

Supporting information

Catalytic activity of silicene bilflake for CO₂ reduction: A theoretical approach

Wilmer E. Vallejo Narváez*, Cesar Gabriel Vera de la Garza, Serguei Fomine*

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México,
Apartado Postal 70-360, CU, Coyoacán, México DF 04510, México.

*E-mail: wilmervall@comunidad.unam.mx
fomine@unam.mx

Table of Contents

1. NBO analysis.....	3
2. CO ₂ chemisorption on silicene monoflake	5
3. Hydrogen absorption on silicene biflake.....	6
4. XYZ coordinates.....	7
3.1 Mechanism with catalyst (silicene biflake).....	7
3.2 Hydrogen absorption on silicene biflake	135
3.2 CO ₂ chemisorption on silicene monoflakes	144

1. NBO analysis

This analysis was carried out for silicene nanoflake (Figure 1 in the manuscript) to know the hybridization of silicon atoms. In the center of the nanoflake, Si (61,19) and Si (23, 65), the percentage of occupation is *s* orbital (26.42%), *p* orbital 2.77(73.29%) and *d* orbital 0.01(0.29%). This character is closer to sp^3 hybridization (25 % *s* and 75 % *p*).

Table S1 NBO analysis for silicene nanoflake.

Atom No	Natural Electron Configuration
Si 1	[core]3S(0.58)3p(1.33)3d(0.01)
Si 2	[core]3S(0.58)3p(1.33)3d(0.01)
Si 3	[core]3S(0.60)3p(1.44)3d(0.01)
Si 4	[core]3S(0.58)3p(1.31)3d(0.01)
Si 5	[core]3S(0.60)3p(1.44)3d(0.01)
Si 6	[core]3S(0.58)3p(1.30)3d(0.01)
Si 7	[core]3S(0.60)3p(1.44)3d(0.01)
Si 8	[core]3S(0.58)3p(1.33)3d(0.01)
Si 9	[core]3S(0.59)3p(1.35)3d(0.01)
Si 10	[core]3S(0.60)3p(1.44)3d(0.01)
Si 11	[core]3S(0.59)3p(1.40)3d(0.01)
Si 12	[core]3S(0.59)3p(1.40)3d(0.01)
Si 13	[core]3S(0.59)3p(1.40)3d(0.01)
Si 14	[core]3S(0.58)3p(1.33)3d(0.01)
Si 15	[core]3S(0.58)3p(1.31)3d(0.01)
Si 16	[core]3S(0.59)3p(1.40)3d(0.01)
Si 17	[core]3S(0.59)3p(1.40)3d(0.01)
Si 18	[core]3S(0.59)3p(1.40)3d(0.01)
Si 19	[core]3S(0.60)3p(1.44)3d(0.01)
Si 20	[core]3S(0.58)3p(1.30)3d(0.01)
Si 21	[core]3S(0.59)3p(1.40)3d(0.01)
Si 22	[core]3S(0.59)3p(1.40)3d(0.01)
Si 23	[core]3S(0.59)3p(1.40)3d(0.01)
Si 24	[core]3S(0.60)3p(1.44)3d(0.01)
Si 25	[core]3S(0.59)3p(1.40)3d(0.01)
Si 26	[core]3S(0.59)3p(1.40)3d(0.01)
Si 27	[core]3S(0.59)3p(1.40)3d(0.01)
Si 28	[core]3S(0.60)3p(1.44)3d(0.01)
Si 29	[core]3S(0.58)3p(1.30)3d(0.01)
Si 30	[core]3S(0.60)3p(1.44)3d(0.01)
Si 31	[core]3S(0.59)3p(1.40)3d(0.01)

Si 32 [core]3S(0.59)3p(1.40)3d(0.01)
Si 33 [core]3S(0.59)3p(1.40)3d(0.01)
Si 34 [core]3S(0.58)3p(1.31)3d(0.01)
Si 35 [core]3S(0.59)3p(1.40)3d(0.01)
Si 36 [core]3S(0.59)3p(1.40)3d(0.01)
Si 37 [core]3S(0.59)3p(1.40)3d(0.01)
Si 38 [core]3S(0.60)3p(1.44)3d(0.01)
Si 39 [core]3S(0.60)3p(1.44)3d(0.01)
Si 40 [core]3S(0.60)3p(1.44)3d(0.01)
Si 41 [core]3S(0.60)3p(1.44)3d(0.01)
Si 42 [core]3S(0.58)3p(1.33)3d(0.01)
Si 43 [core]3S(0.58)3p(1.30)3d(0.01)
Si 44 [core]3S(0.58)3p(1.31)3d(0.01)
Si 45 [core]3S(0.58)3p(1.33)3d(0.01)
Si 46 [core]3S(0.58)3p(1.33)3d(0.01)
Si 47 [core]3S(0.58)3p(1.33)3d(0.01)
Si 48 [core]3S(0.59)3p(1.35)3d(0.01)
H 49 1S(0.54)
H 50 1S(0.54)
H 51 1S(0.54)
H 52 1S(0.55)
H 53 1S(0.55)
H 54 1S(0.54)
H 55 1S(0.54)
H 56 1S(0.55)
H 57 1S(0.54)
H 58 1S(0.55)
H 59 1S(0.54)
H 60 1S(0.54)
H 61 1S(0.55)
H 62 1S(0.55)
H 63 1S(0.54)
H 64 1S(0.54)
H 65 1S(0.55)
H 66 1S(0.55)

2. CO₂ chemisorption on silicene monoflake

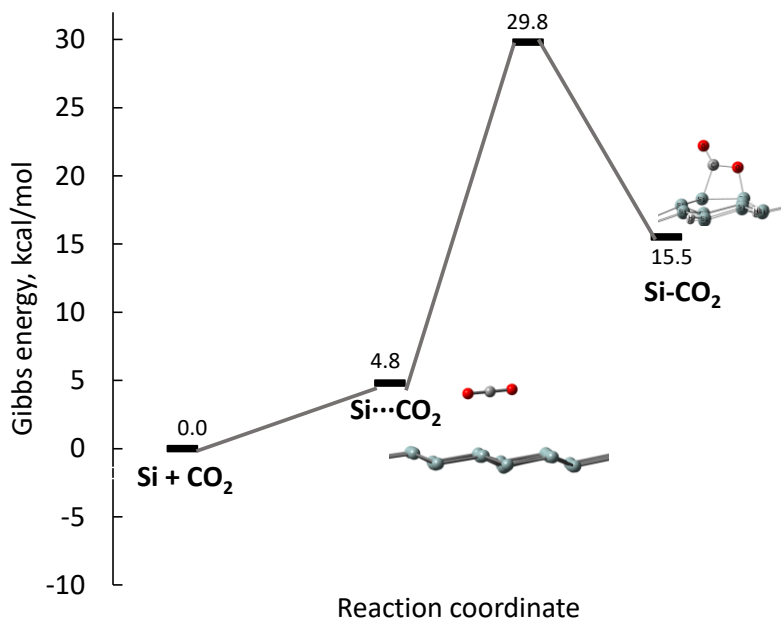


Fig S1 Potential energy profile for CO₂ chemisorption on silicene monoflake (**Si**). The level of theory used was TPSS-D3BJ/def2-SVP. This result is not included in reference 12 (in the manuscript).

3. Hydrogen absorption on silicene bflake

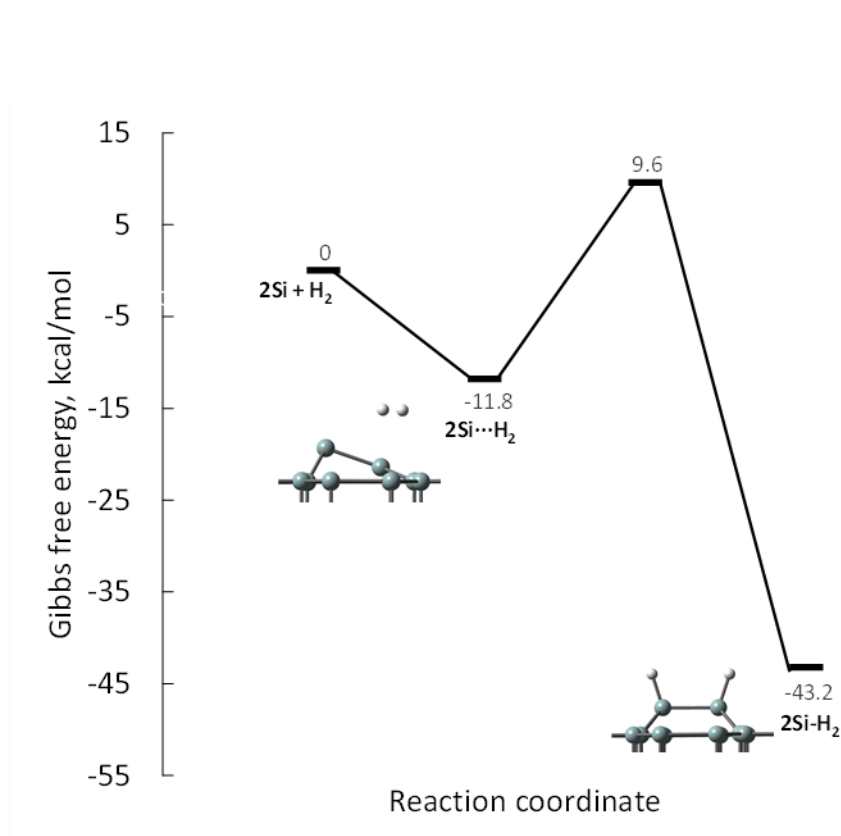


Fig S2 Potential energy profile for hydrogen absorption on silicene bflake (**2Si**).

4. XYZ coordinates

3.1 Mechanism with catalyst (silicene bilflake)

- **H₂**

H	0.0000000000000000	0.0000000000000000	0.37864129793633
H	0.0000000000000000	0.0000000000000000	-0.37864129793633

- **H₂O**

O	0.0000000000000000	0.000000000001365	0.12224060626212
H	0.0000000000000000	0.75884092207211	-0.48857330312557
H	0.0000000000000000	-0.75884092208576	-0.48857330313655

- **CO₂**

C	0.000000000003877	-0.00000000000811	0.00000000034625
O	-0.00000000001938	0.00000000000406	1.17218860700206
O	-0.00000000001938	0.00000000000406	-1.17218860734831

- **CO**

O	0.72386859160196	1.41630899000000	0.00000000000000
C	-0.41574507160196	1.41630899000000	0.00000000000000

- **OCH₂**

C	-0.96315130632712	0.19313304230275	0.00000016130101
O	-2.17147777496584	0.19313304104021	-0.00000005387991
H	-0.35778533121110	1.13974786524547	-0.00000005371055
H	-0.35778532749594	-0.75348177858843	-0.00000005371055

- **HCOOH**

C	-2.56625246748834	1.26938855444683	-0.00000013224816
H	-1.93379358788267	0.35474618035934	0.00000006501346
O	-3.77405473013434	1.29087521951131	0.00000003731286
O	-1.76905832553729	2.36013874680273	-0.00000000336594
H	-2.36664896895735	3.14015120887979	0.00000003328778

- **CH₃OH**

C	-1.27728454145703	1.48779440557192	0.01547922362659
H	-0.90383140730846	0.45006217043377	0.02693716166122
H	-0.91897691224943	1.96518289895033	-0.92247172536452
H	-2.38762161963671	1.44669334912690	-0.02275987825884
O	-0.78405557728129	2.11935654884887	1.18426808084891
H	-1.11083601206709	3.03576316706821	1.17962423748663

- **CH₄**

C	-5.61678135628583	3.93092889385665	-0.00000000028776
H	-5.24949026675156	2.89204824128707	0.00000000021861
H	-5.24947095693913	4.45034751626118	0.89969414926280
H	-5.24947095611715	4.45034751680583	-0.89969414976895
H	-6.71866805390632	3.93093235178927	0.00000000057529

- **2Si**

Si	1.20247474378435	8.21298850854550	-1.20203960607689
Si	-1.20236546242911	8.21301474466727	-1.20203961822291
Si	-2.39793987189789	6.16355900300848	-1.20166638849158
Si	-4.77579335653157	6.29519259348327	-1.20985574134475
Si	-5.82243081173303	4.15602772552052	-1.20200788272549
Si	-8.19501919903191	4.12542210841360	-1.20073360159736
Si	-9.35349527484054	2.02082242973923	-1.20224850739299
Si	2.39800217626514	6.16352043165584	-1.20166937880978
Si	-1.18163670616202	4.13898481715216	-1.20414484156356
Si	-4.66990377206239	2.09232673562123	-1.20304454661666
Si	-8.11720783104630	-0.00026208265043	-1.20330178716950
Si	4.77585386340981	6.29533030501847	-1.20986326918417
Si	1.18162640087755	4.13898165804908	-1.20413769639135
Si	-2.31278356074874	2.06917277021606	-1.19921618146178
Si	-5.76536404991747	-0.00015159172011	-1.20756432203831
Si	-9.35385971951136	-2.02110832931550	-1.20227014328981
Si	-8.19548251141777	-4.12575452676210	-1.20073593859385
Si	-4.67001480697544	-2.09269124566925	-1.20302715506820
Si	-1.17763104542885	0.00003628986566	-1.20231754863542
Si	2.31287807139730	2.06922444265666	-1.19921730252204
Si	5.82262047440966	4.15623650885827	-1.20201011811014
Si	4.66999927763184	2.09257089786833	-1.20303738090949
Si	1.17767351646792	0.00010517329939	-1.20231400429990
Si	-2.31289704534429	-2.06904679468343	-1.19923462321340
Si	-5.82288797978929	-4.15621174192479	-1.20203443123630

Si	8.19520093274564	4.12552543813750	-1.20072494960194
Si	9.35353859705463	2.02085471082503	-1.20224769725915
Si	5.76529938388506	0.00002244849502	-1.20756741995187
Si	2.31286454802670	-2.06901769418007	-1.19923141354859
Si	-1.18165597089288	-4.13881640299150	-1.20414421000559
Si	-4.77596500516839	-6.29523436347123	-1.20988443685167
Si	8.11714330910407	-0.00017259113792	-1.20329190652128
Si	4.66998419325965	-2.09253775965521	-1.20304588091685
Si	1.18159328972542	-4.13878604358010	-1.20414477470594
Si	-2.39812052879592	-6.16329587390971	-1.20170665357243
Si	9.35376595385924	-2.02103923706577	-1.20226078203527
Si	5.82278768814429	-4.15609952301162	-1.20204848814253
Si	2.39804677323940	-6.16327386711324	-1.20171589925789
Si	-1.20244885641653	-8.21268804844669	-1.20207626157564
Si	8.19537013354639	-4.12567803922071	-1.20073751732128
Si	4.77590176079170	-6.29515740965315	-1.20989756789788
Si	1.20238522097610	-8.21267489023015	-1.20208007121505
Si	1.20247881178076	8.21298549087714	1.20207342317193
Si	-1.20236092363978	8.21301122470808	1.20207859783399
Si	-2.39793494232098	6.16355606132353	1.20170163262882
Si	-4.77578969092330	6.29519454286307	1.20989861643816
Si	-5.82243058138265	4.15603382410258	1.20203800241090
Si	-8.19501629825192	4.12542844148134	1.20072234177315
Si	-9.35347943079777	2.02082359154476	1.20226910443775
Si	2.39800239640633	6.16351447983067	1.20169536353900
Si	-1.18163837020749	4.13897854280168	1.20416407543322
Si	-4.66992044859296	2.09232112021098	1.20302695808341
Si	-8.11721283830735	-0.00027132123518	1.20335479433576
Si	4.77585536203944	6.29531467254764	1.20988767215306
Si	1.18162596410140	4.13897676944050	1.20415269194933
Si	-2.31279229485817	2.06916664549350	1.19922685006830
Si	-5.76537164876465	-0.00016088773891	1.20754577019747
Si	-9.35385510255705	-2.02112065339339	1.20227099142843
Si	-8.19548695842354	-4.12577242196291	1.20070789829158
Si	-4.67001501962376	-2.09269684023774	1.20301893329817
Si	-1.17763007562963	0.00003440367467	1.20232403493894
Si	2.31288117163760	2.06922211640898	1.19922671576434
Si	5.82262874448524	4.15622896535853	1.20203798264156
Si	4.67000421779353	2.09256747209213	1.20302735235244
Si	1.17767677716135	0.00010571732653	1.20232254244945
Si	-2.31289576250196	-2.06905202553130	1.19923515708541
Si	-5.82289369020752	-4.15621239907291	1.20201821636327
Si	8.19520398726084	4.12552811813485	1.20073389467221
Si	9.35353687488062	2.02085804136614	1.20226486543845

Si	5.76530859333045	0.00001656061786	1.20753120969182
Si	2.31284923853089	-2.06902190342366	1.19922308948016
Si	-1.18165520132807	-4.13882243048394	1.20413065420820
Si	-4.77596620123541	-6.29522823192935	1.20985462646478
Si	8.11715734917288	-0.00017759339127	1.20336485410077
Si	4.66997810400290	-2.09254035934081	1.20300416470012
Si	1.18160117221733	-4.13879746515024	1.20413646776500
Si	-2.39812029098005	-6.16330664766407	1.20168041499732
Si	9.35375255324523	-2.02105897517683	1.20227472058931
Si	5.82278009316985	-4.15610145293727	1.20199930475307
Si	2.39805649146062	-6.16328953052345	1.20166733273724
Si	-1.20244061739997	-8.21269285084252	1.20204118616598
Si	8.19535980895662	-4.12569828612845	1.20070619256053
Si	4.77590727718250	-6.29515819347649	1.20983990446398
Si	1.20238947878459	-8.21268395691938	1.20203824175676
H	-1.75597781129002	9.33030874383997	2.03415601829368
H	-1.75598449407319	9.33031587498513	-2.03411065432537
H	5.39908749409495	7.35402309893217	-2.06771494285923
H	8.90228392840739	5.14752451792201	-2.03883312750749
H	8.90235244212588	-5.14779393373578	-2.03888882458004
H	5.39906755342164	-7.35384345814459	-2.06771836060915
H	1.75599142981910	-9.33001338991748	-2.03416284494812
H	-1.75604533696193	-9.33002765314719	-2.03416416422638
H	-5.39917195513426	-7.35394611783875	-2.06773111846100
H	-8.90250732911776	-5.14781930518964	-2.03885361737304
H	-8.90203202000284	5.14740876221332	-2.03882669477164
H	-5.39906362730864	7.35383199054494	-2.06769362403268
H	-5.39907992336110	7.35385809786625	2.06776393208494
H	-8.90204117088181	5.14745870764554	2.03883058349581
H	-8.90248686539955	-5.14781741775230	2.03879661445126
H	-5.39914347737120	-7.35391970269045	2.06766026067784
H	-1.75600082926484	-9.32997367669210	2.03408245426225
H	1.75595443141025	-9.32999477989317	2.03408666740098
H	5.39910508958656	-7.35388158265934	2.06766476449719
H	8.90231661212454	-5.14778700976233	2.03883878626187
H	8.90228926193654	5.14752235754995	2.03884296560280
H	5.39907551344207	7.35400912611472	2.06773086979473
H	1.75611463981510	9.33027359032741	-2.03411797058887
H	1.75612143499330	9.33026747403500	2.03415441076599
H	10.59127482904466	2.06786255311518	2.04450755121939
H	10.59127072967306	2.06784855174299	-2.04449570145431
H	10.59148377439335	-2.06795836414018	2.04456461873169
H	10.59146070999249	-2.06791322361768	-2.04452992877486
H	-10.59120005100337	2.06787006294049	2.04453095897393

H	-10.59127532973881	2.06785418473310	-2.04452976385854
H	-10.59159482939339	-2.06797272695400	-2.04458767091450
H	-10.59157984610531	-2.06799941272218	2.04456865450381

• **2Si...CO₂**

Si	1.19855271045677	8.23313366411815	-1.28383415028856
Si	-1.20687127024597	8.23242706579336	-1.28310242049485
Si	-2.40492587530552	6.18413283279655	-1.28761501750322
Si	-4.78366916946267	6.30122775710367	-1.29326915859053
Si	-5.81460269167557	4.15427513702566	-1.28784416911325
Si	-8.18668895499461	4.12172311637965	-1.28377758879926
Si	-9.33592958662051	2.01250065825806	-1.28449115830596
Si	2.39809279335705	6.18572337565747	-1.28933323941680
Si	-1.18397908993604	4.16222074091669	-1.29544924698599
Si	-4.65002734574799	2.09678242951252	-1.29310677142919
Si	-8.08906040940404	-0.00168283929098	-1.28870621419537
Si	4.77685255578082	6.30406038866883	-1.29669012235029
Si	1.17989157747111	4.16219054533756	-1.29630283967666
Si	-2.29233941047265	2.07971855149198	-1.29799392880120
Si	-5.73713380953280	-0.00114063693467	-1.29572494034598
Si	-9.33498244489166	-2.01645488346879	-1.28485689803568
Si	-8.18472808374376	-4.12513057464034	-1.28451055496747
Si	-4.64907644340077	-2.09858070404113	-1.29349750692805
Si	-1.17669592056467	-0.00018366251956	-1.32609215992936
Si	2.29236261656836	2.08190567008637	-1.29859145508410
Si	5.80997920215990	4.15815218418102	-1.29189247276519
Si	4.65010026818106	2.09802155564077	-1.29637061676498
Si	1.17936533652181	0.00025799035282	-1.32624744389330
Si	-2.29138319852608	-2.08058635726733	-1.29805753529745
Si	-5.81261390097921	-4.15664354482236	-1.28849619915650
Si	8.18225771846190	4.12665226440692	-1.28957051327276
Si	9.33405931202926	2.01855789965148	-1.29150236179502
Si	5.73917277826022	0.00129802098146	-1.29982929518031
Si	2.29327770249611	-2.08085857036126	-1.29883982031406
Si	-1.18207000654109	-4.16258885072870	-1.29591862159577
Si	-4.78077255851970	-6.30318849919576	-1.29425222773633
Si	8.09114434877013	0.00178257127151	-1.29473240589212
Si	4.65099507258458	-2.09587662589118	-1.29668984973864
Si	1.18176894974430	-4.16161325647090	-1.29690015035236
Si	-2.40208334186995	-6.18506293907829	-1.28845816366127
Si	9.33506646898657	-2.01436985053867	-1.29168490766748
Si	5.81193532652118	-4.15542517921952	-1.29228643601745
Si	2.40102782527316	-6.18451675652840	-1.29002842505652

