Supplementary Material (ESI) for Dalton Transactions

Supporting information (computational details) belonging to the publication

"The Competition Between Si–Si and Si–C Cleavage in Functionalised Oligosilanes: About their Reactivity with Elemental Lithium"

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Computational Details

All calculations were done without symmetry restrictions. Starting coordinates were obtained with Chem3DUltra 10.0. Optimization and additional harmonic vibrational frequency analyses (to establish the nature of stationary points on the potential energy surface) were performed with the software package Gaussian 03 (Revision D.01 and Revision E.01)[1] on the B3LYP/6-31+G(d) level. Thereby, no imaginary frequencies were obtained. The starting structural parameters for the systems were taken from the X-ray data of (*S*)-**1**·HCl[2] and (*R*)-**3**·HCl.[3] All other compounds were constructed based thereon with *Chem3D*. Each molecule was optimized both, as neutral compound and as radical anion as the first step of the reaction is supposed to be an electron transfer from the metal to the silane (possible interactions between the radical anion and the metal have not been considered in these calculations). The total (SCF) and zero-point energies (ZPE) of all systems can be found in Tab. 1. The calculated standard orientations of all investigated silanes can be found in Tab. 2 to Tab. 13.

Tab. 1 Total (SCF) and zero-point energies (ZPE) of all calculated systems.

compound	Method/Basis	Min./TS	SCF [Hartree]	ZPE [Hartree]
1	B3LYP/6-31+G(d)	Global Min.	–1644.467099	–1643.940472
1$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1644.459014	–1643.938856
8	B3LYP/6-31+G(d)	Global Min.	–1260.987489	–1260.569191
8$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1260.972001	–1260.557901
4	B3LYP/6-31+G(d)	Global Min.	–1629.846083	–1630.339755
4$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1629.836490	–1630.324531
10	B3LYP/6-31+G(d)	Global Min.	–1452.728037	–1452.255706
10$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1452.717959	–1452.251796
3	B3LYP/6-31+G(d)	Global Min.	–1260.569402	–1260.987286
3$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1260.557420	–1260.971240
9	B3LYP/6-31+G(d)	Global Min.	–1069.246902	–1068.883119
9$^{\bullet-}$	B3LYP/6-31+G(d)	Global Min.	–1069.227136	–1068.865497

Tab. 2 Standard orientation of **1** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.3031228494	–0.3953201432	0.1120742207
C	0.1031566784	1.4876478657	0.2054422091
Si	–1.8963989169	–1.3168159805	–0.010492906
C	–2.7649553234	–0.6724306176	–1.5753692863
C	–2.8538164339	–0.7336697608	1.5235305929
N	2.3355431914	–0.0108607956	–1.9627734664
C	–1.9208948812	–3.221130153	–0.0474814947
C	2.8749044555	–0.4867688671	–3.2418870382
C	3.4045759024	0.2149832723	–0.9873843907
C	4.4345779596	1.2283770371	–1.4991611989
C	1.2897781949	–0.9099074646	–1.4683564331
C	3.8774669031	0.5048498061	–3.8403675635
C	5.0142575555	0.7974304853	–2.8524547799

C	0.0566015274	2.2836007597	–0.9568220511
C	–0.142101176	3.665282023	–0.8836076235
C	–0.2977605428	4.287919567	0.3583089128
C	–0.0567817696	2.1376842667	1.4450445695
C	–0.2526894395	3.5195308206	1.5245593057
C	–3.7934523208	0.3124411587	1.4507825907
C	–4.4682277064	0.7691866544	2.5874663943
C	–4.2159523405	0.1879843854	3.8323209375
C	–2.9873424664	–3.9459308125	0.5201374318
C	–3.0453061206	–5.3405886285	0.4423436998
C	–2.0326768721	–6.0499517021	–0.2090400998
C	–0.9642387027	–5.3545893973	–0.7812337308
C	–0.913161813	–3.9600055459	–0.6979471049
C	–3.2872657221	–0.8528316937	3.9314395285
C	–2.6175539272	–1.303777481	2.7910638937
C	1.1582185771	–1.0401329608	1.6848918306
H	–3.8221036151	–0.9664625427	–1.5871293567
H	–2.2969174734	–1.0952509672	–2.4728645493
H	–2.7107545081	0.4199379534	–1.6552068653
H	2.035109405	–0.6350730962	–3.9316226681
H	3.3658874007	–1.4768415049	–3.1142055401
H	3.9161565897	–0.7409882021	–0.7378277014
H	2.9555920818	0.5914515298	–0.0629095819
H	5.2312362955	1.3396014069	–0.7518998533
H	3.9444117057	2.2059135386	–1.6001991314
H	0.5618120215	–1.0348634941	–2.2815824732
H	1.6967388064	–1.9289630292	–1.2773222515
H	4.272274431	0.096982688	–4.7802816368
H	3.3509300154	1.4375161182	–4.0850079095
H	5.6844083825	1.5704568149	–3.2503016218
H	5.6226574987	–0.1100202419	–2.7177561705
H	0.2038992682	1.8247430469	–1.9309221109
H	–0.1688549929	4.2561597988	–1.796549712
H	–0.4498631865	5.3631308262	0.4166866945
H	–0.0313948594	1.5625498899	2.3681093334
H	–0.3721516197	3.9937647391	2.4960372555
H	–4.0080464681	0.7840911691	0.4945204282
H	–5.1896196598	1.5783265328	2.4991948024
H	–4.7396560401	0.5403908188	4.7177404067
H	–3.7845345338	–3.4169869136	1.0374555957
H	–3.8808646924	–5.8722669366	0.8920230207
H	–2.0749797261	–7.1348531515	–0.2688121893
H	–0.1697374718	–5.8964016644	–1.289402936
H	–0.0680617557	–3.4457540758	–1.1508939283
H	–3.0869396371	–1.3151748651	4.8954062221

