of model compound **5”**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.420441	0.628053	-0.220329
2	14	0	-0.953213	2.428198	-0.693613
3	14	0	0.953213	2.428198	0.693613
4	14	0	2.420441	0.628053	0.220330
5	14	0	-3.499137	-0.150594	-2.166861
6	14	0	-3.986779	1.301539	1.415856
7	14	0	3.499136	-0.150595	2.166861
8	14	0	3.986779	1.301539	-1.415856
9	1	0	1.710572	3.699631	0.497045
10	1	0	0.531991	2.379854	2.120987
11	1	0	-1.710572	3.699631	-0.497045
12	1	0	-0.531991	2.379854	-2.120987

13	1	0	-3.298909	1.991586	2.538865
14	1	0	-4.965157	2.240190	0.801609
15	1	0	-4.723616	0.125664	1.951431
16	1	0	-4.172405	0.982744	-2.861269
17	1	0	-2.507811	-0.758484	-3.091633
18	1	0	-4.523955	-1.167355	-1.808129
19	1	0	2.507810	-0.758484	3.091633
20	1	0	4.172405	0.982744	2.861269
21	1	0	4.523955	-1.167355	1.808129
22	1	0	4.723616	0.125664	-1.951431
23	1	0	4.965157	2.240189	-0.801608
24	1	0	3.298909	1.991586	-2.538864
25	52	0	1.129041	-1.315280	-0.887806
26	52	0	-1.129041	-1.315280	0.887806

Reference

1 *Gaussian 03*, Revision B.03, M. J. Frisch, G.W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov,G. Liu, A. Liashenko, P. Piskorz, I.Komaromi, R. L.Martin, D. J. Fox, T. Keith, M. A. AlLaham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.