Si	-1.20304309459793	-8.23277638413710	-1.28411134230328
Si	8.18420934313121	-4.12296733475553	-1.29001362092239
Si	4.77982742941676	-6.30182856647562	-1.29742654351756
Si	1.20238187041789	-8.23244962177902	-1.28479294958328
Si	1.19909105859323	8.22774597100347	1.12008383094288
Si	-1.20572081928607	8.22708159299878	1.12076461466020
Si	-2.40286759259656	6.17851855756280	1.11579915068410
Si	-4.78127974740649	6.29697037951604	1.12626298938246
Si	-5.81122275195878	4.15034233437424	1.11629033969131
Si	-8.18354659672562	4.11976533070085	1.11809720191958
Si	-9.33332070446674	2.01168237342986	1.11986286794711
Si	2.39792687586206	6.18007546393512	1.11398992340283
Si	-1.18253975581593	4.15715938018682	1.11156015766467
Si	-4.64603161662756	2.09400926713946	1.11201151403322
Si	-8.08573602263116	-0.00186483284648	1.11854095642536
Si	4.77622590502484	6.29993297808580	1.12299475924556
Si	1.18017975081071	4.15716455932798	1.11104582608871
Si	-2.28953229859206	2.07542515934987	1.10226751281595
Si	-5.73404617350150	-0.00134751511363	1.12023160650727
Si	-9.33236367780946	-2.01599907443354	1.11950696133246
Si	-8.18159804721443	-4.12354970516507	1.11736019484285
Si	-4.64508234425388	-2.09620306440209	1.11164453679812
Si	-1.17781297926983	-0.00030181586537	1.07420317522472
Si	2.29145539725800	2.07772255148462	1.10173368767469
Si	5.80842749275549	4.15429026081074	1.11217130718473
Si	4.64779232091284	2.09536342823110	1.10872388536199
Si	1.18251408206509	0.00015078633699	1.07316193124194
Si	-2.28859103160671	-2.07654925395399	1.10216275188446
Si	-5.80926248069003	-4.15310377576432	1.11561952378425
Si	8.18089426123018	4.12442950305338	1.11228979198235
Si	9.33340355766213	2.01757962914536	1.11275445815105
Si	5.73776512989450	0.00113672842739	1.11643859021757
Si	2.29236260921383	-2.07694849822808	1.10142818545519
Si	-1.18071769577815	-4.15782246186804	1.11107722605616
Si	-4.77843454175403	-6.29929002962679	1.12529867453257
Si	8.08955583650357	0.00165393004214	1.11250992305120
Si	4.64871026072151	-2.09357909255028	1.10841182657803
Si	1.18201461462591	-4.15686835580688	1.11042693602515
Si	-2.40007252265599	-6.17977129283232	1.11496038163110
Si	9.33438574153046	-2.01366175001638	1.11257456532497
Si	5.81038915060495	-4.15189070245396	1.11176149986333
Si	2.40081226890288	-6.17913669433665	1.11328973322561
Si	-1.20190858528284	-8.22774887236292	1.11975034344659
Si	8.18283059190951	-4.12102569476903	1.11184971073750

Si	4.77915718089593	-6.29796632232151	1.12225864905934
Si	1.20290387938129	-8.22735455639704	1.11911813538408
H	-1.76010262907829	9.34289786124761	1.95432391957050
H	-1.75936331984924	9.35372946716168	-2.11055704285798
H	5.40680452969856	7.36030300088740	-2.15273748132606
H	8.89071827003099	5.14717160285844	-2.12826694359551
H	8.89305117077134	-5.14312628228672	-2.12882609964731
H	5.41024352458820	-7.35767617158800	-2.15361715106856
H	1.75418833694637	-9.35384127042277	-2.11258533453439
H	-1.75496960344036	-9.35426882753980	-2.11169120879943
H	-5.41162545157821	-7.35888091772169	-2.15029035809933
H	-8.89383884355317	-5.14518671280853	-2.12319204285423
H	-8.89630475279448	5.14157439264768	-2.12228258459427
H	-5.41497442776966	7.35680313786645	-2.14912435973222
H	-5.41005532642257	7.35000706789807	1.98706706156913
H	-8.88802805243156	5.14057832545379	1.95976942650285
H	-8.88567038477414	-5.14480853220147	1.95883587209671
H	-5.40683083717487	-7.35269629319009	1.98592960850058
H	-1.75586325297625	-9.34391590970008	1.95312797425251
H	1.75753384826758	-9.34364795168955	1.95186991159747
H	5.40843019573997	-7.35131007669181	1.98234489524799
H	8.88798506321521	-5.14184586001920	1.95297332785657
H	8.88563585218398	5.14543930535449	1.95353285043740
H	5.40509868911645	7.35342022620945	1.98319776345297
H	1.74990833231366	9.35485201170498	-2.11148275202669
H	1.75322228826490	9.34420578729186	1.95294778273621
H	-10.57425449595092	-2.05717167817096	-2.12740349840782
H	-10.56976603949391	-2.05483669377983	1.96484951125874
H	-10.57075393830292	2.04973525878466	1.96519731147073
H	-10.57521696758326	2.05286233175264	-2.12703045929528
H	10.57289218136632	-2.05378633272820	1.95622652029988
H	10.57191669461761	2.05824616246515	1.95637404727749
H	10.57406613587206	-2.05642411743923	-2.13454720049444
H	10.57301999993318	2.06132486793136	-2.13438224759765
C	0.01849171364491	-0.00431425520540	4.37370277520454
O	1.19072869837652	-0.00529658604576	4.39966011206140
O	-1.15407178176609	-0.00335192380242	4.35228769980012

- **2Si-CO₂**

Si	-1.18267514224816	-8.02742476912802	-1.08741772772596
Si	1.20872678843749	-8.00896921984634	-1.08812799231105
Si	2.37621021031325	-5.94670540160543	-1.10026003379922
Si	4.73185959913967	-6.21313780849723	-1.19760606109273

Si 5.89001163227678	-4.13616222865108	-1.25374733831531
Si 8.26203401707588	-4.12626749869339	-1.44055566937854
Si 9.47879748964886	-2.05528073084962	-1.49218629768659
Si -2.36239578874461	-5.97349911923817	-1.10297600310661
Si 1.18271560453602	-3.91459970014715	-1.04449058062573
Si 4.80715713671105	-2.03456865570752	-1.14246229397284
Si 8.30664781971107	0.00126649859374	-1.40229175893900
Si -4.72192732500784	-6.22887554897421	-1.20830591196204
Si -1.16697685001764	-3.94150463099523	-1.06040440738664
Si 2.45135964896254	-1.94516218196800	-0.99121895068541
Si 5.96959732800540	0.00064695999508	-1.23517620177046
Si 9.47831808322805	2.05804577428720	-1.49199563331683
Si 8.26030488661708	4.12826007851914	-1.44007016205091
Si 4.80570072800867	2.03499477886458	-1.14194427995663
Si 1.13165130692233	-0.00081653140176	-0.68600174100331
Si -2.45244073520012	-1.98523178776283	-1.05061441055484
Si -5.88716665627492	-4.15582446014980	-1.26967483973188
Si -4.80569416748370	-2.05154315624495	-1.18739081416764
Si -1.19028632881433	0.00024046178894	-0.80669778572247
Si 2.45002253799132	1.94456397121934	-0.99047905380977
Si 5.88831176814525	4.13666180885957	-1.25327416343919
Si -8.25864667160626	-4.13793151241447	-1.43886485169552
Si -9.46642731337517	-2.05931058753615	-1.49254331999599
Si -5.95243797379701	-0.00054449660643	-1.26585391307953
Si -2.45356372733896	1.98504430935196	-1.05064497142675
Si 1.18083038535362	3.91370106629028	-1.04422934074378
Si 4.72954160650520	6.21324315997823	-1.19713146450028
Si -8.29539825395374	-0.00071729447125	-1.41138932651918
Si -4.80686977365941	2.05115152658671	-1.18762434312049
Si -1.16883312504336	3.94176636592812	-1.06030225739296
Si 2.37399652646202	5.94602653722189	-1.10005033256397
Si -9.46756500838532	2.05719429407508	-1.49292602417626
Si -5.88929029870747	4.15496234087573	-1.27028905116157
Si -2.36489995938502	5.97336446914106	-1.10328770568555
Si 1.20637830257366	8.00822766665204	-1.08829501112857
Si -8.26077587252681	4.13641727056784	-1.43948175053921
Si -4.72448781899790	6.22827700036651	-1.20893713052783
Si -1.18501356213626	8.02719712601703	-1.08773951485933
Si -1.19382489538622	-7.98971031916790	1.31573421449082
Si 1.22081776174671	-7.97665117063092	1.31607632139127
Si 2.44711793890424	-5.94565096532120	1.29985208888486
Si 4.82477754674282	-6.21959513996597	1.22206805956844
Si 6.07150487686499	-4.18888167016892	1.14068946295797
Si 8.43671648240905	-4.16865884565410	0.95366527355454

Si	9.62737714959867	-2.06950046418381	0.90770551362340
Si	-2.43732448905984	-5.96955878508151	1.29628864356129
Si	1.20091214159366	-3.91436546068719	1.37675064724934
Si	5.01611714232984	-2.09580506419823	1.25801568386891
Si	8.46059561050175	0.00113001205572	0.99564947503441
Si	-4.81643133216536	-6.23034130494198	1.21111470310438
Si	-1.20476344862786	-3.93256754520461	1.36486919584681
Si	2.67990573709735	-2.05632800752297	1.38645413361597
Si	6.11059453650174	0.00056130922315	1.17415674685823
Si	9.62677897782160	2.07204225856758	0.90791631219487
Si	8.43489802071895	4.17051071734164	0.95415798295785
Si	5.01446393386429	2.09611516371730	1.25856945797853
Si	1.65605726435078	-0.00070731214116	1.70042861974132
Si	-2.66339641751627	-2.06437557527468	1.33151072943185
Si	-6.05263910630473	-4.19171213476174	1.12619956888540
Si	-4.99862501467186	-2.09557329762472	1.21757305535605
Si	-1.62262100102650	0.00041851075175	1.56227359251175
Si	2.67816176708664	2.05598510869566	1.38722152160452
Si	6.06968370256839	4.18930990294041	1.14116453321665
Si	-8.41967833844959	-4.16968417171603	0.95698880676898
Si	-9.60724100741974	-2.06935595742242	0.90739195246518
Si	-6.09016333846132	-0.00046617540147	1.14736717405048
Si	-2.66480158382200	2.06434433242341	1.33152353502424
Si	1.19874876109762	3.91375211398353	1.37703978155947
Si	4.82229110361255	6.21964050862734	1.22251738778549
Si	-8.43959040383880	-0.00058396366445	0.98582503913592
Si	-4.99996015443394	2.09533917223354	1.21724528908339
Si	-1.20691932964158	3.93303843802190	1.36490833115731
Si	2.44468830406074	5.94521221526752	1.30005391493056
Si	-9.60844100025408	2.06749917508407	0.90700821767966
Si	-6.05482885678276	4.19101237538344	1.12558335397178
Si	-2.44006922405242	5.96964877496090	1.29600721167459
Si	1.21833375282929	7.97620353727891	1.31591822172011
Si	-8.42185578999556	4.16836763139567	0.95635100656692
Si	-4.81921089138311	6.23000086165914	1.21047021733538
Si	-1.19631437877768	7.98964896920611	1.31539596749326
H	1.73946655978382	-9.09710399739492	2.16724617876276
H	1.80586424786846	-9.10190703781745	-1.92195609171590
H	-5.22545458505442	-7.33887554807229	-2.07934234712797
H	-8.88882775193679	-5.16237670043456	-2.33328769893762
H	-8.89132153173715	5.16047187031008	-2.33409170075086
H	-5.22804090627855	7.33821268482810	-2.08004208016560
H	-1.76492744162491	9.12903639774490	-1.92178349694904
H	1.80372944634504	9.10103470079153	-1.92214789905871

H	5.23643206091909	7.31853661171435	-2.07212680417501
H	8.87576590579527	5.15579963510798	-2.34110333866859
H	8.87826185459659	-5.15323943087171	-2.34171182493353
H	5.23906477428953	-7.31831068567599	-2.07256946242079
H	5.39440848223383	-7.33098784861775	2.05011925275379
H	9.21322051256557	-5.20384960720211	1.70973561723264
H	9.21082152467825	5.20602991464662	1.71037868466264
H	5.39154170485893	7.33109255868987	2.05075384174824
H	1.73697926557796	9.09679348493253	2.16691657673645
H	-1.70290816116182	9.11261800606916	2.17020543138459
H	-5.40200082284432	7.33643948376286	2.03589381362184
H	-9.19339225516070	5.20113429585519	1.72082145811202
H	-9.19098221701868	-5.20259488806208	1.72150827177054
H	-5.39880377183315	-7.33679109702804	2.03681672364459
H	-1.76289789389620	-9.12919990881803	-1.92133177691517
H	-1.70054075070620	-9.11255114699081	2.17064254600384
C	-0.60785818056927	-0.00044995961779	3.21082163186427
O	-1.22194597545749	0.00440343944802	4.25789328688165
O	0.74073790273961	-0.00170574714740	3.17888145079362
H	10.66901402229153	2.13292670565331	-2.40098734147682
H	10.91917665383605	2.17524746891606	1.66284825111515
H	10.91993519744444	-2.17222304914728	1.66243290217701
H	10.66960831453462	-2.12961183370057	-2.40108340578153
H	-10.89957593112709	2.16213709664536	1.66510685818117
H	-10.89831959093759	-2.16465200011710	1.66550685429582
H	-10.66153313245065	2.13455509925836	-2.39769314483684
H	-10.66038237471525	-2.13747082003217	-2.39726380209241

• **2Si-CO₂ + H₂**

Si	-1.14339024623262	-8.04984677808741	-1.16004314108279
Si	1.24851010272970	-8.03034999093155	-1.16726388781474
Si	2.41866965525407	-5.96920709557202	-1.16537410290307
Si	4.77595415490892	-6.22279509771427	-1.27128085166847
Si	5.92983742657824	-4.14271511409997	-1.31048090292316
Si	8.30119170523303	-4.13064853183064	-1.50323823937824
Si	9.51245753052790	-2.05632295803430	-1.53665988758359
Si	-2.33190040305194	-6.00062175244283	-1.15509639396155
Si	1.21416241268895	-3.94462880091548	-1.08568826543673
Si	4.83350722774317	-2.04977840409027	-1.17342636661671
Si	8.33338123352885	-0.00501656714055	-1.42079376225447
Si	-4.69237687087745	-6.25335435897526	-1.25424320898478
Si	-1.13525898453340	-3.96993848754043	-1.09549018424166
Si	2.47755366453665	-1.97235060001921	-1.01859028530589

Si	5.99680172179701	-0.01385083476583	-1.24837962049160
Si	9.49991466980118	2.05538573652924	-1.49314463371178
Si	8.27457349699620	4.12005105542524	-1.41640842991169
Si	4.81924753100159	2.01159306339737	-1.12972560631291
Si	1.15449807031861	-0.03456574502549	-0.69147031247083
Si	-2.42732057614587	-2.01863999528736	-1.06303990295962
Si	-5.86412547165927	-4.18338837720592	-1.29260673043470
Si	-4.78015661599546	-2.08165878528220	-1.19186643475454
Si	-1.16749671054149	-0.03429579376394	-0.79793447326984
Si	2.46441067112143	1.91848107004117	-0.97661720485270
Si	5.90345164626276	4.11303401273879	-1.22426892600688
Si	-8.23584679886122	-4.18011835686853	-1.45629737811688
Si	-9.45623561271445	-2.10867825796970	-1.48750040983864
Si	-5.94846402353607	-0.04251417526348	-1.25268987840628
Si	-2.43988463368615	1.94694812047365	-1.02479274883640
Si	1.19170495441986	3.88569371967846	-1.00510420778212
Si	4.74107602995590	6.18671066903019	-1.14383014268957
Si	-8.29223019056570	-0.04708345412694	-1.38863169063463
Si	-4.79324278661164	2.00253043538902	-1.15197105826505
Si	-1.15775906739966	3.90481872947976	-1.01690293203718
Si	2.38557723600809	5.91792746965827	-1.04394789649631
Si	-9.46709818654411	2.01006692987045	-1.44838334000256
Si	-5.88685575715958	4.10094063159064	-1.21391717084263
Si	-2.36369595515326	5.93076612017997	-1.03811050068354
Si	1.20718036992540	7.97385545097584	-1.00972948799910
Si	-8.25857625043988	4.08751033231409	-1.37777833613395
Si	-4.72519247330888	6.17548844058967	-1.13460366207486
Si	-1.18456776954414	7.98497183572543	-1.00418679070784
Si	-1.14810522145959	-8.03272566549663	1.24339626343803
Si	1.26700135182470	-8.01887333983011	1.23696340425983
Si	2.49668788832958	-5.98952538602354	1.23469953792023
Si	4.87595976069330	-6.25295894064728	1.14784671973707
Si	6.11742379673642	-4.21816055041728	1.08250655494283
Si	8.48198475369539	-4.19648885702950	0.89057340435717
Si	9.66825155752005	-2.09511952505372	0.86258877915502
Si	-2.40009887921800	-6.01713000547648	1.24447605094262
Si	1.23924283631562	-3.96634753496353	1.33518305363287
Si	5.04813871886198	-2.13390062574280	1.22544421830885
Si	8.49481733007706	-0.02956625366678	0.97686783183299
Si	-4.78022401665861	-6.27654856686607	1.16549091496487
Si	-1.16579255649313	-3.98186769771020	1.32991344751138
Si	2.71226592498314	-2.10473271038685	1.35827859209419
Si	6.14515371408875	-0.03807816288152	1.15921415902509
Si	9.65489100707463	2.04515708002895	0.90644393130333

Si	8.45443532398062	4.13756002625021	0.97828425647025
Si	5.03223574484848	2.04792897189936	1.27059923563732
Si	1.68092601296499	-0.05666502108829	1.69273304561137
Si	-2.63403437271799	-2.12065959051367	1.31995825864782
Si	-6.02368529960251	-4.24143507482691	1.10245742176660
Si	-4.96736774498136	-2.14785243612090	1.21363218006316
Si	-1.59898228825271	-0.05654768254054	1.56910764365762
Si	2.69598239082056	2.00669553724809	1.40253864860210
Si	6.08972700992151	4.14073246133294	1.16977724235659
Si	-8.39084116765623	-4.23504754193731	0.94028660174934
Si	-9.59103131489845	-2.14198849046428	0.91266812226965
Si	-6.08057536879596	-0.06589425095574	1.15906107045321
Si	-2.64797998128354	2.00401894946959	1.35972883436546
Si	1.21524248439289	3.86334149969293	1.41596057595148
Si	4.83993376753202	6.16872799238846	1.27538921828141
Si	-8.43065069448356	-0.07004073681773	1.00922908853791
Si	-4.98139615533192	2.02192552707283	1.25403557443939
Si	-1.18981768739826	3.87183320191117	1.40827536414737
Si	2.46179904495482	5.89483421675998	1.35600043054793
Si	-9.60208597707478	1.99718511309722	0.95198204496342
Si	-6.04688808838654	4.11248421082326	1.18174717352628
Si	-2.43264053116188	5.90300037849875	1.36126600015802
Si	1.22452426093897	7.91937395774593	1.39397612130706
Si	-8.41413436206706	4.09631386763809	1.01925505553555
Si	-4.81391091350215	6.15217101591873	1.28510229725380
Si	-1.19066218461261	7.92428554558399	1.39863267223679
H	1.78621726162677	-9.14843339289298	2.07571279716546
H	1.84152684282085	-9.11789404445401	-2.01109022240624
H	-5.19695263468329	-7.35623121554390	-2.13377838243598
H	-8.86004290233658	-5.20144774927454	-2.35849070299551
H	-8.88850797387595	5.12217596632808	-2.26057376564195
H	-5.23352813322658	7.29336286919643	-1.99276227252964
H	-1.76664574102375	9.09581042445375	-1.82476730116678
H	1.79699702653347	9.07866762551326	-1.83311786477056
H	5.24395316164632	7.30184925889661	-2.00861979473575
H	8.88109283288238	5.16115043598337	-2.30787397896144
H	8.91471631428672	-5.14873419885541	-2.41622181950570
H	5.28403024979307	-7.31824603964567	-2.15795236391743
H	5.45067879048883	-7.37159427098613	1.96256753294815
H	9.25847192256473	-5.24009786316113	1.63497039739390
H	9.22442073450459	5.17003903033457	1.74466237461527
H	5.41015547391068	7.27255025248839	2.11316580346009
H	1.73933797893636	9.03523575322767	2.25353310907110
H	-1.69734568402444	9.03870695063791	2.26458305271897