H	–1.9064759643	–2.1218228213	2.8915014894
H	1.3413007956	–2.1189027167	1.6029829186
H	0.5335823701	–0.8820657399	2.5719833551
H	2.1225318167	–0.5496310063	1.8634297152

Tab. 3 Standard orientation of **1**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.4528690306	–0.3928116156	0.4294268101
C	–1.1185020297	–2.0572877357	–0.1170828141
Si	1.6407309409	0.2857124299	–0.6281195502
C	1.4311156496	–0.1851770911	–2.4653205697
C	3.121542325	–0.6628912874	0.0704795466
N	–3.1329036513	0.8238095517	0.0470162634
C	1.9321153373	2.1367808611	–0.5029115319
C	–3.860631569	2.0385406118	–0.3192728981
C	–3.6169058615	0.2759219034	1.311797835
C	–5.1147406765	–0.0483610152	1.2482115193
C	–1.6795778397	1.0514414625	0.0199095149
C	–5.3669158977	1.7849701797	–0.452904655
C	–5.935333654	1.1820008028	0.8387364931
C	–2.0940369917	–2.1975266289	–1.145953031
C	–2.4704821026	–3.4428167686	–1.6400926085
C	–1.8867832775	–4.624340946	–1.1397084248
C	–0.5518964376	–3.2697215196	0.3779838483
C	–0.9259578287	–4.5157726933	–0.1188224968
C	3.8888605217	–1.5327522784	–0.7428794518
C	4.9801842931	–2.2456208183	–0.2468016738
C	5.355908009	–2.123397898	1.1019080523
C	2.6492468517	2.7592677722	0.5589366269
C	2.7915467904	4.1393553862	0.6523164586
C	2.2145481991	4.9929103858	–0.3120065043
C	1.503139418	4.4089450026	–1.3738078294
C	1.3649320612	3.0258920123	–1.4672083145
C	4.6046205389	–1.2847551141	1.9363888576
C	3.507389952	–0.5828475256	1.4353776756
C	–0.1560719127	–0.4212895221	2.3208687376
H	2.3128755707	0.0869616299	–3.060570543
H	0.5628831001	0.3223338448	–2.9043652926
H	1.2536776191	–1.2626348483	–2.5679736492
H	–3.4554096821	2.4058525295	–1.270077164
H	–3.6887297213	2.8437772592	0.4313240638
H	–3.4285279763	0.9853861703	2.1502321395
H	–3.054978217	–0.6376938898	1.5253958724
H	–5.4451185614	–0.4274621072	2.2253685285

H	–5.2660559964	–0.8548655269	0.5180643985
H	–1.4346620042	1.4127028588	–0.9877004944
H	–1.3990708315	1.8880834755	0.6969353412
H	–5.8753478857	2.7278017722	–0.7001701567
H	–5.5370199629	1.09216429	–1.2888944675
H	–6.9955888907	0.920366749	0.7133183635
H	–5.8871148037	1.9351337117	1.6410749356
H	–2.576206205	–1.3062114818	–1.5419594614
H	–3.2295090628	–3.50191524	–2.4201387693
H	–2.1750056499	–5.5973840818	–1.5316962614
H	0.2009394499	–3.2302323856	1.164204199
H	–0.464498687	–5.414788228	0.2893525944
H	3.6308482553	–1.65044293	–1.7931472064
H	5.5426162409	–2.8998452222	–0.9115572455
H	6.2062402661	–2.677800742	1.4934886416
H	3.1250091504	2.1415270484	1.317255285
H	3.3614375784	4.562167696	1.4794148373
H	2.3178950824	6.0730081544	–0.2354641587
H	1.0539835126	5.0426464621	–2.1386522618
H	0.8137931364	2.6205616122	–2.3142824913
H	4.8685448909	–1.1875011819	2.9888141215
H	2.9311783918	0.0318151163	2.1235051405
H	0.2263330882	0.5498486336	2.6626913541
H	0.5890847157	–1.1790438818	2.5908882535
H	–1.0734316492	–0.6396461858	2.8825622446