H	-5.39629859408888	7.24932032516042	2.12322646836823
H	-9.17979956090403	5.12434109682723	1.79592496508001
H	-9.15071443638606	-5.28181914411413	1.69736104971568
H	-5.35622503654541	-7.39248983359727	1.98292808082706
H	-1.72229905990049	-9.14765274575469	-2.00020338933638
H	-1.64892496340302	-9.16574979615719	2.08840406288433
C	-0.57875630844953	-0.07120979352444	3.21639858404995
O	-1.17755993013032	-0.07707065841992	4.27436749707728
O	0.76832956025097	-0.07759585622911	3.17367124996558
H	-3.65266564925578	-0.08476735807770	4.09026644120483
H	-4.38845354835121	-0.08688492361766	3.89243350436921
H	-10.87934735802597	-2.24864325099321	1.67167540586514
H	-10.65155896169399	-2.18257951375114	-2.38892440044535
H	-10.89106508029133	2.08205661953693	1.71260594573535
H	-10.66300882974437	2.09475516852986	-2.34806961112242
H	10.96297248181784	-2.20045152396999	1.61095433898163
H	10.70055795742366	-2.11539788601526	-2.44843183509579
H	10.68752561426713	2.14111716196428	-2.40339211664188
H	10.94854918129278	2.14315670392027	1.65763050512872

• **2Si-CO₂ + H₂***

Si	1.13253402805152	8.03675722346917	-1.23073136217528
Si	-1.25950873462094	7.98427246419515	-1.22790257461577
Si	-2.38826871375551	5.90123653416434	-1.22813305200190
Si	-4.74642051188756	6.11301872874563	-1.24768140599604
Si	-5.73960064128356	3.96434038589089	-1.25930250416787
Si	-8.10676278261121	3.98957232290605	-1.29141791249462
Si	-9.24459627166852	1.89126267261175	-1.32102184085196
Si	2.33125412714159	5.99507079898006	-1.25503165293533
Si	-1.16578052892932	3.87915769622935	-1.21244901111106
Si	-4.49987649927891	1.94621627558230	-1.24610648295042
Si	-7.94781455450280	-0.08934734814635	-1.32351128295327
Si	4.68913095025520	6.22522919131837	-1.28433475682022
Si	1.18023387481553	3.93150511441058	-1.24745146367398
Si	-2.15559127634175	1.73556122177310	-1.25043937438665
Si	-5.59330815224730	-0.12391969488354	-1.30821239373799
Si	-9.21017070447357	-2.08108923838443	-1.38041977065128
Si	-7.90114005309042	-4.07319045253560	-1.41946780053554
Si	-4.24271008652414	-1.98713370238430	-1.67352591772705
Si	-1.01466961461522	-0.19648894271225	-1.82817942861605
Si	2.14520279881279	1.78429831411518	-1.30963751701244
Si	5.66696404882403	4.06592646367295	-1.32215384516615
Si	4.49798029642513	2.00547805894388	-1.32661296689791

Si	1.15612506724574	-0.03366726087740	-2.38347529717706
Si	-2.17678708080349	-2.03508394124425	-2.60956211361910
Si	-5.53642390547276	-3.91404292350192	-1.44063636907436
Si	8.03855035927866	4.06310310676702	-1.34919476977701
Si	9.24291506456236	1.99068415006094	-1.39330692235905
Si	5.65870780471334	-0.03483338751642	-1.39281753408839
Si	2.18700229033969	-1.86085798644058	-1.35626677650623
Si	-1.20069754670432	-3.79649790253075	-1.45683200773066
Si	-4.56914936689442	-6.07148903618481	-1.43812498536196
Si	8.01157247015745	-0.02786936190435	-1.40811437824865
Si	4.53608352978931	-2.10027325014449	-1.37908088083562
Si	1.14432897960708	-3.96967724747047	-1.38051088404605
Si	-2.21574343044693	-5.91808589169565	-1.45296004799317
Si	9.27142112460897	-2.02891695990523	-1.45145809433114
Si	5.73034104254532	-4.14116283357940	-1.43898757044873
Si	2.33049818489830	-6.02045011375350	-1.42948785077843
Si	-1.17537939079011	-8.03990755510840	-1.44905040895613
Si	8.10177708944684	-4.12265930795021	-1.46632489457188
Si	4.68951354958156	-6.26828863200852	-1.45560190753033
Si	1.21003878912507	-8.10371499232763	-1.45835729085856
Si	1.13929716695430	8.01304794624082	1.17455159904753
Si	-1.25706023580719	7.97553826275917	1.18083555817295
Si	-2.39241716692346	5.89830289377389	1.17601591158792
Si	-4.75572566299705	6.09764584285271	1.17990213464598
Si	-5.76483693458518	3.95571238766743	1.14255710410085
Si	-8.13091036379033	3.96972578068968	1.11516901603892
Si	-9.26701591562749	1.86553164243061	1.08432996217385
Si	2.34910618451354	5.97446654601905	1.14989148445475
Si	-1.16897628878878	3.87673034804114	1.18141018218462
Si	-4.52987797546332	1.94273364227118	1.13999533026792
Si	-7.97736689548455	-0.11994946555931	1.07689459168706
Si	4.71023241548181	6.19876297668713	1.13655682278482
Si	1.18480391377883	3.91251088093418	1.15018404379256
Si	-2.19035686571115	1.74825075872327	1.17187317245265
Si	-5.62083651077141	-0.13391198527426	1.12550566582271
Si	-9.22124434862959	-2.12632752212431	1.02506070293340
Si	-7.89706421536807	-4.11003252030612	0.97717730844174
Si	-4.28793368072896	-2.01577936379934	1.41585198112989
Si	-1.11597980321025	-0.06567194101547	2.16720095207479
Si	2.19129701745992	1.78669833941252	1.11010199352538
Si	5.69525059580793	4.04154048136224	1.07892215460208
Si	4.53908865777126	1.97867066651098	1.07689404535313
Si	1.21382181885201	-0.10267250269186	2.03982938057016
Si	-2.21810536816829	-2.12538962736803	2.26597159206715

Si	-5.53583392459352	-3.93324870707341	0.96795874435180
Si	8.06770798909513	4.03411375979990	1.05241279716961
Si	9.26950172207019	1.95883532431227	1.01344015472590
Si	5.68918788290906	-0.06589793119888	1.02053171155165
Si	2.24827754865294	-1.93866755513100	1.07491254939466
Si	-1.19541983808233	-3.79061051730424	1.03457209956155
Si	-4.55671726066408	-6.08215386354985	0.96612015057409
Si	8.04119795841303	-0.06137854877276	0.99892366719136
Si	4.58376769576609	-2.13709011967020	1.02886119819082
Si	1.14855629137396	-4.00916672035117	1.01241951738355
Si	-2.20380735800030	-5.91898978557641	0.95056630434796
Si	9.30020031905627	-2.06357347995971	0.95483436763105
Si	5.76354109731479	-4.17928783643290	0.96327684565300
Si	2.34366381647246	-6.05679927034136	0.96841881248730
Si	-1.16449858956040	-8.04509264191756	0.95491088247921
Si	8.13459529458467	-4.15970670601706	0.93476978032117
Si	4.70554868545851	-6.29691762896029	0.96406132931471
Si	1.22084994912729	-8.13677660670794	0.94573029766471
H	-1.83489143536588	9.07062143558431	2.02521260545343
H	-1.86004699037734	9.07349497657214	-2.06396700982183
H	5.27943309144420	7.29287573329652	-2.15409167272194
H	8.70334638595321	5.11349984045323	-2.18667082755377
H	8.78070107543000	-5.13845605048680	-2.33425732551860
H	5.25688463901461	-7.33491897524613	-2.34204867380465
H	1.77887059592035	-9.17870450979697	-2.33373126345999
H	-1.81387474153140	-9.09235538514000	-2.30335920670576
H	-5.22504660735180	-7.06285739011377	-2.34947420300512
H	-8.46969196999759	-5.15806027137008	-2.28173351153951
H	-8.77745704631818	5.02683597105088	-2.13932217521643
H	-5.35301238935001	7.16490026671539	-2.12569570092276
H	-5.37389225026437	7.13695744053429	2.06471623139375
H	-8.83380898096971	4.98541953975417	1.96308078671447
H	-8.44829740276658	-5.22682043081328	1.80951092590543
H	-5.20132188048531	-7.07418964967999	1.88470437255374
H	-1.80746200833927	-9.09273605622485	1.81192196727367
H	1.77861806349760	-9.24445242702390	1.78668913042490
H	5.28375400408087	-7.37959175668879	1.82344716065070
H	8.83473096997228	-5.20140731789549	1.75365568226534
H	8.75694014406313	5.06140324321039	1.89860735739038
H	5.33286834090437	7.23342994974397	2.02343555430489
H	1.67667843414676	9.15686169283762	-2.06433082662248
H	1.68368840937845	9.11968256330188	2.02594304882411
C	0.70323113243676	0.16613608507185	3.94450770048386
O	1.31359609787879	0.25118588228692	4.97663603927650

O	-0.66709929739143	0.31451001033444	3.85537590139315
H	-10.41829421910604	-2.12030074143065	-2.26512013989998
H	-10.43519055031782	-2.23310390114484	1.89620603227732
H	-10.50754581022220	1.86023455340565	1.92464932721023
H	-10.46872329985129	1.88934581437090	-2.18516013714777
H	10.54171063794215	-2.11576323878832	1.79290329594411
H	10.50883089985239	2.00819687826548	1.85494828291202
H	10.49404721461664	-2.05807364114018	-2.31823188614513
H	10.46409402534331	2.06486717579800	-2.25937418559485
H	-3.92766191909337	0.73405913884921	4.15644683767378
H	-3.21569280401742	0.66270915751592	4.41303890721909

- **2Si-COOH**

Si	-1.20335400	-7.95441000	-0.97794800
Si	1.18319600	-8.08207300	-1.02316900
Si	2.42492500	-6.06408200	-1.08509400
Si	4.78275800	-6.28425300	-1.26372500
Si	5.90413300	-4.18092500	-1.33665100
Si	8.27405500	-4.10426200	-1.56959400
Si	9.42257400	-1.99200900	-1.59439000
Si	-2.32080500	-5.86428900	-0.98262600
Si	1.23353700	-4.03795200	-1.00443400
Si	4.78486700	-2.08910500	-1.18989100
Si	8.20937700	0.03483000	-1.42522300
Si	-4.67814400	-6.08501900	-1.05232800
Si	-1.09874900	-3.85202200	-0.96565300
Si	2.41892900	-2.02696000	-1.01022100
Si	5.87508400	-0.00880300	-1.21947300
Si	9.35792700	2.10464500	-1.48429300
Si	8.06164900	4.11749700	-1.37319200
Si	4.59635000	1.94514500	-1.04655600
Si	0.98731200	-0.14670800	-0.67331900
Si	-2.33830600	-1.86666500	-0.94403000
Si	-5.79216000	-3.99587000	-1.13312700
Si	-4.67047500	-1.91833900	-1.07847000
Si	-1.31919900	0.27556300	-0.85185300
Si	2.25116600	1.84987700	-0.82913900
Si	5.70127600	4.02771800	-1.14860100
Si	-8.14963100	-4.03259600	-1.34755400
Si	-9.32539700	-1.95102300	-1.48485800
Si	-5.78199000	0.13762000	-1.18524800
Si	-2.25334900	1.89651800	-2.30591400
Si	0.94445300	3.79855200	-0.86942500

Si	4.53081000	6.08337400	-1.07466100
Si	-8.12217900	0.09137800	-1.42784000
Si	-4.32057300	2.01180500	-1.13827800
Si	-1.40753700	3.63680300	-0.96557900
Si	2.18214100	5.80549800	-0.98254400
Si	-9.37407300	2.08371500	-1.61940700
Si	-5.69561300	3.95828900	-1.29731500
Si	-2.32810600	5.81506100	-1.08260400
Si	1.15236900	7.92994400	-1.04133900
Si	-8.05241300	4.07728700	-1.59171700
Si	-4.66757400	6.09616800	-1.26101800
Si	-1.22417800	7.91312300	-1.09472800
Si	-1.17735800	-7.90066700	1.42524200
Si	1.23813300	-8.02672800	1.37870800
Si	2.56418700	-6.06150900	1.31612900
Si	4.94147100	-6.31801800	1.15318300
Si	6.14417900	-4.26362700	1.05242500
Si	8.50278800	-4.18783400	0.81859000
Si	9.63323000	-2.05682000	0.80031600
Si	-2.36520300	-5.84004900	1.41345200
Si	1.31368500	-4.03559800	1.40464900
Si	5.07469000	-2.18549800	1.19426400
Si	8.41484100	-0.02007100	0.97009700
Si	-4.75526900	-6.04950100	1.36942600
Si	-1.07861000	-3.83179500	1.46273400
Si	2.75826800	-2.17250200	1.35224000
Si	6.06906600	-0.04930300	1.18830000
Si	9.52791000	2.07574300	0.91311000
Si	8.25960700	4.12841700	1.02188500
Si	4.83447500	1.97324900	1.35317600
Si	1.64961200	-0.17724200	1.62757300
Si	-2.54676700	-1.95329600	1.43630100
Si	-5.98022700	-4.00692000	1.25960200
Si	-4.88943300	-1.92300800	1.32994100
Si	-1.71113600	0.26688400	1.55010300
Si	2.48014700	1.98744500	1.54919000
Si	5.89763500	4.06614900	1.24436400
Si	-8.34292400	-4.00367900	1.04787700
Si	-9.52005200	-1.90217300	0.91112900
Si	-6.01537400	0.14614200	1.20876400
Si	-2.77582600	2.14094800	2.45766300
Si	0.98059700	3.83904700	1.52564900
Si	4.63021500	6.08539800	1.34554200
Si	-8.35824100	0.16466200	0.96480200

Si	-4.74338000	2.12227300	1.25967600
Si	-1.41800700	3.78414800	1.49623300
Si	2.24524800	5.86293100	1.41775900
Si	-9.60048800	2.17547000	0.77141900
Si	-5.98037400	4.09365400	1.07983800
Si	-2.46211700	5.90183700	1.30495500
Si	1.12971100	7.95368500	1.36372200
Si	-8.32559000	4.20559000	0.79363600
Si	-4.82700400	6.16228100	1.14938400
Si	-1.27425700	7.94629700	1.30893800
H	1.70426800	-9.16821700	2.23226100
H	1.70435300	-9.21527200	-1.85381200
H	-5.21063700	-7.18617300	-1.91740800
H	-8.73473300	-5.09300400	-2.23013400
H	-8.55747100	5.11455200	-2.54907500
H	-5.16867600	7.15822800	-2.19303500
H	-1.83451100	8.96499000	-1.97017200
H	1.81251000	8.96478100	-1.90058400
H	5.02208100	7.19371700	-1.95248600
H	8.60272600	5.19378300	-2.26474800
H	8.90814000	-5.08629100	-2.50760700
H	5.28008600	-7.38323900	-2.15205300
H	5.55981100	-7.43186000	1.94210200
H	9.30696500	-5.22671400	1.53931800
H	9.01776800	5.16792200	1.79140000
H	5.21218700	7.18208700	2.18573000
H	1.65048300	9.07563800	2.21200100
H	-1.83396600	9.06669800	2.13397000
H	-5.44213400	7.24702800	1.98366400
H	-9.03657700	5.31749200	1.50490200
H	-9.12890200	-5.00294600	1.84240000
H	-5.32951800	-7.12825500	2.23765900
H	-1.86016700	-9.03316900	-1.78497200
H	-1.71067900	-9.00482200	2.28927100
C	-0.59132200	-0.08831800	3.09091500
O	-1.14656300	-0.12429000	4.29369800
O	0.64359400	-0.42073600	3.11011000
H	-2.06980800	0.21428500	4.21834700
H	-2.85502100	2.05204800	3.96138000
H	-10.49565700	-2.01818700	-2.41960200
H	-10.82135600	-1.97991000	1.65294000
H	-10.89805100	2.28699700	1.51416700
H	-10.52032500	2.12007800	-2.58414900
H	10.81802600	2.20201400	1.66665300

H 10.94718500 -2.14253700 1.51792400
H 10.59579600 -2.00934600 -2.52759300
H 10.52869800 2.22159400 -2.41273200

• **2Si-CO-OH**

Si 1.14573946982623 8.04838558052563 -1.32727257023344
Si -1.24538826897019 8.00820582844402 -1.33913245175978
Si -2.36714613738341 5.92385266608734 -1.33436828739229
Si -4.72303795726032 6.12654317289078 -1.36682350400660
Si -5.67614801167428 3.96411950227038 -1.35020262845500
Si -8.04491337776342 3.99479452047193 -1.39113125757397
Si -9.23477833059404 1.92131174099476 -1.40343934657691
Si 2.33764085777925 6.00129860359048 -1.30216701009666
Si -1.15993945258624 3.88743919923825 -1.29830984071770
Si -4.45437134563995 1.93753879942104 -1.31387594436360
Si -7.98312847075359 -0.08408451596291 -1.37265482212061
Si 4.69315067847365 6.24131236333140 -1.31318998766927
Si 1.18651585806960 3.93324837629988 -1.29180815857865
Si -2.09770298733202 1.71755446365242 -1.34263127380468
Si -5.62866674471347 -0.08715372937226 -1.31358141824183
Si -9.26118276272251 -2.06709869424337 -1.40326139266285
Si -7.92705420643490 -4.04682714326330 -1.39469762605271
Si -4.17919965162322 -1.94914243657794 -1.31133063052003
Si -0.97181955402940 -0.22101273719814 -1.95783511892135
Si 2.07234898957630 1.74412111521554 -1.36476791003754
Si 5.64381011282118 4.07225488954534 -1.31553270335797
Si 4.42624689154531 2.03461550348079 -1.29545145686716
Si 1.19370038360208 0.02531000793427 -2.70102383959205
Si -2.25686699997233 -1.98237994264961 -2.64975906489993
Si -5.56256996757897 -3.87690821612944 -1.32615351134775
Si 8.01538646412516 4.06833979675158 -1.33278341619661
Si 9.21805652964487 1.99609867535498 -1.34296834790840
Si 5.60985171899188 0.00535434396380 -1.36288218157218
Si 2.11211073884063 -1.74726563672022 -1.45939443399986
Si -1.24657648442156 -3.69692673722726 -1.41324603482565
Si -4.60513387076077 -6.03701644245453 -1.37688634217046
Si 7.96485616363117 -0.00586932023566 -1.35045554417422
Si 4.46018221130350 -2.04167578944530 -1.34817292341079
Si 1.10767006440380 -3.88209392834951 -1.37085831858878
Si -2.24983455825021 -5.84670165682452 -1.37353183437541
Si 9.22711092474961 -2.00393006054761 -1.36488731395660
Si 5.67253946160847 -4.07236665143340 -1.37205669175736
Si 2.28208199680448 -5.94591830453693 -1.39239095467224

Si	-1.21330008092796	-7.96873485812823	-1.39515383272421
Si	8.04203391074909	-4.08651119368175	-1.36939243833708
Si	4.63907601095128	-6.20017865482689	-1.40236635744430
Si	1.17066607948488	-8.03703691014720	-1.40493751290909
Si	1.13685185381537	8.07239189984028	1.07687007939213
Si	-1.25741420770347	8.02305492076421	1.06807847445310
Si	-2.39303920956005	5.94625936609984	1.07128729312062
Si	-4.75158419857574	6.14888411629357	1.05897780955772
Si	-5.71820824507159	3.99124256742751	1.05478442863430
Si	-8.08569799496212	4.00539607303152	1.01423825722075
Si	-9.27970182237411	1.92930481558872	1.00142673429129
Si	2.34086903296284	6.03474720789872	1.10324705461520
Si	-1.19172239791549	3.90806543411595	1.09334132191386
Si	-4.50287492868892	1.96243754999275	1.07524664143279
Si	-8.03797291992812	-0.08367798174888	1.03559158833857
Si	4.69877273091729	6.25384038775253	1.10460318973323
Si	1.15362209881751	3.98947181047494	1.10781398381242
Si	-2.14795597643870	1.75060194391910	1.08043842360342
Si	-5.68101546296528	-0.06938261957869	1.07867885949504
Si	-9.30174931564799	-2.07853404816136	1.00198231325481
Si	-7.98778612196457	-4.07579796588893	1.00691956518324
Si	-4.30805846931296	-1.98067769141026	1.12977560005063
Si	-1.24326426272221	0.06339355386924	2.44162961507566
Si	2.15446369037924	1.87477259454072	1.07008808643038
Si	5.66606298613303	4.09173550538890	1.08461360649254
Si	4.49201714278510	2.03587336523264	1.11397793659678
Si	1.09142384362254	-0.02202627636977	1.98316833057036
Si	-2.27556851453395	-2.06421317926461	2.28468801484027
Si	-5.62573128666086	-3.93577832399760	1.06996829838924
Si	8.03564797069380	4.07406701326560	1.06847876039536
Si	9.22188409672336	1.99125329045043	1.06442824097155
Si	5.62388583287340	-0.01317046327910	1.05034062472244
Si	2.15179417674549	-1.87165061005552	0.97081697666323
Si	-1.23115891927769	-3.74282004185744	1.02637227848574
Si	-4.61899306357488	-6.07042734483555	1.03736318237827
Si	7.97760033630934	-0.01729169904361	1.05647367626928
Si	4.48875843974994	-2.06107186546792	1.06268937367724
Si	1.10230711224347	-3.94927658858757	1.03438223906152
Si	-2.26356835931906	-5.86634832430493	1.02507711646591
Si	9.23631298648768	-2.01640509690652	1.04197881059560
Si	5.67950373635955	-4.10508788334561	1.02958917055431
Si	2.29777658134711	-5.98689453939011	1.00526046236955
Si	-1.20635358322704	-7.98324055827854	1.01104860766075
Si	8.04916981363675	-4.09825775461441	1.03215072719992