Tab. 4 Standard orientation of **8** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.2440031583	0.2363965553	–0.1751565416
C	–0.3009881089	2.1360953291	–0.2503434625
Si	–2.445420947	–0.6612803256	–0.2062201391
C	–3.2990150887	–0.2770584874	–1.8647492913
C	–3.4826614301	0.1116026826	1.1908175904
N	2.0013226527	0.132602039	–2.0003310886
C	–2.3921064535	–2.54675335	0.0390050383
C	2.3354403031	0.1604454221	–3.4298091333
C	3.013396771	–0.6163107168	–1.2495666578
C	4.4058309223	0.0053154677	–1.4018855633
C	0.6447377024	–0.3863141026	–1.7646467256
C	3.6993775487	0.8138198987	–3.6770509332
C	4.803950321	0.1061497913	–2.8804476502
H	–0.847504507	2.4948355524	–1.1316193467
H	0.7173120362	2.5403003161	–0.3092289082
H	–0.7836317918	2.5606709597	0.6387838076

H	–4.4829285627	–0.3390021563	1.2311555603
H	–3.6097881649	1.1885617682	1.0235178994
H	–3.0208612189	–0.0126349475	2.1777942378
C	–2.5863482201	–3.1313642367	1.305695245
C	–2.5194333142	–4.5157448872	1.4920149365
C	–2.2541930717	–5.3563443339	0.4079141524
C	–2.05918427	–4.8019465898	–0.8604468978
C	–2.1267038382	–3.4172134131	–1.0370198563
C	0.6110784367	–0.2767215731	1.4475902986
H	–4.3283031767	–0.6584318803	–1.8713201148
H	–2.7749306667	–0.7234732485	–2.7184547041
H	–3.3428180627	0.8058904239	–2.0374545384
H	1.5535402339	0.7233698002	–3.952789458
H	2.3344927468	–0.8683069549	–3.8528161373
H	3.0431775942	–1.6747600991	–1.5918253172
H	2.7253957258	–0.6353887829	–0.1951226473
H	5.1342794824	–0.5975524401	–0.8436152067
H	4.398334698	1.0072719872	–0.9512305093
H	0.0078753704	–0.0245026029	–2.5846785246
H	0.6168551919	–1.4937710522	–1.8364563558
H	3.9212837442	0.7930582	–4.752299892
H	3.6441651482	1.868910356	–3.3758563275
H	5.7596877325	0.6349090354	–2.9900148844
H	4.95370328	–0.9060156827	–3.2860896259
H	–2.7996583838	–2.5013735771	2.166737043
H	–2.6763778179	–4.9365050764	2.482722184
H	–2.2024726849	–6.4332466021	0.5490231694
H	–1.8558383882	–5.4472596918	–1.7120959588
H	–1.974110888	–3.0137776829	–2.0364384661
H	0.7900489601	–1.3576492051	1.4923011056
H	–0.0171965818	–0.0110966363	2.3078539987
H	1.5724921939	0.2349947503	1.5800545969

Tab. 5 Standard orientation of **8**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.0179382392	–0.0244233883	0.1866192386
C	0.2381490814	1.8633509248	0.0124328564
Si	–2.2409013992	–0.7640601974	0.0657128862
C	–3.0536241378	–0.0267160813	–1.4951264764
C	–3.1914771178	–0.1510102333	1.6032928808
N	2.1143305671	–0.275864866	–1.8509286952
C	–2.2707019588	–2.6411561296	–0.0246426086
C	2.4704903242	–0.865522467	–3.1422287783
C	3.2488227035	–0.301742257	–0.9302768194

C	4.4592795665	0.4492777384	–1.4974997283
C	0.9065847604	–0.9033376527	–1.2898087228
C	3.6403187238	–0.127373036	–3.8015488725
C	4.861188889	–0.0977512498	–2.8730345837
H	–0.148778411	2.2261446962	–0.9491853752
H	1.3011230142	2.14521385	0.0721072794
H	–0.2951863557	2.3942743974	0.8120069553
H	–4.2421503955	–0.4721958418	1.5640050307
H	–3.1714004598	0.9472630227	1.6535875639
H	–2.756740383	–0.5302151	2.5386198829
C	–2.0573065619	–3.4444896873	1.1336759515
C	–2.0191199423	–4.8348499187	1.0706031978
C	–2.1871146824	–5.503436913	–0.1561305622
C	–2.3517288519	–4.7325560746	–1.3242551627
C	–2.3908761512	–3.3424083671	–1.2570548154
C	0.7667235565	–0.5769212602	1.8568068071
H	–4.0862606405	–0.3856796955	–1.6044539381
H	–2.5083492451	–0.2813273026	–2.41514992
H	–3.0829562341	1.0689962941	–1.4252836125
H	1.5868709351	–0.8209215387	–3.7919563629
H	2.7305010636	–1.9424286783	–3.0288633433
H	3.5413793584	–1.3499810702	–0.6932268661
H	2.9442053612	0.1603162779	0.0148028526
H	5.2959910395	0.374112081	–0.7880821918
H	4.2034442222	1.5142972772	–1.5845406947
H	0.1663046136	–0.9406797889	–2.1016120732
H	1.0939346577	–1.9648531699	–1.0185462264
H	3.8875085062	–0.6148243665	–4.7560519014
H	3.3256912058	0.9001855434	–4.0307846638
H	5.6701446096	0.5059224447	–3.310465165
H	5.2540966667	–1.1200330161	–2.7588034612
H	–1.9341529376	–2.9659531261	2.1047706126
H	–1.8664199665	–5.4083290755	1.9845877469
H	–2.1736602833	–6.5901451648	–0.2040042807
H	–2.4608516512	–5.2257798604	–2.289718855
H	–2.5330223855	–2.7832941434	–2.1810581882
H	0.7758804382	–1.6723421127	1.9472085747
H	0.1744007246	–0.1795146811	2.6916202999
H	1.7964773237	–0.2176370359	1.9898623274