Si	4.65249168556076	-6.23378744112179	1.01508132726913
Si	1.17699444019573	-8.06489150869574	0.99868617743705
H	-1.84435648999419	9.12000933930354	1.90415388918921
H	-1.83240952565885	9.09233586318127	-2.19126058710219
H	5.29826815121976	7.28851340226359	-2.19707491597782
H	8.67922351917546	5.11100400513630	-2.18025727459321
H	8.71675046534890	-5.12132141905893	-2.21757056039075
H	5.22245852071713	-7.25440860131880	-2.29282310732675
H	1.75402122268837	-9.11313848911792	-2.26963530518326
H	-1.84429142619091	-9.02563449699951	-2.25002435400933
H	-5.23133019157682	-7.05292860792821	-2.28489130128348
H	-8.48418254587599	-5.13438375635569	-2.26305532442707
H	-8.69437056136575	5.03980657693145	-2.24710378898446
H	-5.32900517619291	7.16129473594167	-2.26563276580643
H	-5.36776169337333	7.19979923852262	1.93209789827356
H	-8.77459269624666	5.04942223835213	1.84044069713381
H	-8.60388904689976	-5.16884734016688	1.82781693545487
H	-5.19479143772828	-7.12562175138657	1.93442558997764
H	-1.83157007131455	-9.04507688793231	1.86478108146554
H	1.75679240944079	-9.15591092000124	1.84686002407039
H	5.22466126221116	-7.30625243216700	1.89111566610500
H	8.72620508770653	-5.13688269580725	1.87408149648714
H	8.72490816344655	5.10787512756533	1.90672410306169
H	5.31737343437502	7.29126525362789	1.99114413754642
H	1.71245214428756	9.14400307063124	-2.17824961233960
H	1.67744049928213	9.19247807638236	1.91311957774851
C	1.76575335924826	-0.07258054282144	3.70072342757682
O	2.26542492707522	-0.10113073809869	4.74225931028459
O	-1.22583347261255	0.56617234949506	4.07013725450090
H	-10.46678065906227	-2.13254990319954	-2.29065198967155
H	-10.53269751056094	-2.16366755892741	1.85287068237663
H	-10.52600310544964	1.98929417533656	1.83200889663252
H	-10.45212788630459	1.95799102656772	-2.27656742878549
H	10.46661799154453	-2.06546980221289	1.89667416012151
H	10.44971117344081	2.03500355485044	1.92304822470522
H	10.45463816024223	-2.03889272134926	-2.22401838567457
H	10.44636791839303	2.05227290595054	-2.19993786659787
H	-2.42789920029106	-2.49330894253518	3.71481318291886
H	-2.08368633666843	0.48172146809368	4.52516830872141

- **2Si-CO-H₂O**

Si	1.14573946982623	8.04838558052563	-1.32727257023344
Si	-1.24538826897019	8.00820582844402	-1.33913245175978

Si	-2.36714613738341	5.92385266608734	-1.33436828739229
Si	-4.72303795726032	6.12654317289078	-1.36682350400660
Si	-5.67614801167428	3.96411950227038	-1.35020262845500
Si	-8.04491337776342	3.99479452047193	-1.39113125757397
Si	-9.23477833059404	1.92131174099476	-1.40343934657691
Si	2.33764085777925	6.00129860359048	-1.30216701009666
Si	-1.15993945258624	3.88743919923825	-1.29830984071770
Si	-4.45437134563995	1.93753879942104	-1.31387594436360
Si	-7.98312847075359	-0.08408451596291	-1.37265482212061
Si	4.69315067847365	6.24131236333140	-1.31318998766927
Si	1.18651585806960	3.93324837629988	-1.29180815857865
Si	-2.09770298733202	1.71755446365242	-1.34263127380468
Si	-5.62866674471347	-0.08715372937226	-1.31358141824183
Si	-9.26118276272251	-2.06709869424337	-1.40326139266285
Si	-7.92705420643490	-4.04682714326330	-1.39469762605271
Si	-4.17919965162322	-1.94914243657794	-1.31133063052003
Si	-0.97181955402940	-0.22101273719814	-1.95783511892135
Si	2.07234898957630	1.74412111521554	-1.36476791003754
Si	5.64381011282118	4.07225488954534	-1.31553270335797
Si	4.42624689154531	2.03461550348079	-1.29545145686716
Si	1.19370038360208	0.02531000793427	-2.70102383959205
Si	-2.25686699997233	-1.98237994264961	-2.64975906489993
Si	-5.56256996757897	-3.87690821612944	-1.32615351134775
Si	8.01538646412516	4.06833979675158	-1.33278341619661
Si	9.21805652964487	1.99609867535498	-1.34296834790840
Si	5.60985171899188	0.00535434396380	-1.36288218157218
Si	2.11211073884063	-1.74726563672022	-1.45939443399986
Si	-1.24657648442156	-3.69692673722726	-1.41324603482565
Si	-4.60513387076077	-6.03701644245453	-1.37688634217046
Si	7.96485616363117	-0.00586932023566	-1.35045554417422
Si	4.46018221130350	-2.04167578944530	-1.34817292341079
Si	1.10767006440380	-3.88209392834951	-1.37085831858878
Si	-2.24983455825021	-5.84670165682452	-1.37353183437541
Si	9.22711092474961	-2.00393006054761	-1.36488731395660
Si	5.67253946160847	-4.07236665143340	-1.37205669175736
Si	2.28208199680448	-5.94591830453693	-1.39239095467224
Si	-1.21330008092796	-7.96873485812823	-1.39515383272421
Si	8.04203391074909	-4.08651119368175	-1.36939243833708
Si	4.63907601095128	-6.20017865482689	-1.40236635744430
Si	1.17066607948488	-8.03703691014720	-1.40493751290909
Si	1.13685185381537	8.07239189984028	1.07687007939213
Si	-1.25741420770347	8.02305492076421	1.06807847445310
Si	-2.39303920956005	5.94625936609984	1.07128729312062
Si	-4.75158419857574	6.14888411629357	1.05897780955772

Si	-5.71820824507159	3.99124256742751	1.05478442863430
Si	-8.08569799496212	4.00539607303152	1.01423825722075
Si	-9.27970182237411	1.92930481558872	1.00142673429129
Si	2.34086903296284	6.03474720789872	1.10324705461520
Si	-1.19172239791549	3.90806543411595	1.09334132191386
Si	-4.50287492868892	1.96243754999275	1.07524664143279
Si	-8.03797291992812	-0.08367798174888	1.03559158833857
Si	4.69877273091729	6.25384038775253	1.10460318973323
Si	1.15362209881751	3.98947181047494	1.10781398381242
Si	-2.14795597643870	1.75060194391910	1.08043842360342
Si	-5.68101546296528	-0.06938261957869	1.07867885949504
Si	-9.30174931564799	-2.07853404816136	1.00198231325481
Si	-7.98778612196457	-4.07579796588893	1.00691956518324
Si	-4.30805846931296	-1.98067769141026	1.12977560005063
Si	-1.24326426272221	0.06339355386924	2.44162961507566
Si	2.15446369037924	1.87477259454072	1.07008808643038
Si	5.66606298613303	4.09173550538890	1.08461360649254
Si	4.49201714278510	2.03587336523264	1.11397793659678
Si	1.09142384362254	-0.02202627636977	1.98316833057036
Si	-2.27556851453395	-2.06421317926461	2.28468801484027
Si	-5.62573128666086	-3.93577832399760	1.06996829838924
Si	8.03564797069380	4.07406701326560	1.06847876039536
Si	9.22188409672336	1.99125329045043	1.06442824097155
Si	5.62388583287340	-0.01317046327910	1.05034062472244
Si	2.15179417674549	-1.87165061005552	0.97081697666323
Si	-1.23115891927769	-3.74282004185744	1.02637227848574
Si	-4.61899306357488	-6.07042734483555	1.03736318237827
Si	7.97760033630934	-0.01729169904361	1.05647367626928
Si	4.48875843974994	-2.06107186546792	1.06268937367724
Si	1.10230711224347	-3.94927658858757	1.03438223906152
Si	-2.26356835931906	-5.86634832430493	1.02507711646591
Si	9.23631298648768	-2.01640509690652	1.04197881059560
Si	5.67950373635955	-4.10508788334561	1.02958917055431
Si	2.29777658134711	-5.98689453939011	1.00526046236955
Si	-1.20635358322704	-7.98324055827854	1.01104860766075
Si	8.04916981363675	-4.09825775461441	1.03215072719992
Si	4.65249168556076	-6.23378744112179	1.01508132726913
Si	1.17699444019573	-8.06489150869574	0.99868617743705
H	-1.84435648999419	9.12000933930354	1.90415388918921
H	-1.83240952565885	9.09233586318127	-2.19126058710219
H	5.29826815121976	7.28851340226359	-2.19707491597782
H	8.67922351917546	5.11100400513630	-2.18025727459321
H	8.71675046534890	-5.12132141905893	-2.21757056039075
H	5.22245852071713	-7.25440860131880	-2.29282310732675

H	1.75402122268837	-9.11313848911792	-2.26963530518326
H	-1.84429142619091	-9.02563449699951	-2.25002435400933
H	-5.23133019157682	-7.05292860792821	-2.28489130128348
H	-8.48418254587599	-5.13438375635569	-2.26305532442707
H	-8.69437056136575	5.03980657693145	-2.24710378898446
H	-5.32900517619291	7.16129473594167	-2.26563276580643
H	-5.36776169337333	7.19979923852262	1.93209789827356
H	-8.77459269624666	5.04942223835213	1.84044069713381
H	-8.60388904689976	-5.16884734016688	1.82781693545487
H	-5.19479143772828	-7.12562175138657	1.93442558997764
H	-1.83157007131455	-9.04507688793231	1.86478108146554
H	1.75679240944079	-9.15591092000124	1.84686002407039
H	5.22466126221116	-7.30625243216700	1.89111566610500
H	8.72620508770653	-5.13688269580725	1.87408149648714
H	8.72490816344655	5.10787512756533	1.90672410306169
H	5.31737343437502	7.29126525362789	1.99114413754642
H	1.71245214428756	9.14400307063124	-2.17824961233960
H	1.67744049928213	9.19247807638236	1.91311957774851
C	1.76575335924826	-0.07258054282144	3.70072342757682
O	2.26542492707522	-0.10113073809869	4.74225931028459
O	-1.22583347261255	0.56617234949506	4.07013725450090
H	-10.46678065906227	-2.13254990319954	-2.29065198967155
H	-10.53269751056094	-2.16366755892741	1.85287068237663
H	-10.52600310544964	1.98929417533656	1.83200889663252
H	-10.45212788630459	1.95799102656772	-2.27656742878549
H	10.46661799154453	-2.06546980221289	1.89667416012151
H	10.44971117344081	2.03500355485044	1.92304822470522
H	10.45463816024223	-2.03889272134926	-2.22401838567457
H	10.44636791839303	2.05227290595054	-2.19993786659787
H	-2.42789920029106	-2.49330894253518	3.71481318291886
H	-2.08368633666843	0.48172146809368	4.52516830872141

• **2Si-HCOOH**

Si	-1.18202400633036	-8.03952148979941	-1.07993295352590
Si	1.20770268932462	-7.97159967826550	-1.05141626187628
Si	2.35221221684135	-5.89708974255549	-1.02673532883939
Si	4.70700959386633	-6.16108102463070	-1.09736446592287
Si	5.82253461964034	-4.06783052012340	-1.16022596343555
Si	8.19143353743500	-4.09610355277387	-1.34076266104330
Si	9.44357591728411	-2.05239875686329	-1.43632806896740
Si	-2.38463215822380	-5.99903755535598	-1.11409212625906
Si	1.14805364746641	-3.86556598631671	-1.00404877891348
Si	4.72339636708017	-1.97737763850358	-1.07549592530095

Si	8.27345327227421	0.00446743888117	-1.39481993077874
Si	-4.74242020225066	-6.26236474358719	-1.25083295477525
Si	-1.19823013578058	-3.96309286125790	-1.05147647867303
Si	2.37736136980282	-1.86909000164076	-0.89885293589557
Si	5.93575233202766	0.02313727129062	-1.23279333648474
Si	9.46779273864824	2.04516387095073	-1.53410059686907
Si	8.31542894190851	4.15653661599030	-1.52395998182736
Si	4.86175682229815	2.11279239123068	-1.21020115003765
Si	1.14276986249620	0.13246561663702	-0.69809554505517
Si	-2.49121991292813	-2.01723449915466	-1.04688225352359
Si	-5.92445179976467	-4.19468758824608	-1.30286299246089
Si	-4.84850790983211	-2.08667743035961	-1.18569491326165
Si	-1.17197746383671	-0.08400357691500	-0.68648248852150
Si	2.49851239765492	2.03675961082672	-1.08305893386766
Si	5.94265026027355	4.21994475419107	-1.33743502553063
Si	-8.29667088796490	-4.14275097432379	-1.50046118532428
Si	-9.48103880607559	-2.04897584323996	-1.52738767081158
Si	-5.96534827202618	-0.02066377896034	-1.23863218756967
Si	-2.41215320000954	1.91265457076229	-0.96248263486739
Si	1.21997731589086	3.99427483341629	-1.06437022719035
Si	4.76191603978886	6.29106662414815	-1.28327610924620
Si	-8.30419298816430	0.00234555371078	-1.40376731379980
Si	-4.75981669858190	1.98668890276876	-1.11479345020641
Si	-1.12702614421434	3.87167636539516	-1.03224934310085
Si	2.40412693327817	6.02946122867250	-1.13794037494031
Si	-9.45406876578612	2.07135072608426	-1.46230960446733
Si	-5.83327418469860	4.09125917615944	-1.19443055873742
Si	-2.32364523885545	5.90343679711244	-1.06296020096308
Si	1.19588975873702	8.06767446473989	-1.09558653808374
Si	-8.20186188522449	4.11823943309084	-1.37812441399293
Si	-4.67893136890361	6.16575407140574	-1.13213695283679
Si	-1.19333690439628	7.98511914567707	-1.06572293397423
Si	-1.21891560070369	-8.00451679255123	1.32275232581271
Si	1.19532868505996	-7.95650726489896	1.35267653046526
Si	2.40092687211888	-5.91247137032291	1.37168467327172
Si	4.78161890116428	-6.14426430100323	1.32030906451282
Si	5.98657659717271	-4.08744239395902	1.23542246213666
Si	8.35375160915692	-4.09678633441190	1.05439045767966
Si	9.57909114864107	-2.01925998879343	0.96430421053643
Si	-2.49012949934853	-6.00321141915847	1.28528088450366
Si	1.15009778764111	-3.88699423205115	1.41351814751397
Si	4.90586491669805	-1.99660516704031	1.33064147920772
Si	8.42932839666188	0.05610649053214	1.00242819956285
Si	-4.86593760908894	-6.28966149082045	1.16966720841781

Si	-1.26566117046434	-3.96298197411219	1.36548933011555
Si	2.55004662759753	-1.95551126773949	1.48561398035233
Si	6.08053807116197	0.06163832489788	1.17865314992415
Si	9.63093703128018	2.10522982768060	0.86510593104947
Si	8.49963852144667	4.23582325370344	0.86725835241071
Si	5.09580191586271	2.20487672181533	1.18425532173579
Si	1.62295834522925	0.19293491663523	1.68989526563040
Si	-2.76224417137334	-2.12765515127502	1.32973739351688
Si	-6.12426398421758	-4.26561174340014	1.08782805455667
Si	-5.08658755230292	-2.16746412278174	1.21232118134308
Si	-1.65784241391405	-0.13180882004675	1.69292888298739
Si	2.77592948061429	2.15350378862039	1.28959310876458
Si	6.13698010167353	4.29927122019035	1.05624682277181
Si	-8.48757446131340	-4.21261702129807	0.89120413581983
Si	-9.64323820473536	-2.09333254311433	0.87150856368922
Si	-6.11344012643969	-0.04175857730508	1.17367203232512
Si	-2.60035499722404	1.98813207093742	1.41742382152874
Si	1.28435338801207	3.98671048239619	1.35728572082356
Si	4.88540779655135	6.32600890281635	1.13618789945717
Si	-8.46246998902736	-0.03121628602733	0.99198974404773
Si	-4.94731400870648	2.01883926310564	1.29121434072783
Si	-1.12043962359121	3.85591917699802	1.39916614925711
Si	2.51158253974363	6.02708898414292	1.26205656652855
Si	-9.59821133692206	2.05316824776941	0.93787085450864
Si	-6.00073440656888	4.11829141579370	1.20079729451135
Si	-2.36750242933879	5.89055047046372	1.33548977939983
Si	1.23414167574000	8.02338047043999	1.30643350207079
Si	-8.36790532366855	4.12993036080539	1.01779342595622
Si	-4.74904767454362	6.14802525263682	1.28707047201160
Si	-1.17947366861768	7.94692211694348	1.33850310493650
H	1.71618096319445	-9.07992693152165	2.19870016495261
H	1.83771376227956	-9.04694278377352	-1.88396695478956
H	-5.22966580174821	-7.37230543798836	-2.13150407596511
H	-8.93281565456136	-5.14089015399644	-2.42009910675834
H	-8.79900152492217	5.16956424209593	-2.26410125857962
H	-5.19792333311605	7.27233747094358	-1.99840304714385
H	-1.82884351778512	9.06420774259417	-1.88936093205426
H	1.74000658365643	9.18328164919805	-1.93551803538208
H	5.24853315761167	7.39996677539522	-2.16555667027877
H	8.96899232945654	5.13790588484076	-2.44931327118487
H	8.78074669473916	-5.15776090893909	-2.21951273604969
H	5.23304580297020	-7.26178433660562	-1.96674681828377
H	5.36053745766197	-7.23448403267662	2.16980873102175
H	9.11981973432522	-5.12145371521463	1.83579659210860

H	9.29465244047661	5.26955786249843	1.60543823476531
H	5.46827101916720	7.45373939912883	1.93255882337132
H	1.72644782168025	9.15244297787423	2.16173613000515
H	-1.71064487845922	9.05686361900846	2.19622221086810
H	-5.31263939596457	7.24694481754153	2.13602825319065
H	-9.13451757278206	5.16022317654049	1.79132348688382
H	-9.28059513560548	-5.24897331020135	1.62820078363061
H	-5.44379757676461	-7.41574044331917	1.97196483194011
H	-1.73147474496136	-9.15101592749300	-1.92183683542559
H	-1.72301628435441	-9.13205000351274	2.17297711885456
C	-0.55243197583351	-0.19701388335770	3.29840667290425
O	-0.28893955257055	-1.46278255191661	3.82968879077184
O	0.63356743843210	0.56316646108147	3.01734684814696
H	-1.07581217952357	0.35817774480949	4.09680458861427
H	-0.02471068446784	-2.06626508764670	3.10226735652886
H	-10.94528178387952	-2.18866933737091	1.61145758845846
H	-10.67309740708503	-2.10421326770682	-2.43676155831039
H	-10.88827894599960	2.16726702662683	1.69577849102970
H	-10.64390668082337	2.17645529638406	-2.36981664396267
H	10.86416366294152	-2.12177625210372	1.73207410535485
H	10.63238818438784	-2.15746814161872	-2.34499710389223
H	10.93401084528304	2.19097926833503	1.60450790855110
H	10.66144206565715	2.07485028458491	-2.44273342851290

- **2Si-CO**

Si	-1.17641290332217	-8.31036460961193	-1.25561236119560
Si	1.22519645266937	-8.23773138785175	-1.25282968383446
Si	2.37154721266102	-6.16095259767821	-1.23087599478809
Si	4.74841585070972	-6.25953974360654	-1.23589966963622
Si	5.76548592967413	-4.10941413555782	-1.21621243182957
Si	8.13793617722938	-4.10298007360279	-1.22567767027084
Si	9.31792868035921	-2.01443057887319	-1.22313848326931
Si	-2.41525818635400	-6.28458670118223	-1.24186675089630
Si	1.13584673683960	-4.14727121387690	-1.21941352189859
Si	4.58192725204870	-2.06228082315166	-1.20491388894608
Si	8.07613739050461	0.00121661991838	-1.21808217869015
Si	-4.79241252953398	-6.37858150414578	-1.24904219299018
Si	-1.22186676179471	-4.24691401283803	-1.21881068815276
Si	2.22420291527882	-2.05285910041443	-1.18405380338625
Si	5.72502687697614	0.00056993659906	-1.20969257216366
Si	9.31746180850420	2.01733937265572	-1.22242499218369
Si	8.13680893221414	4.10544780948690	-1.22451227763298
Si	4.58125179383944	2.06286046101458	-1.20460755069833

Si	1.06092289043139	0.00020918932396	-1.21781868639352
Si	-2.24489640552860	-2.11727578359198	-1.33362537910900
Si	-5.75623660542298	-4.20102490530707	-1.23554529963705
Si	-4.59806767012229	-2.14011322663162	-1.23192274703117
Si	-1.27329887296606	-0.00020889349326	-1.27860053189540
Si	2.22351499848800	2.05358572393469	-1.18364881070863
Si	5.76416996287224	4.11053352790788	-1.21525400082479
Si	-8.12772082435492	-4.12726758594879	-1.22303204284731
Si	-9.22913872253399	-1.99596841847761	-1.21855555625969
Si	-5.60223815758605	-0.00098278559658	-1.24539675220264
Si	-2.24575013757482	2.11649121136410	-1.33329828622374
Si	1.13401172509816	4.14744857617485	-1.21946809742755
Si	4.74651807520329	6.26037416696821	-1.23507616848882
Si	-7.95566028352949	-0.00108019853413	-1.22178857436821
Si	-4.59901809218335	2.13859149523476	-1.23242367248680
Si	-1.22351582224723	4.24673246073894	-1.21914733572863
Si	2.36955742019378	6.16138479272815	-1.23055059175584
Si	-9.22981456309917	1.99322175678821	-1.21938690981610
Si	-5.75764436081905	4.19907602704348	-1.23694574768655
Si	-2.41725573244540	6.28416098567767	-1.24307606603340
Si	1.22309608631811	8.23809138475092	-1.25295638496577
Si	-8.12904669747914	4.12497962923700	-1.22460944323422
Si	-4.79438104378163	6.37697330103439	-1.25068233294963
Si	-1.17863356217908	8.31018143362112	-1.25668610427512
Si	-1.18064242668935	-8.33321027793423	1.14379060029375
Si	1.22184543143132	-8.25860219248721	1.15385266419375
Si	2.36842319907606	-6.17905306090893	1.17223688640275
Si	4.74733825318995	-6.27170083854034	1.18455559234096
Si	5.77348995223324	-4.12359359953514	1.18634772022759
Si	8.14555635506864	-4.11179863972165	1.17645963752534
Si	9.32151099578992	-2.01826635631039	1.18135819169701
Si	-2.41779952781615	-6.30795344466499	1.16010755142023
Si	1.13303561562250	-4.16454759839097	1.18816642216712
Si	4.59500248557641	-2.07343722738173	1.20113653485221
Si	8.08282699852876	0.00091652628646	1.19094928296181
Si	-4.79386492332217	-6.38799753835076	1.17130335642161
Si	-1.22085011428036	-4.27889697590941	1.18511315666927
Si	2.23778260890566	-2.07482407303116	1.21591269043248
Si	5.72874442039071	0.00039392518820	1.20146556089574
Si	9.32080907380915	2.02066871200638	1.18214468462766
Si	8.14401713047842	4.11362201477859	1.17779015231509
Si	4.59422139899619	2.07382117899643	1.20156139531410
Si	1.11831719683073	0.00009987526249	1.17964153294646
Si	-2.24104050495328	-2.16003881098637	1.07619980887277

Si	-5.75310984430352	-4.20645516721467	1.16972733052004
Si	-4.59891673545076	-2.14495631252293	1.16595912287486
Si	-1.24790835637979	-0.00003239010561	1.33468589406055
Si	2.23689581135580	2.07553311386039	1.21640274485491
Si	5.77180140310852	4.12456211223607	1.18750041730394
Si	-8.12323474282982	-4.13198393729896	1.17769252406333
Si	-9.22060052291764	-1.99766720251018	1.18692190428542
Si	-5.59210382497065	-0.00067468127501	1.18035225284380
Si	-2.24201639544045	2.15954018933038	1.07629607579197
Si	1.13101834052227	4.16461927029327	1.18822547721228
Si	4.74487231001552	6.27225622224262	1.18549628811588
Si	-7.94649082774435	-0.00068796795847	1.18378608881589
Si	-4.59977948155219	2.14404951218810	1.16534873727718
Si	-1.22295218371478	4.27892024342623	1.18475184505211
Si	2.36577554590226	6.17945663977045	1.17249528783665
Si	-9.22129701999016	1.99567950378675	1.18609141716261
Si	-5.75468719547913	4.20510234973234	1.16826546364442
Si	-2.42022337231470	6.30777978811809	1.15887078006518
Si	1.21889370766296	8.25884082003340	1.15378160521928
Si	-8.12461533945882	4.13038735861435	1.17603365752803
Si	-4.79621981278542	6.38708064615983	1.16957710585380
Si	-1.18354075426364	8.33327229078616	1.14275380717648
H	1.80658326719808	-9.36970114089125	1.97308536874323
H	1.81404190233132	-9.33347753204786	-2.08951918413093
H	-5.45234869281432	-7.41809478989241	-2.10292891216322
H	-8.85294644591687	-5.13147092746710	-2.06688160980905
H	-8.85418334156126	5.12889873807274	-2.06885718661417
H	-5.45446035818721	7.41613395067358	-2.10485431806227
H	-1.70633643274245	9.43119473424564	-2.09977359586070
H	1.81202178000726	9.33397182178205	-2.08938983755802
H	5.38132755785817	7.30179714878153	-2.10556739845485
H	8.82220077355694	5.13664423775582	-2.06943659481646
H	8.82348479640584	-5.13383740359091	-2.07082905629547
H	5.38327542531784	-7.30053770129623	-2.10682971434590
H	5.37899785413419	-7.32360333008667	2.04492737787346
H	8.84530871987253	-5.14386081937984	2.00825506955093
H	8.84326819781656	5.14582009911454	2.00991008659978
H	5.37627133830950	7.32398381697376	2.04624650477006
H	1.80327413143494	9.36989071532128	1.97330853227999
H	-1.71575447492726	9.47132294133753	1.95971609459209
H	-5.46454053721385	7.42716872099498	2.01640926190844
H	-8.84803806592593	5.13766018898683	2.01774067496285
H	-8.84640197910397	-5.13926068857973	2.01965235567439
H	-5.46155077515340	-7.42819804282736	2.01852582768173

H	-1.70398099868466	-9.43163686071324	-2.09843137532240
H	-1.71253848170540	-9.47116646017907	1.96103589701080
C	-1.33898583744532	0.00076394960930	3.26684618353576
O	-1.50477467248713	0.00129034478958	4.40990266211030
H	-10.45381786611922	-2.00996024559482	2.03932376394998
H	-10.46759847207252	-2.00711244282674	-2.06343012005240
H	-10.45452796918271	2.00755462117877	2.03849325940845
H	-10.46835480118605	2.00351473376256	-2.06414591507281
H	10.55937566567465	-2.07088825045094	2.02505503975155
H	10.55306991057505	-2.05859898745730	-2.07102832170552
H	10.55857002508910	2.07340646379173	2.02593535772616
H	10.55271695575444	2.06207548382071	-2.07016914318948

- **2Si-CO + H₂**

Si	1.27704740887920	8.05944768564028	-1.29401284378615
Si	-1.12223306446154	8.09153623494149	-1.29148620198872
Si	-2.31551170642228	6.04616767279858	-1.28569665258283
Si	-4.68733158795269	6.21149135567310	-1.28561238473711
Si	-5.74642000340085	4.08504584883968	-1.26230990713930
Si	-8.11961277536633	4.12252729884836	-1.25836373350837
Si	-9.37476763538724	2.07374613781150	-1.24903009832793
Si	2.45704406642084	6.00090480209922	-1.28766814677043
Si	-1.10994641308583	4.01389893572414	-1.28291758725514
Si	-4.60640833915271	2.01316727704665	-1.26569127295388
Si	-8.19105940891073	0.02303060374021	-1.25162388548421
Si	4.82149482343437	6.16589224242922	-1.29957596823670
Si	1.24356867073664	3.96766654848686	-1.27762007543253
Si	-2.24478410534956	1.95687860623148	-1.25840042883403
Si	-5.83842649093541	0.01000119096007	-1.25831423760946
Si	-9.39933272514965	-2.01507154977260	-1.23855577049250
Si	-8.16796283892060	-4.07773844602395	-1.23716220672453
Si	-4.62014550598560	-2.00611298677823	-1.26102241064029
Si	-0.97208923883406	-0.03301163963705	-1.37408444834716
Si	2.23896966989050	1.82381742238694	-1.38672861275972
Si	5.77737119485281	3.99683555729022	-1.28805992157868
Si	4.58142621093412	1.95783398344581	-1.30997354434294
Si	1.26165364931756	-0.20217215528986	-1.88203788758150
Si	-2.26648427194448	-1.99078996385557	-1.28469705131088
Si	-5.79534935178025	-4.05491435544061	-1.24291037180405
Si	8.14725408827539	3.97269259751880	-1.28248693537437
Si	9.27937205829091	1.86321273110696	-1.27912696645045
Si	5.65295231479755	-0.13346710349737	-1.32158605558677
Si	2.28726948698180	-2.07006736894221	-2.61580442487523

Si	-1.08750581353465	-4.01672755508268	-1.30366615481713
Si	-4.71170975075983	-6.16864107965608	-1.25415296348127
Si	8.00945898598383	-0.13297121811302	-1.29733720770610
Si	4.26488621270878	-2.03481221287626	-1.37460483818180
Si	1.25088481091978	-3.75423486528083	-1.36812865964922
Si	-2.33874610190081	-6.02403912079537	-1.26919945799895
Si	9.28356484687869	-2.12107691965331	-1.28875231780232
Si	5.61512446667450	-3.96995228681608	-1.31927971646066
Si	2.25346705308448	-5.89045087057468	-1.31012599158643
Si	-1.22204954719028	-8.10807088179791	-1.26499512528129
Si	7.97740390071154	-4.12253191552447	-1.28927590595056
Si	4.60928160884076	-6.11020909988136	-1.30545108767473
Si	1.16746307963409	-7.99425764800496	-1.27475345582275
Si	1.28053348222283	8.06934061461108	1.11029702305963
Si	-1.11789181628663	8.09758186788839	1.11555681216707
Si	-2.30763097969365	6.04941704817722	1.12159832031485
Si	-4.67921270494483	6.21781636288689	1.13852228657324
Si	-5.74038853178533	4.09268435788792	1.13765201766601
Si	-8.11301162854637	4.12952553553828	1.14454920418958
Si	-9.36548543228669	2.07925416160571	1.15564584510795
Si	2.45792732508304	6.01014795394103	1.11472158545467
Si	-1.10414321371027	4.01549361153419	1.11577106006310
Si	-4.60237488863087	2.01981309617981	1.13781933298859
Si	-8.18181885958130	0.02805487223488	1.15677998471650
Si	4.82135483651354	6.16496488576186	1.12497751185795
Si	1.24673152795140	3.97897359133191	1.12749333144826
Si	-2.24330540570054	1.96290079352295	1.14227654442799
Si	-5.82860849838093	0.01292886802493	1.14879492254368
Si	-9.39179459054542	-2.00886521612541	1.16440635787667
Si	-8.16143383262380	-4.07250889544462	1.16694949669057
Si	-4.60955367681885	-2.00374043679101	1.14657561208048
Si	-0.97781379087323	-0.02230375004829	1.05621753356879
Si	2.23879866475581	1.84396213482628	1.04414031218076
Si	5.77378438096515	3.99409917107828	1.11527169566328
Si	4.58432840939206	1.95254998333268	1.08351516880247
Si	1.25037961349891	-0.16416724565813	1.86133428559566
Si	-2.25566253709347	-1.99273369834135	1.11043285440796
Si	-5.78867256032519	-4.04908075218522	1.16171515846902
Si	8.14206149584460	3.97406739779030	1.12266289881659
Si	9.26152176829974	1.85963013862689	1.12610367931118
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Si	2.35122003115334	-2.15794697983841	2.53771825996340
Si	-1.05154949813760	-4.00367009636739	1.09095144058678
Si	-4.69175557379065	-6.15410524940584	1.16820939754159

Si	7.98772505452111	-0.13495531313589	1.10706372063010
Si	4.20188067920141	-2.02701553677153	1.10525703182440
Si	1.28666880916727	-3.69152783747910	1.11572414750914
Si	-2.31770768931089	-6.00342998558309	1.13188374708540
Si	9.27233331013382	-2.11532431394138	1.11710044338986
Si	5.59229475083990	-3.94070542795383	1.08228007658951
Si	2.24791131685549	-5.85323780348649	1.09265212827358
Si	-1.21400887916068	-8.09357074329381	1.14008871652078
Si	7.95596577158458	-4.10676084460291	1.11253767946261
Si	4.60070828298524	-6.08617802881074	1.10345056063366
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H	-1.66494680298510	9.20619232547203	-2.13364170525047
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H	8.84020072335269	4.99823618888229	-2.12772882525427
H	8.58573509754220	-5.21051682177872	-2.12193122271118
H	5.20533693064357	-7.15805164148518	-2.19668760700083
H	1.79017505072426	-9.07594029281199	-2.10526417966171
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H	-8.84622221686774	-5.12424206614034	-2.06881519133346
H	-8.78461894042825	5.17461248574271	-2.09367023916066
H	-5.29547619745387	7.27004001757992	-2.15422038773897
H	-5.27832990240887	7.28274771386422	2.00560806751022
H	-8.77483859396334	5.18590102890929	1.97694897180976
H	-8.83703539798791	-5.11419949961884	2.00667983508048
H	-5.27842997434419	-7.22140852071023	2.04138328804518
H	-1.76277371170325	-9.18394830855087	2.00961608199021
H	1.81946667668143	-9.01438132864421	1.98290614332297
H	5.19627725499326	-7.11900915200834	2.01229715964021
H	8.52897985900251	-5.19582969737815	1.96846054577572
H	8.83354449826638	4.99834469955165	1.97037456457923
H	5.44789623845354	7.20537684597555	2.00235566456411
H	1.84715164016709	9.16018730607387	-2.13635803235516
H	1.85543863184293	9.17538790611245	1.94230432907834
C	0.77884463048162	0.64582921146441	3.48697845028332
O	0.47274261066166	1.17151920552496	4.46904972349226
H	10.49185217721803	1.87150387766927	1.98218201914154
H	10.52191003265433	1.89301875603892	-2.11705499573106
H	10.48626764284704	-2.17508934218820	1.99385326546789
H	10.50657404511957	-2.18809825143101	-2.15255370934894
H	-10.61321361010524	2.17057514939125	-2.08742388529355
H	-10.59753997322294	2.17843872408619	2.00314791174790
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H	-10.62419141185557	-2.08307082973197	2.01377324763275
H	1.78986109812315	-0.98249866192978	6.26925671164669
H	2.04681054727549	-1.45448874473721	5.73295501574527

• **2Si-OCH**

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Si	-2.29685682875639	6.02890819881033	-1.25580087120553
Si	-4.66724094252220	6.19647966851663	-1.24973222325496
Si	-5.72490822068220	4.06856850112863	-1.23806456288222
Si	-8.09679212331449	4.11098344407876	-1.22602773538951
Si	-9.36205995161093	2.06750712857283	-1.22649223383128
Si	2.47673014847395	5.98313608924288	-1.27769040974791
Si	-1.09648701671236	3.99517895854620	-1.27993375292123
Si	-4.59459281203899	1.99161926505011	-1.25702887482035
Si	-8.18953358545868	0.01038283047513	-1.24017401169572
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Si	-2.23343541829933	1.94372932200896	-1.26057161303232
Si	-5.83731605246494	-0.00501284203970	-1.25196571638311
Si	-9.40643909058953	-2.02254635784088	-1.23348601253117
Si	-8.18998241051914	-4.09529410212557	-1.24158228048110
Si	-4.64154128285113	-2.03448366168730	-1.26325651126361
Si	-0.97272603359758	-0.05224152808148	-1.34291909717411
Si	2.25667307912824	1.81623076932288	-1.34878368246067
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Si	-2.28756301995513	-2.00018559781353	-1.27428864159814
Si	-5.81662077164120	-4.08330122490845	-1.25443974114438
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Si	9.31412253981123	1.87472898988050	-1.29589726794548
Si	5.68779874691941	-0.10874624364281	-1.28920508166381
Si	2.28630753626661	-2.07219740645428	-2.54156720019084
Si	-1.12610916368597	-4.03501667437067	-1.26689835941305
Si	-4.73854241621968	-6.19989449787401	-1.27389479441188
Si	8.04562353965205	-0.12358976371945	-1.29701877550800
Si	4.27473168644775	-2.00067956905466	-1.30136387586994
Si	1.21665453697557	-3.74364157476173	-1.28584654539100
Si	-2.36345113558298	-6.05289530943998	-1.27195635117571
Si	9.29985009739470	-2.12478130119909	-1.28769378445105
Si	5.61370513328957	-3.95551506225463	-1.26014880589488
Si	2.24153040930270	-5.87998218799243	-1.24835560574160

Si	-1.22460918378544	-8.12566608265299	-1.26530893917349
Si	7.97677849369940	-4.11591721837834	-1.27559009548719
Si	4.59956455500363	-6.09354329192378	-1.26716484188393
Si	1.16430904599226	-7.99011998344579	-1.26346128918940
Si	1.30535982836071	8.02681561043368	1.14423508836932
Si	-1.09322213532602	8.05937347165364	1.15513361588269
Si	-2.27977657250644	6.01067164574081	1.15060398320025
Si	-4.64967041142406	6.18492352815120	1.17423945879342
Si	-5.70954910289697	4.05868779968584	1.16212778574748
Si	-8.08223756518057	4.10280441805048	1.17713720741300
Si	-9.34984669466521	2.06150139969216	1.17836700660371
Si	2.48041584459222	5.96704082916357	1.12425606929878
Si	-1.07902337403614	3.97565500864610	1.12754671496819
Si	-4.57334984471282	1.98488361112936	1.14787447473958
Si	-8.17581949911807	0.00616325010338	1.16750270551004
Si	4.84164814647973	6.16304552372665	1.13128898811088
Si	1.26392208590585	3.93696355455347	1.13093910551540
Si	-2.21226760655516	1.92815508797644	1.14260768360977
Si	-5.82367765469078	-0.00745338050558	1.15418225568959
Si	-9.39559181243774	-2.02498952298186	1.16962781640078
Si	-8.17997117875402	-4.09669733010781	1.16221804710254
Si	-4.62766387710548	-2.03568532962014	1.14350107552719
Si	-0.93263521539025	-0.05031289562852	1.09198087912558
Si	2.24175475296887	1.79453171465297	1.08592756246604
Si	5.80682319019801	3.99914097371075	1.11489261979747
Si	4.58886127845964	1.97129025369394	1.09642957146470
Si	1.12491981308480	0.05944979384751	2.20512452909078
Si	-2.27149141007217	-1.98675454029708	1.11735089343343
Si	-5.80700954570224	-4.08356449366611	1.15021066667168
Si	8.17669271400506	3.97932534498704	1.11491991593900
Si	9.32040702451903	1.87740097983140	1.10992472908163
Si	5.69324861698792	-0.09916090819535	1.10790182428912
Si	2.26403385969568	-2.00898576529812	2.30192008808741
Si	-1.13104533323291	-4.03263891830331	1.12565706322863
Si	-4.73653310579622	-6.20254103335956	1.14864155139533
Si	8.04777101869355	-0.11673778123473	1.10905179935362
Si	4.30135120793843	-1.99544221860781	1.14364884923898
Si	1.20567660820279	-3.76840040122509	1.16381368661219
Si	-2.36366333125826	-6.04969298476020	1.13113398215550
Si	9.30304695627743	-2.11528390666378	1.11835835629118
Si	5.61705236261473	-3.95538928663410	1.13690425469053
Si	2.24920719722889	-5.88578496738786	1.15031402759338
Si	-1.22614017907757	-8.12156110147729	1.13999137818029
Si	7.98262110325529	-4.10650703992296	1.12653568948742

Si	4.60543193367141	-6.09253811640906	1.14435660410021
Si	1.16196418480315	-7.99242957088667	1.14158537593578
H	-1.63416109469714	9.16941919650871	2.00453443785542
H	-1.64681183194244	9.19349552741718	-2.08611310315333
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H	8.87036235120701	5.00598948000598	-2.13373082598475
H	8.56640899265937	-5.20855703434727	-2.11532391900807
H	5.19289066202984	-7.13927699969348	-2.16262379156864
H	1.80249964011371	-9.05462966289240	-2.10409708887893
H	-1.75847056933944	-9.23448494463284	-2.12058611658683
H	-5.34596623380741	-7.26466818487117	-2.13573675677909
H	-8.87750748986298	-5.13502265085238	-2.07410741143716
H	-8.76385254818047	5.16844020661184	-2.05315037866344
H	-5.27910402065888	7.25822149023234	-2.11191640049446
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H	-5.33365927783300	-7.27280899321388	2.01093346993552
H	-1.76563607764823	-9.22168408703872	2.00297212266823
H	1.79921672669944	-9.05762183133831	1.98251767175128
H	5.20485952367927	-7.12746327628018	2.04846719119108
H	8.57185976630785	-5.19437666966775	1.97313138906905
H	8.86863081279779	5.00528087530590	1.96032445506836
H	5.45844278459855	7.20630007648276	2.01230316792203
H	1.86197229261659	9.14919339577062	-2.09682065679105
H	1.88454446430488	9.12280554792398	1.98681790252242
C	0.66276323028375	0.82555501302609	3.94526979118831
O	0.12028815222624	1.91702258671276	4.00337952303779
H	0.89151804467709	0.25353064501820	4.88963859336359
H	2.46728201962731	-2.33871819227063	3.75152363917380
H	10.55811371953459	1.89719241587177	1.95499876021059
H	10.54852624989242	1.90426466825222	-2.14555157093285
H	10.52050883956844	-2.18886191008801	1.98903778031552
H	10.51798228357078	-2.21071972470977	-2.15625953986415
H	-10.60052861373190	2.17461408165118	-2.06383079970176
H	-10.58011353808678	2.16247988602629	2.02841629802959
H	-10.64650387405173	-2.09611714501848	-2.07184481540540
H	-10.62820138503735	-2.09633309754100	2.01906208763535

- **2Si-(OH)₂CH**

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Si	2.14642024171217	-5.89295363375973	-1.09122529352977

Si	4.49519451031938	-6.18386279640088	-1.15584119997142
Si	5.63670878302621	-4.11275421894449	-1.23101375640349
Si	7.99126490852212	-4.23444275096517	-1.43246829024128
Si	9.24586402920312	-2.20402454993502	-1.58463664879907
Si	-2.60827013800619	-5.98963980605114	-1.21047602151297
Si	0.98678024756563	-3.84079337056712	-1.06854909662774
Si	4.57520233405350	-2.00803487368784	-1.16077672431934
Si	8.10479578513972	-0.12639642546658	-1.53340394984238
Si	-4.97303557584912	-6.12611968817430	-1.39267000222551
Si	-1.34503745106284	-4.00758164668585	-1.10453818654318
Si	2.25646743850980	-1.86932093403841	-0.93842936757676
Si	5.76877903348223	-0.00402712066294	-1.28582613935970
Si	9.41917446034969	1.82075711474219	-1.75956079593142
Si	8.18018799534732	3.86883167178490	-1.75086303031428
Si	4.39130036724144	1.93334472172536	-1.24228920855912
Si	1.32592643231688	0.31639015183749	-0.90460807693659
Si	-2.44160358360454	-1.95037571564120	-1.07091762006198
Si	-6.00085006122944	-3.97810535373552	-1.44212192141492
Si	-4.80583047340644	-1.92923842639541	-1.27243113630484
Si	-0.97896145697928	-0.10233156237181	-0.68019482166150
Si	2.31252901105228	1.86214571597375	-2.40052628556797
Si	5.82178103640227	3.83950774040340	-1.43722132823723
Si	-8.36620899360379	-3.83633747435146	-1.68848968369662
Si	-9.47057597535366	-1.70177249913680	-1.69992787932772
Si	-5.86742314347598	0.16514407967702	-1.30858405094122
Si	-2.18299177063394	1.92101734164585	-0.94272220014791
Si	1.51293815881862	3.64206864402905	-1.08641634720788
Si	4.84224585502786	6.00258656268490	-1.40220333649010
Si	-8.19956601692490	0.28642127075579	-1.51966929875824
Si	-4.52594014816786	2.07434986749635	-1.13257402871123
Si	-0.83448848912923	3.83644471473941	-0.97530095797533
Si	2.49499564790982	5.79428900595617	-1.20820092728720
Si	-9.27972095041253	2.39284676379547	-1.56926203462868
Si	-5.56313740986498	4.19323095141456	-1.22362638743143
Si	-2.00170410887311	5.88335744958718	-1.06722501151189
Si	1.44916197349884	7.92289192948313	-1.19551919732511
Si	-7.91797581342878	4.36023464490367	-1.45104082321594
Si	-4.34219954960420	6.21850013708165	-1.14643948235118
Si	-0.92616977736406	7.98416067262441	-1.12483077850929
Si	-1.47381957532020	-8.01365238166984	1.22471972149674
Si	0.94449137765766	-7.94123744497691	1.27461165517137
Si	2.19223627561633	-5.91755079704227	1.30667370743196
Si	4.57533790245586	-6.15720343895543	1.26463029320398
Si	5.80822344065045	-4.11983132265232	1.16183126217514