Tab. 6 Standard orientation of **4** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.1788719554	–0.205713627	0.1302657184
C	–0.0331465067	1.6794478932	0.0773861979
Si	–1.9814822772	–1.1984536555	0.0205945493
C	–2.8848822863	–0.5389754824	–1.5321918438
C	–2.9666493604	–0.6232302001	1.5577161756
N	2.2785091318	–0.0089029432	–1.9094032118
Si	–1.9901626092	–3.5738963579	–0.0449849694
C	2.8460288109	–0.5956568096	–3.1286104284
C	3.3212100784	0.2732250696	–0.9207868394
C	4.387125796	1.2230639237	–1.4786637729
C	1.1935560878	–0.8405964635	–1.3825593116
C	3.8893798946	0.3235083916	–3.7716043035
C	5.000486374	0.6732717829	–2.7726675909
C	–0.0377036406	2.3905838869	–1.1392333353
C	–0.2504173341	3.7717615895	–1.1733239296
C	–0.4643762365	4.4800065187	0.0127007639
C	–0.2491998722	2.4157583794	1.2593947632
C	–0.4611483652	3.797432177	1.2321889621
C	–3.7925984096	–4.1917005685	–0.0024846111
C	–1.0727873256	–4.3217316491	1.4468337168
C	–1.179546197	–4.2284407061	–1.6389361029
C	1.0121816012	–0.6942120303	1.7734616915
H	–3.9218745134	–0.8979341829	–1.5600498876
H	–2.3984481393	–0.8619219036	–2.4608821227
H	–2.9124162599	0.5577797013	–1.5351028685
H	–4.0022199306	–0.9847530166	1.5158055961
H	–2.9999187008	0.4720591022	1.6147233317
H	–2.5243665549	–0.9932828377	2.4909413064
H	2.0242495632	–0.7808582009	–3.8309847937
H	3.309115368	–1.5827040868	–2.9074702128
H	3.8054751057	–0.6687823923	–0.5798821012
H	2.8526067821	0.7303210353	–0.0437201027
H	5.1622858325	1.3810305351	–0.7172408464
H	3.9202873034	2.1976725609	–1.6747812275
H	0.4798312758	–0.9971203237	–2.2032967068
H	1.5587736759	–1.8593190129	–1.1168027604
H	4.3045765943	–0.1678276902	–4.6615252005
H	3.3923949049	1.2434111052	–4.1089196006
H	5.7000073081	1.398334603	–3.2084113239
H	5.5834167831	–0.2322724657	–2.5450727866
H	0.1536354057	1.86422707	–2.0705325291
H	–0.2426592729	4.2959661505	–2.1264329023
H	–0.6282283928	5.5547269184	–0.0128533951

H	–0.2484968606	1.9093894207	2.2227991135
H	–0.6222370977	4.3391594995	2.161582128
H	–4.3714915397	–3.815927225	–0.8554756418
H	–4.308421608	–3.8779313544	0.913535919
H	–3.823890913	–5.2892608016	–0.039983948
H	–1.4909044103	–3.9741477961	2.3998750881
H	–0.0060623092	–4.0659666757	1.4395947741
H	–1.1493026592	–5.4174530033	1.4329448352
H	–0.1234501358	–3.940657066	–1.7097332037
H	–1.6876879016	–3.8520751743	–2.5355978306
H	–1.2267629183	–5.3254879572	–1.6692189746
H	0.342702316	–0.5295291643	2.6265420558
H	1.9305824455	–0.1246162453	1.958216792
H	1.2751501443	–1.7591982448	1.7707177387

Tab. 7 Standard orientation of **4**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.122798125	–0.0357816729	0.1104865857
C	0.0488062984	1.8276858261	0.0913614631
Si	–1.9609802412	–1.2471540457	0.0057184347
C	–2.9132072209	–0.5916726164	–1.5323081803
C	–2.9584813458	–0.6815596713	1.5519319377
N	2.2655578102	0.0295131248	–1.9420097814
Si	–2.0711463194	–3.6351675093	–0.0593171976
C	2.8506797	–0.6432243276	–3.0988954817
C	3.2786366351	0.3425244534	–0.937869737
C	4.3840664158	1.2353324534	–1.5142665978
C	1.1221503208	–0.7197380852	–1.4067840505
C	3.9380872282	0.2080895589	–3.7656462415
C	5.0251119189	0.5972231754	–2.753801942
C	0.0017269747	2.5860284286	–1.1237523944
C	–0.2222455474	3.9564999188	–1.1318640088
C	–0.4180633123	4.6712284909	0.0710900628
C	–0.1245375527	2.5843466528	1.2962298156
C	–0.3481858745	3.9554344494	1.2863169467
C	–3.7984504822	–4.4797915764	–0.0212497179
C	–1.1092884277	–4.3798392978	1.4216694527
C	–1.2161139595	–4.2987386945	–1.6400622024
C	0.9672714108	–0.6017627186	1.7375271095
H	–3.9617303713	–0.9172019742	–1.5194590633
H	–2.4672342076	–0.9468396392	–2.4715606951
H	–2.8964365871	0.5060397781	–1.5496345792
H	–4.0015285617	–1.0200603571	1.4979501176
H	–2.9592972276	0.413982813	1.626913578