Si	8.17285140516885	-4.19479612770914	0.96289491992410
Si	9.44144285842318	-2.14679119099655	0.81049677900858
Si	-2.75572695135915	-6.01919977519380	1.19056657076993
Si	0.95550214289917	-3.88639258860573	1.34586926932846
Si	4.76832330571228	-1.99879903901851	1.24472298268173
Si	8.36137157123344	-0.03871737003119	0.85701650831180
Si	-5.14009813073053	-6.17990940737685	1.02295662349433
Si	-1.44844212369932	-4.03639502422156	1.30294655164367
Si	2.40747539134282	-1.98345023137359	1.44771828418947
Si	6.01932955511707	0.00651665288427	1.11051935141300
Si	9.66828755971447	1.92974441902810	0.62783686451276
Si	8.48052765986092	4.01378490728319	0.63032740670966
Si	4.86305665082021	2.04903255676859	1.14711074583409
Si	1.75298834767443	0.27022718076776	1.49057435803010
Si	-2.79944923229279	-2.10483891494430	1.28461032765040
Si	-6.25534069658527	-4.07578551176559	0.94385291814059
Si	-5.11458632450116	-2.03475842875702	1.10956746169503
Si	-1.61713656228876	-0.15991657236838	1.65046842636818
Si	2.90380295289937	2.12138419050812	2.33540420830622
Si	6.13739872450471	3.98990014436707	0.93561094967402
Si	-8.60869728159649	-3.93414358902464	0.69848268503473
Si	-9.68305156868804	-1.77434093925799	0.69320984474555
Si	-6.06327484025904	0.12556018068212	1.10035827338871
Si	-2.40464995676516	2.02840089106513	1.43047422096324
Si	1.55114496500405	3.77133567322206	1.36662519685333
Si	5.01620674756476	6.07453159651037	1.00748927672467
Si	-8.40792894184314	0.22658970041320	0.87488898537656
Si	-4.75946728541640	2.10465265911418	1.26729428189551
Si	-0.85284043424553	3.85052142673740	1.42766229490736
Si	2.64537486125053	5.86432745534586	1.17952360591050
Si	-9.45068428734679	2.35837545619366	0.82729343759192
Si	-5.75653038860586	4.22980979708638	1.17009222056591
Si	-2.04753895738304	5.92137618828414	1.33260174141769
Si	1.51232673726433	7.93794131780277	1.20799342667869
Si	-8.11486198765802	4.36853481766678	0.94489620962427
Si	-4.42740612780334	6.20948351113367	1.27339229381982
Si	-0.89058283022615	7.99069798157347	1.28017953175264
H	1.45202981327632	-9.07685765653134	2.11328485213095
H	1.61309083658787	-9.03214468298536	-1.94827476170483
H	-5.50662797983074	-7.19535231346218	-2.29633574878997
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H	-8.42264173045979	5.45734236038016	-2.33874314696542
H	-4.81120553734007	7.34295396399271	-2.01868462855185
H	-1.57582760616178	9.03489640244684	-1.97298517610233

H	2.07591913984739	8.96770031078395	-2.06800180172337
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H	8.72387934166452	4.87054343206623	-2.72504882536371
H	8.53188332812820	-5.33019656726066	-2.30013876492995
H	5.00150014574650	-7.29406058925949	-2.02534195738145
H	5.12999730242576	-7.24369893662876	2.13591171810010
H	8.91961600502076	-5.21450347522792	1.76984031723437
H	9.24202972678837	5.10431961378649	1.32218185914547
H	5.65563738418844	7.15374354951299	1.83094711469787
H	2.10273666581931	9.03876924511371	2.03821557609911
H	-1.38021343339240	9.12004785138889	2.13783773884804
H	-4.97261866416346	7.31677155308107	2.12465301607233
H	-8.84383086455144	5.42751408107295	1.71669993762143
H	-9.44503848566304	-4.95834709329519	1.40404435897678
H	-5.80216519222634	-7.27628074701380	1.80097019078049
H	-1.95973961549241	-9.14606506482298	-2.02517243710612
H	-1.96444110469433	-9.15499225265875	2.06450920576219
C	-0.62557824218622	-0.31930271987821	3.31141255075880
O	-0.23800228609347	-1.52880868376618	3.81858742517255
O	0.58497021220626	0.56087026257737	3.01695950081646
H	-1.14041104444895	0.23574919153743	4.11412819125904
H	-0.04000402056859	-2.14933796602369	3.07765305595823
H	-10.99770793292378	-1.82915987382566	1.41183319295185
H	-10.64202273231612	-1.68589965622797	-2.63478746945885
H	-10.73659279267664	2.52657785085492	1.57947037487812
H	-10.44748720028352	2.54794253379367	-2.49540327003538
H	10.73678110166885	-2.27937104722912	1.55423797141450
H	10.40959031425942	-2.30938191710148	-2.52324666693851
H	10.97709211598816	2.00170023576327	1.35520909185296
H	10.56145375247457	1.79996535701367	-2.72909801281698
H	2.91571731078616	2.03523058233786	3.84205359609120
H	1.14076545217843	0.71684378580067	3.81709401182877

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Si	2.36724534082407	-6.18805943873846	-1.23737744530657
Si	4.74798614872244	-6.28907526660344	-1.22252434934720
Si	5.75672567690069	-4.13261876240630	-1.20083155381108
Si	8.12935403393901	-4.09913727777547	-1.16970940132651
Si	9.29777937748549	-1.99913339248111	-1.15721887778767
Si	-2.44205481587098	-6.10598575152428	-1.26745522238787
Si	1.14673320430574	-4.16815413513631	-1.25309186141329

Si	4.58445656266654	-2.07668524714608	-1.22266265150030
Si	8.05745430555888	0.01742732337787	-1.17793291311032
Si	-4.81308175128092	-6.22817357379226	-1.28954126142610
Si	-1.20873678305042	-4.08793767566148	-1.26782952641898
Si	2.22319037817317	-2.07669468444317	-1.24613980773869
Si	5.70538956607980	-0.00243344782654	-1.20730617679412
Si	9.27786389720469	2.04741014419431	-1.15843714222037
Si	8.07418477847975	4.12580363582623	-1.17400845668162
Si	4.53293104830408	2.04568120737117	-1.23120393373333
Si	1.03102230563300	-0.03650492527733	-1.31163172255788
Si	-2.28229193823941	-1.98130688594245	-1.28148151135476
Si	-5.80924783072162	-4.07156190544577	-1.27796188049066
Si	-4.62961449386505	-2.02482457258441	-1.26933249568731
Si	-1.30056573070798	0.14312306492283	-1.53927281143500
Si	2.18582123305212	2.00426979045526	-1.25900605143307
Si	5.70330731521085	4.09617291747853	-1.20666027278985
Si	-8.17797231199919	-4.07781102296602	-1.28841797987351
Si	-9.32549140456922	-1.97618769430012	-1.28892775492521
Si	-5.72650297169191	0.05153376148605	-1.27308056875853
Si	-2.34022188464407	1.98626696847539	-2.44170910395239
Si	1.01712770288427	4.03196851375047	-1.29708325077288
Si	4.61008083268873	6.20556523665939	-1.23490476331364
Si	-8.08220480295837	0.03924684716897	-1.27891255321726
Si	-4.37034383093626	1.97473075491615	-1.31940145741642
Si	-1.32064217113040	3.76736462765897	-1.34822749002599
Si	2.23096647619124	6.06185916400205	-1.25297350901773
Si	-9.37916048474390	2.01262789390368	-1.28505845058125
Si	-5.72884269187322	3.89723467163184	-1.26708118995715
Si	-2.370404444673102	5.87550820276457	-1.27616084272546
Si	1.08495461264857	8.13185773716872	-1.26639523332986
Si	-8.09556439037700	4.02681685783581	-1.27894429383575
Si	-4.73238165339455	6.04348083734609	-1.28342601743254
Si	-1.30341894638395	7.99224364939064	-1.27823835359923
Si	-1.27989035621793	-8.16491994018957	1.14772042050478
Si	1.12271795483846	-8.21492996986092	1.16321650247877
Si	2.34627196104723	-6.18322566963942	1.16827859736840
Si	4.72474828351461	-6.28742194087840	1.19838971259220
Si	5.72622417858124	-4.12844678659182	1.19987116808936
Si	8.09852804764301	-4.09580493358508	1.23183436474426
Si	9.26609741567585	-1.99664011030054	1.24740478067996
Si	-2.45436731793588	-6.10175825152257	1.13438384829542
Si	1.12953553356254	-4.16326568565783	1.14480164630489
Si	4.55220117635166	-2.07259761915463	1.17953129912642
Si	8.02380047572065	0.01897660937932	1.22947408599068

Si	-4.82449092153082	-6.22897326852325	1.13797175552875
Si	-1.22247031173820	-4.08386700626080	1.13756923206193
Si	2.19281528084433	-2.06824422396509	1.15000591897278
Si	5.67114992350302	0.00114565313266	1.20535208828909
Si	9.24581339222947	2.04740424274659	1.24523225327600
Si	8.04046394849819	4.12410602130328	1.22930679474865
Si	4.49310633454769	2.04705409117930	1.17934160934347
Si	0.99642359592039	-0.03415614734139	1.09672127666154
Si	-2.29440448260018	-1.97744449051721	1.13533532115861
Si	-5.81961357811995	-4.07286657427555	1.12509366199093
Si	-4.63876746730547	-2.02726362198108	1.12588646461120
Si	-1.33325811390697	0.16077596139976	1.32909648890170
Si	2.14446148875755	2.00850589892163	1.14828104478608
Si	5.66909917510350	4.09486498529250	1.20036185447344
Si	-8.18756086904517	-4.07913572662427	1.11869007655138
Si	-9.33636497753280	-1.97832360062112	1.11669561581480
Si	-5.73439048650060	0.05169379026951	1.13592643950907
Si	-2.33741417839854	1.99181407354874	2.30647444792952
Si	0.99203588198523	4.03637856577789	1.10907267434386
Si	4.58007942445235	6.20525581884838	1.18650446582654
Si	-8.09155113684561	0.03723163710419	1.12420495997091
Si	-4.38307861542287	1.98278405742271	1.20599820856834
Si	-1.34066815753998	3.76493990406405	1.17572118081635
Si	2.20437454316897	6.05942785688255	1.14730785461366
Si	-9.38679814453745	2.01238694260969	1.12034030223725
Si	-5.74010476769315	3.90748689988889	1.13211499238630
Si	-2.38009825330533	5.87603030331360	1.12507237234520
Si	1.06995856912767	8.13400401595789	1.13752500621715
Si	-8.10671974524412	4.02977506760631	1.12248234855167
Si	-4.74065510765021	6.05336331345264	1.12364433439875
Si	-1.31672700307895	7.99583387049500	1.12593628745226
H	1.64795849314789	-9.34259089375592	1.99944267972073
H	1.67011865128335	-9.35229856309008	-2.06578583417000
H	-5.44275933804701	-7.26960761246121	-2.16395933594820
H	-8.86734870609827	-5.10017278132207	-2.14045060924869
H	-8.68896321642677	5.11109144738592	-2.12669227942933
H	-5.34323929514673	7.06316287727526	-2.19643516297663
H	-1.94772221333091	9.05007579351333	-2.12284090942445
H	1.61686182308010	9.24114028637857	-2.12235014767472
H	5.22586264800667	7.27399581617054	-2.08693336508679
H	8.76901765043697	5.16290917876373	-2.00375862739223
H	8.84313230987548	-5.12499324152552	-1.99741589077171
H	5.39545036269724	-7.33874947766147	-2.07355185049981
H	5.35483620706475	-7.33606997579515	2.06360005860443

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H	8.71032187132518	5.16147583836594	2.07903104022939
H	5.16855654256491	7.27998117366840	2.04951185573541
H	1.60289506767825	9.24018474584003	1.99646941012180
H	-1.97526460481498	9.05367641220739	1.95942963685329
H	-5.34651597854572	7.08903660257688	2.02192570030242
H	-8.71413327685700	5.11289830232048	1.96189961507673
H	-8.88047751670170	-5.10489698083516	1.96371453536218
H	-5.45550913522955	-7.27463248993110	2.00637554582532
H	-1.83077072208816	-9.27678707228106	-2.09156338254488
H	-1.86202902721412	-9.26926529202348	1.97768124966238
C	0.46873962485137	1.66173818961841	4.19940983056682
O	1.33458144214346	2.38951250010138	3.74552615403501
H	0.39156370474936	0.58135399279243	3.91673258040952
H	-0.29442061417216	2.03271506538030	4.92444045978523
H	-10.60873902899458	2.06786501697254	1.98638368459501
H	-10.59482931641169	2.06721019066067	-2.15979909789060
H	-10.57799212606545	-2.01269630244136	1.95631692095751
H	-10.55970394453040	-2.00600209457990	-2.13949356235187
H	10.46930198825590	2.11059293709441	2.10920542165494
H	10.52398405105352	2.11137063986007	-1.98929731023868
H	10.49283668737585	-2.04596798711281	2.10792015193924
H	10.54692298997325	-2.05199395090734	-1.98457246117612

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Si	1.13981837693389	8.10325274459358	-1.19634141804489
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Si	-2.31636313768660	5.79679977618658	-1.09336006043462
Si	-4.67592344699354	5.98613506925738	-1.14512538248598
Si	-5.74712532877294	3.88069713003149	-1.22638009426083
Si	-8.10486724867079	3.93589821464422	-1.41068885601944
Si	-9.29733973449956	1.86933473638098	-1.55908034905797
Si	2.42630463604659	6.11365293522372	-1.20622408627235
Si	-1.07309999163752	3.79795880268431	-1.05348793935490
Si	-4.60617391400697	1.82031197426832	-1.15317879249763
Si	-8.08354019744039	-0.16683807209231	-1.51438936843737
Si	4.78327839984127	6.31881458891414	-1.40927286157120
Si	1.24735203621889	4.07755628114075	-1.08852250744701
Si	-2.28495682768830	1.79726203975356	-0.91463510483464
Si	-5.74381285937244	-0.21423513363286	-1.27658688295397
Si	-9.33883856784537	-2.15302128754230	-1.74233502687197
Si	-8.03852862280635	-4.16197740279038	-1.73692237374049
Si	-4.30855585222187	-2.10847456202911	-1.23452251478740

Si	-1.33578348058416	-0.38152402881221	-0.84261223007609
Si	2.36660479098635	2.02732870796827	-1.05179082837607
Si	5.85597273583671	4.19350121717925	-1.45686933663639
Si	4.72371076448107	2.10715695725295	-1.28876100622275
Si	0.97071016258952	0.10242127298175	-0.76975112684360
Si	-2.23792081250678	-1.93590926721085	-2.39691206441032
Si	-5.68234495439870	-4.05584547372963	-1.42818003749336
Si	8.22247820541130	4.11364324562252	-1.71156527133359
Si	9.38651760414521	2.01189493186475	-1.72996389682807
Si	5.83572588784245	0.03564332683327	-1.32933594721645
Si	2.22647442659843	-1.88756575639791	-1.01656778625401
Si	-1.39656735583066	-3.69552240418698	-1.07664725272733
Si	-4.63004651633915	-6.18437232709775	-1.38714781810045
Si	8.17357049864954	-0.01194375368987	-1.54686784433475
Si	4.57421518029563	-1.93238498053978	-1.15992057731482
Si	0.95526179941526	-3.85250466153484	-0.98438175087743
Si	-2.29513132772519	-5.88265270760723	-1.19620259529147
Si	9.32731250020528	-2.07826297630812	-1.59926145990943
Si	5.68493666657512	-4.01563594040504	-1.22305807790608
Si	2.19435057632451	-5.85648188451961	-1.06749690465971
Si	-1.18738454323299	-7.98014422452432	-1.17962228664712
Si	8.04178494807273	-4.09495736884122	-1.46957470041268
Si	4.54632910072137	-6.08859960766046	-1.14747892093363
Si	1.18838431496173	-7.99088810392903	-1.11356125735623
Si	1.20832948773574	8.10960114024374	1.20570341072939
Si	-1.20297684293605	7.90406102241154	1.26954318303510
Si	-2.34606441249707	5.81802929048249	1.30261963434160
Si	-4.73913904164692	5.95178923134709	1.27727759649223
Si	-5.90305117094307	3.87486699684018	1.16632066112585
Si	-8.26971022150821	3.88467775511124	0.98642653285032
Si	-9.47875957625172	1.80217007474359	0.83669293254263
Si	2.58454378540695	6.17851152660511	1.19029023478106
Si	-1.03435299842811	3.83415796309974	1.36787656983364
Si	-4.78944263246222	1.79475926122543	1.25945543817442
Si	-8.32921687193657	-0.26855823880720	0.87690338151808
Si	4.96245393201371	6.38631241416619	1.00321317698614
Si	1.34905904206705	4.15169064364909	1.31333741837560
Si	-2.43268386703597	1.89082876669473	1.47717986806852
Si	-5.98585210811883	-0.24259420872756	1.12362711314860
Si	-9.58158802558922	-2.27205732107226	0.64505518638540
Si	-8.32721225668572	-4.31567128038913	0.64555087139416
Si	-4.75190048913186	-2.24109048352375	1.15717918203379
Si	-1.73295059840460	-0.35654898243363	1.56973731300843
Si	2.73044693687604	2.23229304443168	1.30928463255883

Si	6.11724165208015	4.30151610152342	0.92936245837035
Si	5.04387246126647	2.22231137045440	1.09175899040993
Si	1.65001208440720	0.20424018028481	1.50030923441849
Si	-2.82395575476850	-2.23088913992835	2.40457061474483
Si	-5.98625006520311	-4.20700395411354	0.94424565495958
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Si	9.60661741450094	2.09127433185530	0.66218317802429
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Si	-1.42821426107970	-3.81611512634017	1.37927077248442
Si	-4.79789063460660	-6.25397524470020	1.02424645506079
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Si	4.84617093288341	-1.95570470642080	1.24114981704210
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Si	-2.43571226209092	-5.95415155507656	1.19294119679149
Si	9.51259249101355	-2.03697173906893	0.79689029333960
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Si	2.24625739719318	-5.88388502303160	1.33261321682896
Si	-1.24627479302187	-7.99567237873832	1.22391683623767
Si	8.26040395564402	-4.09869826979854	0.92367196172095
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H	9.03408639387944	-5.13085289728725	1.68739496726293
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H	1.62954183507134	9.22794215179345	-2.05676871074494
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H	10.80791330421494	-2.14917740488632	1.54281845864730
H	10.49311642715456	-2.19379248457470	-2.53336353590957
H	-10.77219855408658	1.89580225818149	1.58928360243019
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H	-0.65592540087009	2.16360282102392	3.85810743142970

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Si	-5.78941882116500	3.92294628845814	-1.26349174957082
Si	-8.14844569891032	3.93985266087661	-1.46973259892326
Si	-9.30589493257908	1.84733421849547	-1.58941197977473
Si	2.40243889844613	6.09052764327634	-1.17051169095256
Si	-1.09819250635124	3.81962676918561	-1.05198330234167
Si	-4.65659419573518	1.85121722544728	-1.18786228963937
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Si	-2.32563106181538	1.82732783958098	-0.99086847429273
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Si	-1.36977722576058	-3.69006717655546	-1.07591866982669
Si	-4.62046179382529	-6.17167466180620	-1.34243090060099
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Si	-2.28312204656252	-5.87412032331136	-1.18373183946324
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Si	1.18439129332874	-8.02689730489703	-1.13121309288478
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Si	1.30320223378871	4.08120498587662	1.34277429992951
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Si	1.68724050495854	0.13278455893748	1.40876938460274
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Si	1.01758542949544	-3.90601972287206	1.40313429929852
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Si	1.16771969781663	-8.02783625636842	1.27368311826689
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H	-1.81476741301520	-9.03417654592005	-2.04238382677747
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H	1.68956958340671	-9.14249688087375	2.13054340028598
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H	1.62781005000480	9.23016704969758	2.09075558573447
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H	-10.48623906114788	-2.21543530801624	-2.66164755766742
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Si	4.82932779120508	-6.29903522125097	-1.38546580135203
Si	5.83219868446337	-4.13950540631711	-1.35169403752857
Si	8.20396028605688	-4.08510105825502	-1.33828739771326
Si	9.33294194463776	-1.96556718188723	-1.31223258984222
Si	-2.34976565603587	-6.24468914729425	-1.40874842811593
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Si	4.64573627008663	-2.09516446106480	-1.33211451517441
Si	8.06492623317758	0.03528384444436	-1.29967554498041
Si	-4.72743142044430	-6.38126401028490	-1.42675206589299
Si	-1.15010444171691	-4.21057408204090	-1.38394397651924
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Si	5.71291608274836	0.01251169529627	-1.31614496937730
Si	9.28845833821921	2.06354160332048	-1.27090991063320
Si	8.11824148145098	4.16120026942609	-1.25150236566198
Si	4.60620833963786	2.10077786134397	-1.29527227262696
Si	1.16373320121979	-0.02505395159263	-1.32892696687906
Si	-2.28338760666730	-2.14088469642608	-1.36251866826988
Si	-5.78194890182666	-4.24591844737806	-1.39663615986904
Si	-4.64083135681388	-2.17580082038650	-1.37066041560724
Si	-1.18718617718709	-0.05028915135864	-1.36432953523100
Si	2.24775711056405	2.06502269376379	-1.33352332006826
Si	5.74571235870904	4.17211351108825	-1.26524587937677
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Si	-8.11299867756604	-0.11850075479527	-1.35265289530846
Si	-4.68586346368703	2.00821968579077	-1.31664975298471

Si	-1.23971378008094	4.10816757348068	-1.28247772787479
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Si	-8.24375983491661	4.00189555959458	-1.29679697228182
Si	-4.86227261163701	6.20938857880318	-1.26678280291351
Si	-1.30839927069469	8.17790498638736	-1.22819851479053
Si	-1.14405208075469	-8.30867428675664	0.97794967775411
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Si	2.43963302160674	-6.22992728553338	1.01492731148812
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Si	5.82066861893377	-4.16336441871531	1.05231537452313
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Si	1.20410251082362	-4.21744475256197	1.03721892197160
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Si	8.05327576474177	0.01020026441601	1.10739207934389
Si	-4.73591917120844	-6.40976644344547	0.99273683943978
Si	-1.15842583818210	-4.23654750995980	1.02377240149538
Si	2.27647140670859	-2.11666306705532	1.05198089782120
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Si	-2.28995683651479	-2.16797441274270	1.03824008458982
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Si	-4.64649910561749	-2.20464937581149	1.03337890886412
Si	-1.19318997161655	-0.08147897233912	1.03171556223695
Si	2.23899570784163	2.03451879447173	1.05915514650480
Si	5.73482111996300	4.14262279710670	1.13827475090700
Si	-8.16071867458826	-4.26980450997135	1.00050513591271
Si	-9.34073529845594	-2.17818132936739	1.02392165920538
Si	-5.76772008499727	-0.12558124289398	1.06453637729701
Si	-2.33618239549257	1.98463520620972	1.08864828996764
Si	1.12124535641955	4.11300403691848	1.12465596500103
Si	4.69355019357778	6.28371426488358	1.16905784751071
Si	-8.11982586638037	-0.14831966474520	1.05464331708271
Si	-4.69290006914718	1.97812579339019	1.08783178443173
Si	-1.24438420922953	4.07911785622992	1.12447348923214
Si	2.31666660147067	6.14768162511257	1.15384519374679

Si	-9.38468603862398	1.85443974334530	1.07539680555796
Si	-5.87899370887186	4.02235296230397	1.11360655097215
Si	-2.48770483552389	6.08721155570939	1.14850085824041
Si	1.09173297435635	8.17940329960683	1.17875876755706
Si	-8.25116567968627	3.97160256821324	1.10510982915375
Si	-4.86776735976234	6.17781276754576	1.15250313173895
Si	-1.31295311029691	8.14952324797293	1.17578947955436
H	1.81912095631549	-9.41312263269846	1.80809974496450
H	1.83551735241491	-9.36970177445954	-2.25527587520641
H	-5.34687835294039	-7.43018770698548	-2.29946241563989
H	-8.84891971627063	-5.26000461445334	-2.25439395563477
H	-8.95681986385371	5.02731392034728	-2.12569906303769
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H	-1.87386628240809	9.30065973805404	-2.04491141055269
H	1.63509858449901	9.34628510441923	-2.03825862949267
H	5.32486800101652	7.38298134212339	-2.09179380038520
H	8.82260109094855	5.19644968535342	-2.07566880619935
H	8.92559420101327	-5.08973702579880	-2.18504456674535
H	5.47610792224518	-7.33789174245763	-2.25040227457079
H	5.45792416508560	-7.37949922749030	1.88394803457720
H	8.90520957885317	-5.13210348697225	1.89657987862071
H	8.79869099313745	5.15173001364332	2.00534528373585
H	5.31573853500503	7.33229762128026	2.04043193355708
H	1.63108982218430	9.29415215453889	2.02372518349594
H	-1.88049559400031	9.25171769873693	2.01882749870231
H	-5.50957319259362	7.21474295894482	2.02349746751762
H	-8.96839627424087	4.97618407653210	1.95568200549809
H	-8.85719963184530	-5.30937842759483	1.82597266860679
H	-5.36011206933966	-7.47931084477818	1.83662530943629
H	-1.67579655859892	-9.39791300665839	-2.26977978843005
H	-1.69228417604506	-9.44092135941539	1.79350726368046
C	0.35873440963048	1.21688213045632	4.08020872952301
O	0.06555510620435	1.60157304709049	5.32737276672723
O	0.91298693117787	0.17012346360962	3.79661177048769
H	0.02913634447535	1.98059503791605	3.34348019504647
H	0.37813067063107	0.89176764292630	5.93149171825787
H	-10.58125147786442	-2.24475860805385	1.86305522591577
H	-10.56859525585690	-2.19433811128145	-2.22807003273195
H	-10.62611373061358	1.87351200179822	1.91564179639806
H	-10.61370299996030	1.92685321872812	-2.17527719684851
H	10.55585991928498	-2.02582565480228	1.94164009621167
H	10.57588584221650	-1.98469108871477	-2.15025528614697
H	10.51333164372481	2.08057220383536	1.98296824160952
H	10.52995835525979	2.12623944596745	-2.10892490203444

- **2Si-OCH₂**

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Si	-2.49094654880064	6.03646425617818	-1.16422033368139
Si	-4.84773318904571	6.22340637490015	-1.38109337446566
Si	-5.89984145525699	4.09130663006567	-1.45624734596858
Si	-8.25857987464356	3.94447127547842	-1.71552507360169
Si	-9.32881023407670	1.79581422403531	-1.71998588397650
Si	2.25877125571359	5.89721534970125	-1.07585596129668
Si	-1.24670399722331	4.04485550319953	-1.02001584440395
Si	-4.72874594786029	2.02569589844493	-1.28372382284278
Si	-8.07080999391554	-0.20154866330577	-1.54094882389513
Si	4.60894088613130	6.13627581454106	-1.17239258839809
Si	1.07167452639716	3.87413288040942	-0.98728620160032
Si	-2.38308509736869	2.01162501713494	-1.04716750606545
Si	-5.73405939391003	-0.09211060992998	-1.32654940554318
Si	-9.25954842151104	-2.24178840139426	-1.59347908227858
Si	-7.91392442875419	-4.21123131888275	-1.47056591650213
Si	-4.36850503748153	-2.00669229738677	-1.23362600917305
Si	-1.09983947787124	0.05560011255583	-0.60575504110900
Si	2.26486123636786	1.88043820064994	-0.85723572684189
Si	5.69137995852324	4.03383027194086	-1.25171862265188
Si	4.58599157654801	1.94706770989839	-1.12272622367556
Si	1.23992949407235	-0.23902184050429	-0.61379369850039
Si	-2.08873269816660	-1.81466379711758	-1.56459132163351
Si	-5.55655130051371	-4.04596593334297	-1.29329966129751
Si	8.04187754636711	4.07553100685957	-1.53035621523843
Si	9.23104510681243	2.00554643525678	-1.66893910876233
Si	5.70805121709563	-0.09488269546695	-1.25436324829869
Si	2.13998969970913	-1.77869062891513	-2.19918412719978
Si	-0.98340531719064	-3.74429485452878	-1.04305444534802
Si	-4.42505333232929	-6.10986793374455	-1.15646475538340
Si	8.03718380341168	-0.03843853100987	-1.56193982194284
Si	4.27717551358142	-1.98566530973902	-1.15793154580647
Si	1.36471250796235	-3.63197980209827	-1.00053822678846
Si	-2.09160506833007	-5.80647141518863	-1.10076758136033
Si	9.30739295260373	-2.01443204985363	-1.78182302128105
Si	5.66289859486514	-3.91966698866173	-1.37329066221684
Si	2.30689809789462	-5.79713208582518	-1.12251924381209
Si	-1.07635443712137	-7.93536246093117	-1.04934166105527
Si	8.01374466373805	-4.02391375419511	-1.72897837940258
Si	4.64467404687660	-6.05629410430276	-1.29369725334452
Si	1.29082604182199	-7.93100609644323	-1.09694821864736

Si	1.08973508755828	7.95813272781779	1.28794467845257
Si	-1.33284827920609	8.06986649763332	1.23807592111212
Si	-2.64098044955666	6.09096241215183	1.22958411946615
Si	-5.02334526461394	6.27897681553385	1.03700054368907
Si	-6.17700263637727	4.19479170827400	0.93876252167335
Si	-8.52328254933249	4.06037440771846	0.66891353321986
Si	-9.53854181055771	1.87670112224519	0.67661175506179
Si	2.31520466768358	5.91562849535274	1.31923845355666
Si	-1.34071177147061	4.09806385376364	1.39853829652661
Si	-5.07108882205188	2.13735427481108	1.08860055432950
Si	-8.26965037390952	-0.13258035549071	0.85346215055215
Si	4.70941295094224	6.12784326782574	1.24884475871091
Si	1.05775105607677	3.88838340519002	1.44795962261332
Si	-2.76815859838655	2.22535142410683	1.29210062199570
Si	-5.91846766499665	-0.05309625637564	1.06678752997105
Si	-9.42670271090849	-2.19311713169398	0.80389527330413
Si	-8.07148802473449	-4.17435622726444	0.92664776078926
Si	-4.52893763716407	-1.98475247365227	1.21340149388465
Si	-1.73266448235759	0.20942851322893	1.74671717832106
Si	2.51412699389959	2.00318433322940	1.52684067109628
Si	5.93098701973754	4.08024292368126	1.13542746998689
Si	4.85084730190236	1.99326315790607	1.27373542236393
Si	1.73551526976260	-0.19548088472796	1.76883148520136
Si	-2.46494636355426	-1.94531003966507	2.32182620354523
Si	-5.70947554782623	-4.01087620127611	1.09731925944918
Si	8.28739110065855	4.07977038366430	0.86052290920425
Si	9.47306370821427	1.97948312942103	0.72427350177491
Si	5.98830138727207	-0.07781464088234	1.13557243880553
Si	2.82308381543489	-2.12358191251288	2.44882960727720
Si	-1.02066197725381	-3.61478011691930	1.43568706740219
Si	-4.47497416171239	-6.02497852908765	1.25316315906507
Si	8.32802699894351	-0.09632961700684	0.82612737607998
Si	4.76591107655074	-2.09069246855017	1.22568801724716
Si	1.38310291369939	-3.69090759360866	1.43875184247921
Si	-2.10540765228779	-5.73282745076009	1.29705899100587
Si	9.58646358293607	-2.09747148074803	0.60268051185669
Si	6.01124753213256	-4.04556875494318	0.99522819366139
Si	2.43359867162608	-5.81916712378415	1.26467644053976
Si	-1.04205217064509	-7.85180179844929	1.35185753095931
Si	8.34690558718326	-4.15214818699559	0.64785204719619
Si	4.80824743177592	-6.07753868738951	1.12046795862083
Si	1.34845780690292	-7.91140681503660	1.30820564394195
H	-1.79666851629384	9.23353159533661	2.06295557373472
H	-1.82210586906184	9.16995052234344	-2.02409349537870

H	5.12436130049552	7.22979559319462	-2.05757555056374
H	8.59373741012143	5.13070164426141	-2.44049354354743
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H	5.13592885009776	-7.13633606263517	-2.21065253781050
H	1.91777923404360	-8.97144266181262	-1.97319628846185
H	-1.77100192160898	-8.98170688988790	-1.86584692900918
H	-4.90813098030113	-7.23298516327063	-2.02185804739122
H	-8.41499798817748	-5.33172481147620	-2.32992440347987
H	-8.90674663254769	4.88282731976393	-2.68715774597053
H	-5.35259626379588	7.30419695264263	-2.28726684694857
H	-5.70856466703041	7.36904364711884	1.80391012872822
H	-9.38329374719593	5.06685239071358	1.36994475992676
H	-8.71998091775983	-5.25184744289080	1.74194319122540
H	-5.02015177371692	-7.07363490567080	2.17478496496360
H	-1.64896864817531	-8.88290430882773	2.25536407997828
H	1.90155437374878	-9.00329470440532	2.17385506731882
H	5.38998931956414	-7.16791089954545	1.97203143907002
H	9.09153323729720	-5.25515056354254	1.33831592439390
H	9.10183707400668	5.08511651092248	1.61865359358328
H	5.29788217442665	7.21608941858061	2.09606296377108
H	1.76347021177915	9.03561834997356	-1.94065918737295
H	1.60040524917278	9.09509494922802	2.12372056066206
C	0.44062856897370	-0.17698109437859	3.19196293862282
O	-0.61469783071554	0.73315968308551	2.90438238868599
H	0.97448813441135	0.17495823096855	4.09512430505088
H	10.79021768214195	2.08212240526225	1.43419896105795
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H	10.90167115484590	-2.20111927367979	1.31455330308488
H	10.43197258196997	-2.03309667787377	-2.77167979098101
H	-10.85524940069511	1.89569445928194	1.39332313817457
H	-10.50416373250490	1.76838615149337	-2.64990834048516
H	-10.69892443708173	-2.33476225973778	1.58257600827709
H	-10.41548846445033	-2.35885686280029	-2.53858663824511
H	-2.65627708078432	-2.12522619530295	3.79608055879679
H	2.90179469371344	-2.26123047504705	3.93816770977762
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Si	-4.59128563936474	6.24260030645753	-1.14944000392027
Si	-5.67036873088145	4.13581920384521	-1.24143328750310

Si	-8.02784158463803	4.16389830766969	-1.48181657033791
Si	-9.23270896543284	2.10142318930859	-1.62186165703689
Si	2.52081098406989	5.98378851568268	-1.14458153646712
Si	-1.05782869216334	3.96408637022622	-0.97380701441491
Si	-4.57845977655340	2.04034529030467	-1.14072402369072
Si	-8.05748840837321	0.04363115273676	-1.55458707056229
Si	4.88149592506179	6.11514619072695	-1.34935959603869
Si	1.26442931326533	4.00337813801792	-1.02357521417660
Si	-2.25452976591329	1.96208212670704	-0.89299994193440
Si	-5.72349937173521	0.00843313312410	-1.29692183494283
Si	-9.31707707617549	-1.94137545204412	-1.76189384552953
Si	-8.08143960093478	-3.99225531281306	-1.73499007457688
Si	-4.44547658826799	-1.97387903324820	-1.25530483742830
Si	-1.14063121136566	-0.08966426430512	-0.62023005873842
Si	2.38586773318286	1.96806526467182	-0.96684773806894
Si	5.90121712527636	3.96933463462623	-1.40180690467938
Si	4.72717240682830	1.90626936955364	-1.22312347029612
Si	1.20312722512252	-0.06227490501326	-0.63130699928459
Si	-2.16997254723307	-1.84077054099400	-1.76801123104515
Si	-5.72193283724732	-3.96448110838813	-1.44126310474626
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Si	9.29356809796537	1.66687009979640	-1.73529561619300
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Si	2.03343246600098	-1.77888386917925	-2.05219804232743
Si	-1.19435896234186	-3.79056821895887	-1.04966461789045
Si	-4.63823755098149	-6.06921441236136	-1.34594042483070
Si	8.01608418370535	-0.31380834465787	-1.53130113820608
Si	4.18106842577504	-2.05131098925243	-1.09651886085390
Si	1.13913853396797	-3.64538440808291	-0.95982399468963
Si	-2.29579854815847	-5.85659706818510	-1.18248580254813
Si	9.22972295581065	-2.33694934730838	-1.62049886425295
Si	5.49505329795140	-4.03120220974393	-1.21274624872583
Si	2.10730701999206	-5.79371412047194	-1.04209699725976
Si	-1.27609971390860	-7.98713073132635	-1.10709846739520
Si	7.84013360670466	-4.26977881967126	-1.48695727338894
Si	4.43470970276509	-6.13491831625656	-1.10611018856930
Si	1.09069744055532	-7.92349211532467	-1.05326390528087
Si	1.40389482174576	8.02796173891397	1.27184697814781
Si	-1.02114423150857	8.03073722247247	1.31867608993173
Si	-2.30658621815896	6.02829528251292	1.35458156345498
Si	-4.69501637184095	6.22648871554600	1.27274451053872
Si	-5.88688993167556	4.15870714257722	1.15566112055720
Si	-8.24791221841411	4.15192903295737	0.91102620679175
Si	-9.43719076389311	2.05572031237406	0.77478923089973

Si	2.66876501905401	6.01661698704340	1.24801077186338
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Si	-4.82468604106170	2.05568761437978	1.24509264898097
Si	-8.29859130488718	-0.02790371673774	0.83562685073633
Si	5.06142140549944	6.17118571905729	1.07098284364727
Si	1.35957053553411	4.03180359464329	1.40018623977610
Si	-2.47919821323390	2.07800597305389	1.48356028216241
Si	-5.95274867899337	-0.02120298374211	1.09731719074484
Si	-9.56091422453131	-2.02744290293170	0.62840562765101
Si	-8.35890770590140	-4.10648922748097	0.64877008970356
Si	-4.79609398567027	-2.07933496713751	1.15509691443288
Si	-1.75096941578423	-0.15215564732166	1.75999636533959
Si	2.79670880214095	2.14992043960295	1.38349593937307
Si	6.21461395121970	4.08857596707180	0.97786276511957
Si	5.09192915943142	2.04064814664965	1.15185034423457
Si	1.74352203379974	0.10644795053417	1.72365194806087
Si	-2.80032006428437	-2.14180454687819	2.29928647307504
Si	-6.01126995189813	-4.05633840106478	0.93843759883458
Si	8.55455830300202	3.93906188945735	0.66809233552879
Si	9.55055281902194	1.74437960935152	0.65660016992687
Si	5.92882081627383	-0.15772677249240	1.13872207215803
Si	2.48302282441310	-1.98475825216725	2.44526627301834
Si	-1.30268753765960	-3.73600383426093	1.41879726112833
Si	-4.78470032323859	-6.07720623096527	1.06500888675396
Si	8.27303342531065	-0.25462374381978	0.85941671212556
Si	4.52240374566945	-2.07052396933705	1.31837790043558
Si	1.09029978170084	-3.64913027636759	1.48777818791522
Si	-2.40660233911519	-5.83341868429961	1.21372567830898
Si	9.44449767977631	-2.30788619065546	0.77196549131377
Si	5.73490983004882	-4.06865723272978	1.16953000015251
Si	2.14041120087572	-5.78503565882147	1.34887799442092
Si	-1.33094575012403	-7.93497890665874	1.29449855095392
Si	8.08137540551132	-4.28115693321357	0.90525117518499
Si	4.50982102216475	-6.08913554225083	1.30831959025095
Si	1.06053168624092	-7.89236619049087	1.35294799413456
H	-1.49133434726758	9.18603566757198	2.15262825953047
H	-1.66153645022254	9.12315801255739	-1.91234948013595
H	5.40441117050945	7.18271236520221	-2.26185588708017
H	8.87785890064509	4.76788303190464	-2.69519706446849
H	8.27631534948177	-5.39010495744495	-2.38238747494388
H	4.92246753813244	-7.24650113546669	-1.98597611257861
H	1.78013803453999	-8.95451147649522	-1.89341694166502
H	-1.90382352258425	-9.03847021117489	-1.96970113980545
H	-5.12484593998185	-7.15108693561678	-2.26147393376795

H	-8.62184962297001	-5.00641978104971	-2.69723168223445
H	-8.59512908642465	5.22368749755536	-2.37624672753429
H	-5.11769663437326	7.34191712680902	-2.02046372856090
H	-5.31748531253762	7.30285321671929	2.10986617243173
H	-9.05239185228758	5.15428619468570	1.68252242545740
H	-9.10150672754185	-5.19676390402135	1.35954835845688
H	-5.37029045449341	-7.16523384452639	1.91452535586230
H	-1.93196850322399	-8.99137383629058	2.17176753206482
H	1.61475361676888	-8.97134461142155	2.23468792964010
H	5.04410411915985	-7.15498566118193	2.21944886876891
H	8.75702923014228	-5.37406925247272	1.67868856697167
H	9.43489018260379	4.93695701892915	1.35747774328240
H	5.72028569422928	7.27376204504986	1.84424028285419
H	1.92390273788090	9.13504293446138	-1.97932324378196
H	1.90851720921297	9.17214727552016	2.10018983591764
C	0.44837477413318	0.60387509058222	3.04775993033838
O	-0.62283252206018	-0.33475290341096	3.01591055061049
H	0.07537333696649	1.64160556619834	2.91339409656243
H	10.87978959259025	1.76729142897879	1.35079757834565
H	10.45006210857669	1.62324336569942	-2.68848321421708
H	10.73050265114640	-2.44536790594674	1.52967893104820
H	10.36704665580847	-2.44322342037038	-2.58974733308983
H	-10.74470372399068	2.14431011445805	1.50324722406210
H	-10.39831876940099	2.17652613541589	-2.56093835675235
H	-10.86880469967203	-2.12366078606581	1.35365560151731
H	-10.45779427755618	-1.95441697377166	-2.73302491426765
H	-2.95386524261019	-2.27409827103170	3.77888619558486
H	2.56260381330182	-2.09123899497480	3.93593142737574
H	0.94311822257777	0.54813945685609	4.03606796047776