H	–2.527241739	–1.0802111254	2.4804679998
H	2.0467254809	–0.8533665421	–3.8152527787
H	3.2833611988	–1.6290737996	–2.807140548
H	3.733749303	–0.5896922377	–0.5292417072
H	2.7869026817	0.8580066478	–0.1087648222
H	5.1408065479	1.4220697664	–0.739465125
H	3.9434759052	2.2051587877	–1.7809827096
H	0.4052451329	–0.8414306128	–2.2311354834
H	1.4256316477	–1.7560303621	–1.1305966443
H	4.3713733143	–0.3474990523	–4.6097814829
H	3.4736556375	1.1163866365	–4.1739153008
H	5.7561125109	1.2790005385	–3.211174532
H	5.5789829883	–0.3062803869	–2.4528419958
H	0.1665484229	2.0766936214	–2.0718972879
H	–0.2377445409	4.4883542561	–2.0840246906
H	–0.6017547056	5.7433079877	0.0621869989
H	–0.0818342965	2.0740111499	2.2587337415
H	–0.4679022478	4.4838862604	2.2329130181
H	–4.4131469835	–4.1782157047	–0.8791301079
H	–4.3550298413	–4.2223144467	0.889273243
H	–3.6950316623	–5.580967911	–0.0520114573
H	–1.5338842007	–4.0578270802	2.3816775922
H	–0.052794813	–4.0828004003	1.4109607118
H	–1.1521735316	–5.4783541219	1.3929585963
H	–0.1654615255	–3.9876769996	–1.6982650744
H	–1.7194291	–3.9415856676	–2.547997526
H	–1.2448666628	–5.3981083327	–1.6567196956
H	0.3015153885	–0.4603433501	2.5986291183
H	1.8929898567	–0.048044052	1.9410623406
H	1.2127542348	–1.6708504038	1.6911619759

Tab. 8 Standard orientation of **10** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.1178854713	0.1315880124	0.0328558462
C	–0.0829648283	2.0276130536	–0.0312488388
Si	–2.3809862198	–0.6037506085	–0.0552352652
C	–3.235595799	0.0870545281	–1.6065299745
C	–3.3254045041	0.009290641	1.4776927796
N	1.959256657	–0.0025157483	–2.0396111916
C	–2.439791767	–2.5048247913	–0.1037071766
C	2.3958668652	–0.6672941224	–3.2731499354
C	3.0542776677	0.087850203	–1.0716888413
C	4.2591010383	0.8438354176	–1.64434148
C	0.7638861353	–0.651349491	–1.4919657831

C	3.5684378122	0.0663250235	–3.9316702283
C	4.7429933296	0.2096179532	–2.9549550493
C	0.0846356128	2.725436562	–1.2440880714
C	0.0461473162	4.1223412363	–1.2899888679
C	–0.1589003479	4.8591484744	–0.1202046665
C	–0.2841063642	2.7927495976	1.1353503876
C	–0.3212114433	4.1895394642	1.0960254781
H	–4.3687972641	–0.3307689433	1.4509464848
H	–3.3310216596	1.1057699346	1.5103901851
H	–2.8838502021	–0.3456853278	2.4166651599
C	–2.5039069792	–3.2683864205	1.0786597274
C	–2.5184572638	–4.6660371384	1.0486253184
C	–2.4665434578	–5.3405098854	–0.1743401714
C	–2.4029153862	–4.606873943	–1.3622318894
C	–2.3888116742	–3.2096566221	–1.3225715104
C	0.6470598836	–0.4682679787	1.6708725243
H	–4.2821832356	–0.2409445847	–1.6517985095
H	–2.7477001815	–0.2310807563	–2.5356792791
H	–3.2255355499	1.1837637399	–1.5916272332
H	1.5420324064	–0.7034862778	–3.9608511064
H	2.6872513632	–1.7205888668	–3.0665236855
H	3.3741987936	–0.9262908865	–0.7448768495
H	2.6880464258	0.611473943	–0.1829962925
H	5.0636428115	0.8560088339	–0.8972748158
H	3.9667538507	1.8872380341	–1.8241183737
H	0.0207786787	–0.6904424567	–2.3006634088
H	0.9629263915	–1.7146706305	–1.23081937
H	3.8754487779	–0.4794492325	–4.8336720004
H	3.230420723	1.0613611145	–4.2521316304
H	5.5479474903	0.8081592508	–3.4007929948
H	5.1659525628	–0.7848424439	–2.7459077467
H	0.2752584842	2.1720018944	–2.159624238
H	0.1826562619	4.6351201661	–2.2395743064
H	–0.1878655949	5.9456600033	–0.1548754305
H	–0.4110086758	2.2966084579	2.0959359682
H	–0.4759383615	4.7536140019	2.0131110595
H	–2.5511571642	–2.7690082546	2.0443506191
H	–2.5722343051	–5.2270187572	1.978967626
H	–2.4786441868	–6.4274363426	–0.2015172665
H	–2.3659131895	–5.1219168026	–2.3195398805
H	–2.3433436112	–2.6638189791	–2.2628815081
H	0.717367228	–1.5630053353	1.6799758546
H	0.0315645842	–0.1752545358	2.5303361867
H	1.6533655363	–0.0651933776	1.8340136621

Tab. 9 Standard orientation of **10**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.0280214454	0.079600749	0.0050356719
C	0.0840629181	1.9453158241	–0.0069804056
Si	–2.2499238148	–0.8663538457	–0.0106116475
C	–3.2037553635	–0.056032571	–1.4564972027
C	–3.088532626	–0.2988149449	1.6133645688
N	1.979586353	–0.037850347	–2.1732550113
C	–2.396276193	–2.7297422471	–0.1505056474
C	2.4366084435	–0.7671484756	–3.3540588058
C	3.0770348423	0.1977949183	–1.23900313
C	4.2121805763	0.9932416844	–1.8958736783
C	0.814299025	–0.6923780127	–1.5611795772
C	3.5428465507	–0.0120870142	–4.10104777
C	4.7202931384	0.2970736065	–3.1660082002
C	0.0078058551	2.7066635163	–1.2158322906
C	–0.076785703	4.0939962894	–1.2116562763
C	–0.0936385391	4.8178363263	–0.0001512696
C	0.0835945023	2.7069306264	1.2035871472
C	–0.0005600352	4.0950878898	1.2076616435
H	–4.1500848319	–0.5821403664	1.6240766581
H	–3.0228143008	0.7919061213	1.7181852119
H	–2.6171451632	–0.7440633496	2.4988787396
C	–2.283021645	–3.588654112	0.9868899921
C	–2.2472190737	–4.9738366177	0.8732699829
C	–2.3154480959	–5.5989763759	–0.3899491755
C	–2.4394313244	–4.7789082957	–1.5309920944
C	–2.4759418361	–3.3938294861	–1.4142580048
C	0.8263839917	–0.5944095664	1.5821442187
H	–4.2567561102	–0.3700653785	–1.4562897974
H	–2.7796393589	–0.3172040151	–2.4347498244
H	–3.1693540549	1.0372098648	–1.3671000917
H	1.5753231846	–0.9211738233	–4.0159429669
H	2.8077725563	–1.7804586373	–3.0745357976
H	3.479907132	–0.7649658186	–0.8472938834
H	2.6845980827	0.7592123315	–0.3866328382
H	5.0292602862	1.1242844475	–1.1725808559
H	3.8348873823	1.9936807425	–2.1467726138
H	0.0425794154	–0.7590403584	–2.341084288
H	1.0463278686	–1.747830199	–1.2958445704
H	3.8751960904	–0.6085537383	–4.9628489923
H	3.1276679415	0.9271351236	–4.4923197218
H	5.4716440464	0.9159335996	–3.6769687171
H	5.2199607728	–0.6450917443	–2.8899898353
H	0.0377562667	2.1873228465	–2.1721919155

H	–0.1223707871	4.6288334149	–2.1608150101
H	–0.1668468268	5.9031691466	0.002007606
H	0.1532925054	2.1900833016	2.1606646049
H	0.0093253596	4.6286468124	2.158608883
H	–2.229566267	–3.1500377283	1.9832683153
H	–2.1699190562	–5.5826810881	1.7745685256
H	–2.2804534409	–6.6823473613	–0.4805510155
H	–2.5134782164	–5.2344250667	–2.5189396295
H	–2.5773390561	–2.801118151	–2.3231864599
H	0.8792299713	–1.690053763	1.5416408545
H	0.2582406368	–0.3312337829	2.4838020483
H	1.8458574699	–0.2074529009	1.7086443397

Tab. 10 Standard orientation of **3** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.0348412909	–0.066759064	0.1593340107
C	0.0818823891	1.8295860739	0.0985478619
Si	–2.2121088147	–0.8092755937	–0.0657819057
C	–2.9828113426	–0.1172589723	–1.661755614
C	–3.2517145256	–0.2185013877	1.4148397317
N	2.2369094997	–0.197504168	–1.7858455679
C	–2.2800733945	–2.7125318124	–0.1293640218
C	2.7643892216	–0.8844416467	–2.9708005241
C	3.2643242722	–0.0579323438	–0.7518570886
C	4.4870362334	0.7087432038	–1.2691384774
C	1.0173120739	–0.8518685439	–1.3036474954
C	3.9632404719	–0.1452152396	–3.5735484436
C	5.0677358201	0.0498182661	–2.5268673317
C	0.3087816251	2.5287193831	–1.1036568374
C	0.277541449	3.9257926565	–1.1487104064
C	0.0191679416	4.6615048341	0.0112836354
C	–0.1730828526	2.5934555478	1.2552615795
C	–0.2043256817	3.9904505219	1.2169116275
C	0.7101242987	–0.6689485286	1.8381295568
H	–4.0322308607	–0.4297759909	–1.7491059459
H	–2.4582533335	–0.4723499413	–2.5578296453
H	–2.9584522063	0.9791593075	–1.6753809294
H	–4.2929808909	–0.5520652972	1.30882956
H	–3.2606536094	0.8756576771	1.492152987
H	–2.8733616681	–0.6181256322	2.3641163508
H	–3.3184566003	–3.0582559242	–0.223848433
H	–1.8633083311	–3.1631337921	0.7801967235
H	–1.7201072489	–3.1119997897	–0.9842712498
H	1.9569246857	–0.9565504322	–3.7096066485

H	3.0624694352	–1.925736999	–2.7173064056
H	3.5828777918	–1.0556073618	–0.3765376516
H	2.8308803582	0.4825604806	0.0954848276
H	5.2416281314	0.7613070381	–0.4733145876
H	4.1833994368	1.739165502	–1.498007625
H	0.3251600734	–0.9076547476	–2.1557727902
H	1.2131981076	–1.9110288669	–1.0187456359
H	4.3390387928	–0.7097910083	–4.4371152796
H	3.6281336042	0.8329992554	–3.9446360609
H	5.8879334198	0.6536627348	–2.9363359063
H	5.496618927	–0.9290036789	–2.2629369206
H	0.5390920264	1.9757547759	–2.0101897803
H	0.4611138765	4.4398882904	–2.0896373345
H	–0.0039449572	5.7481807029	–0.0228312751
H	–0.3485066562	2.0955502418	2.20720691
H	–0.4016443115	4.5533800932	2.1264932137
H	0.0584010945	–0.3633840345	2.665837116
H	1.7143527765	–0.2826146476	2.0486756141
H	0.7640081609	–1.7650211415	1.8564825129

Tab. 11 Standard orientation of **3**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.7189991774	–0.3982822655	0.6131388016
C	–0.6564497282	1.4161717075	0.1574515895
Si	–2.6882250398	–1.3908633448	–0.3056634155
C	–2.6351988785	–1.3150162476	–2.212514169
C	–4.2160681274	–0.4007491517	0.2674692432
N	2.0903605549	–0.7733786396	–0.2236363483
C	–2.9626884326	–3.2125666807	0.2003353423
C	3.0444592132	–1.6687183212	–0.8780854393
C	2.6001298886	–0.2976416575	1.060250228
C	3.9348251598	0.4395181621	0.8968954622
C	0.7609438644	–1.3906141289	–0.1356352375
C	4.3933029761	–0.9832383691	–1.1232754689
C	4.9750911152	–0.4369255069	0.1872315307
C	–0.0093342176	1.8796925326	–1.0245397347
C	–0.0295816329	3.2228948842	–1.391784742
C	–0.7053054265	4.1755468283	–0.6055565755
C	–1.3726313571	2.3921309679	0.908528602
C	–1.3961115974	3.7343681955	0.5400577848
C	–0.8113110571	–0.623026502	2.5095855827
H	–3.5736400216	–1.7040959837	–2.6342274444
H	–1.8151229741	–1.9212625472	–2.6201545995
H	–2.5030487065	–0.2859656207	–2.5736329256

H	–5.1271517428	–0.8049831744	–0.1981594385
H	–4.1376040913	0.6605269409	–0.0039844094
H	–4.3477961676	–0.4594789845	1.356192678
H	–3.8990974577	–3.592424923	–0.2430327054
H	–3.0402349871	–3.3216848288	1.2908259488
H	–2.1451956084	–3.8622176268	–0.1412720429
H	2.6082418307	–1.9939882657	–1.8315586723
H	3.2037719801	–2.5887953817	–0.2709432788
H	2.7272816422	–1.1418245308	1.775530533
H	1.85753799	0.3820676695	1.491569066
H	4.2989901847	0.7507958661	1.8861734663
H	3.7592388408	1.3526200979	0.3120202683
H	0.4706644274	–1.6707413654	–1.1601577531
H	0.8035945849	–2.3521882314	0.4246822766
H	5.0860306776	–1.6986816583	–1.5896035647
H	4.2475028872	–0.1581103659	–1.8342530857
H	5.8985442132	0.1297403736	–0.0027462822
H	5.249362947	–1.279630452	0.8411792671
H	0.5448322899	1.1753984131	–1.6408736968
H	0.4954819821	3.538508379	–2.2930267972
H	–0.7094519516	5.2265149445	–0.8866289219
H	–1.9092088796	2.0915712341	1.807866589
H	–1.9467189307	4.448751081	1.15150655
H	–1.7555418415	–0.2271662068	2.9100780003
H	0.011793078	–0.1211697532	3.0346190766
H	–0.7768243732	–1.6914947006	2.7657152791

Tab. 12 Standard orientation of **9** [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	–0.0486360076	0.0663129609	–0.0507008795
C	–0.1131583044	1.9604530463	–0.191159887
H	–0.5954313922	2.4127810721	0.6844881064
Si	–2.2383904012	–0.8547439215	0.0241214792
C	–3.230975045	–0.3698232576	–1.5280293438
C	–3.1685819257	–0.2061203521	1.5550257297
N	2.0183018953	0.0264520679	–2.1053831943
C	–2.1726820112	–2.7562983957	0.1231032153
C	2.2924759858	–0.2919795406	–3.5120400928
C	3.1807790643	–0.2760919598	–1.267560256
C	4.4211192577	0.5082947862	–1.7113507993
C	0.7978682787	–0.6395028373	–1.631680961
C	3.4938541627	0.4936736934	–4.0477102722
C	4.7405267454	0.2450857628	–3.188618025
H	–0.6656581355	2.2802351453	–1.0831235699

C	0.8552150373	–0.4018754226	1.5641506534
H	–4.2473858116	–0.783665553	–1.4806008301
H	–2.7639630235	–0.748869214	–2.4458505822
H	–3.3223348393	0.7189924226	–1.6277145854
H	–4.1800978065	–0.6319202007	1.6020249573
H	–3.271086431	0.8861432387	1.533631696
H	–2.6551696803	–0.4732969027	2.4872518483
H	–3.1864371187	–3.1762867149	0.1742584679
H	–1.6289663886	–3.0979971794	1.012850751
H	–1.6786076037	–3.1918120475	–0.754551366
H	1.3973479381	–0.0494806635	–4.0967653359
H	2.4768887018	–1.3817697667	–3.6382613287
H	3.4059740987	–1.3658221643	–1.2927628057
H	2.9377623667	–0.029002925	–0.2303746015
H	5.2710171214	0.2305258567	–1.0739793596
H	4.2356287965	1.5803575766	–1.5583305475
H	0.0431710376	–0.5274443781	–2.4231869639
H	0.9498639716	–1.7363043488	–1.5243624649
H	3.6769993145	0.2072823443	–5.091811158
H	3.247405949	1.5642450363	–4.0414202248
H	5.574539607	0.875461644	–3.5233720325
H	5.0641972747	–0.799865077	–3.3103597246
H	0.900352129	2.3718820925	–0.2724125468
H	0.2291594924	–0.1679977328	2.4349691636
H	1.7974836935	0.1457701315	1.6892186129
H	1.0849300064	–1.4741783223	1.6035790577

Tab. 13 Standard orientation of **9**$^{\bullet-}$ [global minimum, B3LYP/6–31+G(d)].

atomic symbol	x	y	z
Si	0.8595217752	0.7036961374	0.1841930644
C	0.5754451298	1.1883531226	2.0020034327
H	1.3489085722	1.8858957772	2.3509788121
Si	2.9343128586	–0.423689302	–0.0836564435
C	2.9685907682	–2.0283936197	0.9451792008
C	4.361247451	0.698847705	0.4940406465
N	–1.8885498351	–0.32656532	0.0713640106
C	3.215092843	–0.8721204966	–1.9159116654
C	–2.7112128996	–1.5198977121	–0.1349335365
C	–2.4931209812	0.8465807851	–0.5574260894
C	–3.9029492382	1.1179424804	–0.0197991732
C	–0.4992695189	–0.5557799845	–0.3525045544
C	–4.1231066761	–1.3424859816	0.4327098039
C	–4.8068667448	–0.1110040128	–0.1741980275
H	0.5966696475	0.3059531957	2.6570412597

C	0.8839973683	2.2691309818	–0.9103654255
H	3.9413744506	–2.5296451854	0.84215552
H	2.1944565383	–2.738983338	0.6211233835
H	2.8107057524	–1.8267086183	2.0144088201
H	5.327589827	0.1901828341	0.3608229424
H	4.2643039051	0.9581039663	1.557903128
H	4.3962370969	1.6375350357	–0.0771498469
H	4.1945474081	–1.3518746051	–2.0496403503
H	3.1905512155	0.0201265093	–2.557825257
H	2.4499835215	–1.5706982296	–2.2838586843
H	–2.2132056507	–2.3658480239	0.3575022223
H	–2.7774720586	–1.7734664735	–1.2171644053
H	–2.5357950612	0.723753691	–1.6631627864
H	–1.8556434311	1.7155503547	–0.3632052963
H	–4.3279750669	1.9844955302	–0.5465343215
H	–3.8287891183	1.390491752	1.0421472719
H	–0.1895029745	–1.5144819606	0.0907903665
H	–0.4356834181	–0.7068803876	–1.4537611704
H	–4.7104995099	–2.2519290026	0.2376857748
H	–4.0533685683	–1.2263573913	1.5230989842
H	–5.7856274419	0.064409976	0.2973224174
H	–4.9976908457	–0.2919094799	–1.2433822339
H	–0.4002087483	1.6750691577	2.1306286587
H	1.7992219696	2.8500490571	–0.726421007
H	0.0346595222	2.9365692656	–0.7150712569
H	0.8691295604	2.0093834109	–1.9790128844

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