• **2Si-OHCH₂***

Si	1.32503612397098	8.03204172928495	-1.11424756414705
Si	-1.06333597621751	7.99120269549649	-1.06542388183515
Si	-2.24709039893640	5.93894540671405	-1.02883502965671
Si	-4.59676321926938	6.19630811713555	-1.13086949727153
Si	-5.67491378783654	4.09012413052624	-1.23325125598373
Si	-8.03290776623646	4.13533372241193	-1.45421841079661
Si	-9.24054868464220	2.07575941733864	-1.59390523652340
Si	2.51458762657851	5.98089525953905	-1.14292190832720
Si	-1.06364956127082	3.90641935595831	-0.98460914441521
Si	-4.57198481148365	1.99772651668951	-1.14726415082010
Si	-8.05924128463661	0.02146479189136	-1.54749269684256
Si	4.87709592218766	6.10957448296349	-1.34669101678531

Si	1.25823842672052	3.99984384167544	-1.03190743777250
Si	-2.24750435471141	1.89449051290368	-0.90428878661178
Si	-5.72144551541551	-0.03028284174609	-1.32457291266034
Si	-9.32960404318193	-1.95488400392178	-1.76096644571550
Si	-8.06589279403077	-3.98745364432493	-1.74981155846075
Si	-4.37863759956334	-1.96186714940733	-1.37026477226599
Si	-1.16110414462204	-0.18748841546771	-0.74406770717346
Si	2.36934142546219	1.95427892202244	-1.01425086669971
Si	5.89587786723396	3.96240281182972	-1.40549444119252
Si	4.71628982374729	1.89988441347126	-1.23982491684801
Si	1.18715844855578	-0.08673899789737	-0.69606482909994
Si	-2.16407827871035	-1.84958826451584	-2.04167673905401
Si	-5.70214728141507	-3.91454769415933	-1.51792209150031
Si	8.24865460560339	3.82023978945528	-1.69394995284543
Si	9.28170461519063	1.65555040191407	-1.71632520317411
Si	5.66391843971094	-0.24596463725739	-1.24914152240973
Si	2.03389252538206	-1.79112684546314	-2.12824380203105
Si	-1.22589460621092	-3.72348769402321	-1.13211644456301
Si	-4.62224234003603	-6.01858469952947	-1.38475185748026
Si	7.99989030981127	-0.32387640154085	-1.51646506709196
Si	4.14396235092295	-2.05450200387473	-1.08203766875990
Si	1.11086731329601	-3.61560238039422	-0.96167968176736
Si	-2.27994193276930	-5.80350513778348	-1.21768737522964
Si	9.20950393664208	-2.35015241433843	-1.59638061374022
Si	5.46689389091451	-4.03186899736360	-1.18975590521209
Si	2.07006701646520	-5.77392445513687	-1.02235536691908
Si	-1.29927696308287	-7.95038778962649	-1.10725003495934
Si	7.81114843468563	-4.27778507028921	-1.46209297804933
Si	4.39634496069541	-6.13032135464154	-1.08877698947897
Si	1.06655212276970	-7.90918627082181	-1.04845545954119
Si	1.38571019808793	8.00720226566796	1.28608889160519
Si	-1.03743858072161	7.97592479728364	1.33861166792378
Si	-2.30463913564426	5.96203675902663	1.36822458745028
Si	-4.69074086216814	6.16392939283218	1.29045232726983
Si	-5.87307285829903	4.09435823760824	1.16278671941899
Si	-8.23447808179161	4.11010630573811	0.94177053647284
Si	-9.42269713967313	2.01733413169729	0.80393360602934
Si	2.66602388171508	6.00786175079811	1.25290632634595
Si	-1.05155833354310	3.93338685561834	1.43552702846384
Si	-4.81018564703511	1.99226356223138	1.23404601561318
Si	-8.27830180892500	-0.06262758890241	0.84383160360239
Si	5.05638430261628	6.16315148081193	1.07205047607245
Si	1.35578080547804	4.02492215672960	1.38710173767986
Si	-2.46490348218322	1.99333397404965	1.47414147093947

Si	-5.92954997997166	-0.08033575967687	1.07673173710147
Si	-9.55494820848155	-2.05019058711512	0.63060501975744
Si	-8.30276567425626	-4.09366407082442	0.63821713328168
Si	-4.65892124575576	-2.05698816065311	1.14379018209890
Si	-1.88409895641148	-0.29027090460606	1.58751755149119
Si	2.76395861858391	2.12883304353912	1.33028170671951
Si	6.19115399716914	4.07289856337384	0.97822474185046
Si	5.06332585799497	2.02613673459676	1.14153403108291
Si	1.71461677974749	0.07810515286942	1.65427173287964
Si	-2.84294222953540	-2.17291941231589	2.53738831057273
Si	-5.95312896091717	-3.97278058492625	0.86924802774098
Si	8.53397066433172	3.92249949646940	0.68899001106739
Si	9.53335714238059	1.73027958169871	0.67536782097777
Si	5.90754710233253	-0.16653925503175	1.14692733581688
Si	2.44797277425882	-1.99534356491566	2.43461454965458
Si	-1.36101941309757	-3.62851752268810	1.42400081618061
Si	-4.75726888400319	-6.00489508167381	1.01742472404458
Si	8.25159278299085	-0.26441202585377	0.87456401145442
Si	4.49854554263044	-2.07399127272342	1.32732623316435
Si	1.04183081321310	-3.64118246274700	1.46933504468837
Si	-2.38604297697293	-5.75727050150439	1.18758722059829
Si	9.41824172779388	-2.32042571930142	0.79631756253119
Si	5.70638112240908	-4.07611442047650	1.19318455565396
Si	2.10618765224908	-5.77416899556186	1.36626068121791
Si	-1.35786625681871	-7.87966338607785	1.29118049180140
Si	8.05162894189212	-4.29059743512930	0.93036885242368
Si	4.47188095508404	-6.09045302998279	1.32617235336935
Si	1.03124974191238	-7.88124968659745	1.35785505343218
H	-1.52354706023057	9.12143608736745	2.17677575455963
H	-1.69806760936603	9.07501354798678	-1.88307819198203
H	5.40028594030502	7.18127906664373	-2.25394929296891
H	8.88857329253617	4.76423956150140	-2.66627704460047
H	8.24763835398912	-5.39830261310751	-2.35709008203716
H	4.88162425425095	-7.24516742577217	-1.96618734390541
H	1.75727242173197	-8.93495639271037	-1.89424138351366
H	-1.94560004840125	-8.99669115694052	-1.96241225987908
H	-5.09655769409711	-7.10158879150433	-2.30525998779114
H	-8.61103826634425	-5.01336365594846	-2.69680153119502
H	-8.60347758060726	5.20245620070065	-2.33779021277620
H	-5.10866538635798	7.30348887740355	-2.00054799555378
H	-5.30395350480909	7.22899611999505	2.14865511769193
H	-9.02292006348566	5.11346816349438	1.72838365354598
H	-8.98653750737287	-5.20631368579841	1.37293774274046
H	-5.35949859206595	-7.06401412893705	1.89069377137824

H	-1.98953782777154	-8.91353207074181	2.17374577044428
H	1.57369822815206	-8.96432653688061	2.24225052175053
H	5.00482522845048	-7.16086985915861	2.23312708172033
H	8.72679539690331	-5.38261779543579	1.70553108935186
H	9.40246718009557	4.92248472227411	1.39018419020813
H	5.71920807687699	7.26152705059547	1.84763599527755
H	1.88453901328728	9.13390841927616	-1.96159808012898
H	1.88039674943601	9.15003354856226	2.12187006527045
C	0.49434564812386	0.62099675127033	3.0355155772698
O	-0.58591169230467	-0.37876773334567	3.03321645268653
H	0.04639193147257	1.62460419672215	2.91867020959962
H	10.85954586994251	1.75376767957707	1.37533766453022
H	10.44021740871058	1.60993060653768	-2.66693770029602
H	10.70230852209201	-2.45365448604052	1.55806867861698
H	10.34939528672009	-2.46369014855685	-2.56181160614385
H	-10.72289728923321	2.09531449737288	1.54647289294665
H	-10.41372976200279	2.15651638188891	-2.52299215609023
H	-10.85249786108425	-2.15628153796610	1.37267549969832
H	-10.47167953330568	-1.96095756978396	-2.73049669105349
H	-1.10287417710341	-0.44968369579017	3.86855980887474
H	2.49029702206605	-2.04684315645311	3.93298680074382
H	1.01262809986785	0.54844399265023	4.00689495472300

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Si	1.83720510071643	0.16014683251723	-0.20962590496860
Si	-0.56275962525972	0.18761676721428	-0.20462313058841
Si	-1.76258182083913	-1.85415643687483	-0.20570248087017
Si	-4.12754066155597	-1.66629639361718	-0.21465504284809
Si	-5.19133698214501	-3.78853582781422	-0.19686041479738
Si	-7.55678919019150	-3.71985490333685	-0.19444835872367
Si	-8.75591586924741	-5.79244323727379	-0.18741040254080
Si	3.01798483852218	-1.89719956073450	-0.20372098009359
Si	-0.57573136484133	-3.89717842556964	-0.20941569984816
Si	-4.04806350156057	-5.85576950130052	-0.19408812766235
Si	-7.54877509921448	-7.83183496297043	-0.17652202960065
Si	5.38153632304883	-1.75759047424352	-0.21260933210744
Si	1.77110055584420	-3.91038879052518	-0.19024655604681
Si	-1.70203965912779	-5.95607042925199	-0.22020313614492
Si	-5.19263051571761	-7.90035337501244	-0.19200082665029
Si	-8.83853739773914	-9.81045123665377	-0.16261188324880
Si	-7.53972712142879	-11.81443897134312	-0.14660064418481
Si	-3.82146930039465	-9.78234258266145	-0.43785797417658
Si	-0.67647645387586	-8.08375749538663	-0.27270833830750

Si	2.68135287695990	-6.08733038820405	-0.20497006464167
Si	6.27351881228302	-3.95299717993668	-0.19907902905551
Si	5.02807587097911	-5.96436901524358	-0.18668009917422
Si	1.60741339501117	-8.06586697017780	-0.70742091817372
Si	-1.74187639188051	-9.83603536301047	-1.38823699455861
Si	-5.17407740633535	-11.67325574068357	-0.14841304609330
Si	8.64233429161367	-3.99847879247538	-0.21453644330174
Si	9.77667022261777	-6.10569899462268	-0.22206972483781
Si	6.12218562668551	-8.03563783093637	-0.21340081162915
Si	2.65420211294678	-9.91803242167439	-1.40884416842042
Si	-0.80406766631219	-11.59453679839245	-0.20556522346724
Si	-4.20674161335700	-13.82863957083844	-0.14739646416488
Si	8.47861596620216	-8.08297123403228	-0.22517900364227
Si	4.67930546132443	-9.90136517231245	-0.23184855516106
Si	1.56527479476166	-11.59976848327712	-0.18778601685550
Si	-1.84750587315985	-13.70390028250547	-0.16168297676119
Si	9.69809825245637	-10.10527993665726	-0.22590016200063
Si	5.98528510765097	-11.87682064612198	-0.20395442094747
Si	2.56542216034396	-13.74976169236975	-0.17735654717017
Si	-0.86277264704214	-15.84997726062327	-0.16729684834434
Si	8.34502405079334	-12.07642766953436	-0.21833224083659
Si	4.92134217221266	-13.98723707017410	-0.20579267962764
Si	1.51823827698315	-15.86817428971691	-0.18198601665197
Si	1.84238467783276	0.16624032799543	2.19495598263149
Si	-0.55810222683188	0.18415550012290	2.20101495361538
Si	-1.75871188741836	-1.85885719273296	2.19878614510346
Si	-4.12389092352768	-1.66293560652539	2.21440698099341
Si	-5.18557509292233	-3.78619066915473	2.20461874882988
Si	-7.55212525928235	-3.71672658685376	2.21342720422985
Si	-8.75846446293506	-5.78446864437721	2.21754590712071
Si	3.02019125034599	-1.89174704110525	2.19953313424849
Si	-0.57078494436050	-3.90320244453580	2.19644237200176
Si	-4.03905269295292	-5.85181647234462	2.19729408942435
Si	-7.54840898415545	-7.82050170445595	2.22513896126872
Si	5.38496054547970	-1.75839408473605	2.21052658456153
Si	1.77839910926808	-3.90481702530333	2.20668317881706
Si	-1.69537177145573	-5.96458050016644	2.18468626774988
Si	-5.19501233923880	-7.88919975205353	2.23624485541637
Si	-8.83690242198454	-9.79936165689148	2.24056804379289
Si	-7.54831014866592	-11.81056224756945	2.25140746414917
Si	-3.84112345975525	-9.77622759782354	2.51187304910096
Si	-0.63119039774312	-8.07358639568700	2.16273350954195
Si	2.67115004489832	-6.08663686410697	2.23198986797658
Si	6.28474989649955	-3.95166367846508	2.20340280285763

Si	5.02748776747073	-5.96060794261122	2.20592622122804
Si	1.46588167517489	-7.84746292018416	3.20606119337621
Si	-1.71022232395001	-9.76646869264124	3.33698667224695
Si	-5.18265268813783	-11.67978398676081	2.27622201866774
Si	8.65470822384188	-3.99550708442747	2.19150260279969
Si	9.78251974435611	-6.10623237200238	2.18353985737040
Si	6.12919093181905	-8.03256055027560	2.18772204481624
Si	2.65413595992427	-9.88241293657514	3.33254393097027
Si	-0.79978871684670	-11.60450835467634	2.27046481390313
Si	-4.20631920080717	-13.83202957551460	2.25257583130877
Si	8.48454300185246	-8.08310623599118	2.18169289790929
Si	4.70169487432695	-9.90093500614893	2.20417283079017
Si	1.56392760055036	-11.62450021412053	2.22064289635466
Si	-1.84711249023157	-13.70770902626602	2.24602582410933
Si	9.70877325234087	-10.10179135560966	2.17920134722206
Si	5.99262679633625	-11.87446017345680	2.19695300119376
Si	2.58296948690338	-13.75394105759618	2.22027647822348
Si	-0.85521882473038	-15.85097077131273	2.23583367793723
Si	8.35367563241955	-12.06969702667562	2.18418658889145
Si	4.93617234324050	-13.98607145446238	2.20582521642018
Si	1.52641636451856	-15.86645990080846	2.22346478478135
H	-1.10406506297464	1.29615039299705	3.04508341218097
H	-1.10761170853646	1.30440100968375	-1.04287334919335
H	6.02969374998046	-0.73367360664943	-1.09391768188629
H	9.33457970556867	-2.97351238335617	-1.06126715987465
H	8.92261275684303	-13.17476751101342	-1.05933259771463
H	5.49207534536615	-15.04674983597550	-1.10030995729713
H	2.11728316928793	-16.93877545876899	-1.04301269182821
H	-1.51172973464900	-16.89115727709795	-1.02774284400002
H	-4.86204774259216	-14.82292065010956	-1.05595391577590
H	-8.11673172895301	-12.91607310476641	-0.98224121509344
H	-8.23047321977171	-2.68236963129326	-1.04066435287182
H	-4.72999381812023	-0.60835645717635	-1.08851284271516
H	-4.72068278677182	-0.60216080137298	3.08899667139455
H	-8.21558533990477	-2.67275726850773	3.05986999236702
H	-8.14531714781032	-12.90146290659938	3.08721531920940
H	-4.84449790752581	-14.83575800531780	3.16321839643896
H	-1.48872942630563	-16.89611612850813	3.10328611363655
H	2.13944356524580	-16.93026157566789	3.08338366918077
H	5.52077837924946	-15.03605171282495	3.10284290917448
H	8.92514076798582	-13.16886375130899	3.02855509079626
H	9.36286886407700	-2.97478105317289	3.03038178666065
H	6.02801741821344	-0.72812542017268	3.08840914310180
H	2.40126178037607	1.26274953713970	-1.05396112296565

H	2.40774418564083	1.27480485883569	3.03074943517367
C	0.91363016726862	-7.48333364929060	5.02090146714327
O	0.24644954804317	-8.67343665680601	5.46564291602665
H	0.24052046536347	-6.59971243171136	5.02043274028434
H	11.01886276683522	-6.09605578864954	3.03093243994863
H	11.00907274831667	-6.08484632450471	-1.07484705663454
H	10.92666185353158	-10.19875224974494	3.04713201710317
H	10.91178954494320	-10.20464162049320	-1.09929314456889
H	-9.99642402643915	-5.72766005954054	3.06065852973506
H	-9.99256398443346	-5.74467412552616	-1.03291953503554
H	-10.04995162704424	-9.84894467074569	3.11827608060071
H	-10.05138363881749	-9.87936478157437	-1.03909886635077
H	-0.24256773678279	-8.47423278985266	6.28483603444441
H	2.86515573253985	-10.19879799651491	4.78036838480961
H	1.78986527255824	-7.24620984079251	5.66025752936905

• **2Si...CH₃OH**

Si	1.43072854648584	8.02330689578989	-1.24127699629906
Si	-0.97281414241223	8.07848704564367	-1.22060390206276
Si	-2.21122773389977	6.05551695369475	-1.23358199235504
Si	-4.57825322325160	6.21165594696778	-1.22802737354483
Si	-5.59313170438455	4.06162559749489	-1.22964475393193
Si	-7.95889516425365	4.12711865967431	-1.21438208836517
Si	-9.15371367580766	2.05496726473141	-1.22193663560559
Si	2.56717481509163	5.94113810125622	-1.28360386207639
Si	-1.06080929507532	3.99065198611675	-1.31128643105521
Si	-4.43097863984916	2.00295015479445	-1.29918635499312
Si	-7.92564451187842	0.02977276545153	-1.25733584580190
Si	4.93855498076884	6.00155498765384	-1.30880962944771
Si	1.29322511421364	3.94945390758688	-1.30035012080615
Si	-2.09802810797938	1.89580882522936	-1.30958069532595
Si	-5.57135047200940	-0.04442596635794	-1.30513266787701
Si	-9.23342387126959	-1.93815054245894	-1.25842504264718
Si	-7.98526300550707	-3.97353284069378	-1.28131595599823
Si	-4.26986892696789	-1.96925178857433	-1.59039807073071
Si	-1.13241420577764	-0.23717720143258	-1.43750339244361
Si	2.27561423457636	1.81475219930948	-1.35677646358827
Si	5.86566867099886	3.81463307321667	-1.32854423988424
Si	4.62344440291094	1.80245923248162	-1.34463300348962
Si	1.23172697672761	-0.29288420361712	-1.43199751149592
Si	-2.17373658517394	-2.01462182947739	-2.50681568856111
Si	-5.61887195713009	-3.86428162134035	-1.31046356350837
Si	8.23252836552459	3.77031046794127	-1.34151716787798

Si	9.34601971933864	1.65123864691418	-1.36815076486362
Si	5.69858412863214	-0.28292142744325	-1.38303547518231
Si	2.21380964700041	-2.08613122266287	-2.51170235422168
Si	-1.20893865400779	-3.80044653962202	-1.37879169995526
Si	-4.64084065639049	-6.01557699394202	-1.33323590633305
Si	8.05468083995360	-0.33396166272651	-1.38122258620529
Si	4.28023785407371	-2.15003794802327	-1.48223536361626
Si	1.15600335250345	-3.83090591152818	-1.42465666409156
Si	-2.28015496908119	-5.89788232825736	-1.35236816126087
Si	9.28812199718397	-2.34830172900483	-1.40409835111229
Si	5.57863240286541	-4.10221289737723	-1.39889227920753
Si	2.14171818399001	-5.96784141470152	-1.39001712325053
Si	-1.30144167817581	-8.04641044473046	-1.37825738306123
Si	7.93738141510668	-4.31878631118052	-1.40912146393721
Si	4.49524834708381	-6.20222694675289	-1.40950298359286
Si	1.07980722972011	-8.07804760693098	-1.39793674593683
Si	1.44876176863866	7.98791739134700	1.16308769023685
Si	-0.95351475770584	8.04319548606018	1.18224368472727
Si	-2.18738026265831	6.01754860844334	1.16933416347918
Si	-4.55252434235937	6.17590684934798	1.19798283474418
Si	-5.56704288696170	4.02831796406616	1.17027120144414
Si	-7.93238430914521	4.10074167297313	1.19370429126876
Si	-9.12628833325606	2.02977640193592	1.18319291140752
Si	2.58241663202465	5.90476734809903	1.11865488781639
Si	-1.04553509570067	3.94934509282268	1.08941942856808
Si	-4.40634362094473	1.97159016803628	1.09431727579459
Si	-7.89707600236080	0.00568438171764	1.14274299470102
Si	4.95273416728199	5.97097732802669	1.11816170120953
Si	1.30751556988712	3.91463399160128	1.09937999001493
Si	-2.07597399296376	1.84290291023515	1.15530605612254
Si	-5.54460739676932	-0.07332479037927	1.13824114004345
Si	-9.21050700781297	-1.95657813926201	1.14424992441880
Si	-7.96076974474365	-3.98939948195958	1.11668794076785
Si	-4.21981178596656	-1.99348589971858	1.34730325790345
Si	-1.11930251844951	-0.29587073117767	1.00998390570852
Si	2.28302114621534	1.77823481262816	1.05505316918446
Si	5.87613829789188	3.78416766575493	1.07448276631847
Si	4.63064544730689	1.77408608814339	1.04689359057169
Si	1.24454052402506	-0.33296876496475	1.05886210832181
Si	-2.09964099029632	-2.01616474104896	2.23643022757943
Si	-5.59258327758051	-3.88039730334809	1.10598672575471
Si	8.24341851365838	3.74294969531879	1.06741462760254
Si	9.35908176778764	1.62650911412204	1.03659562160861
Si	5.70898372412058	-0.30865516908878	1.03815865471739

Si	2.22833521971118	-2.10532068937266	2.17238503652436
Si	-1.18812403349080	-3.81553312924656	1.08438636557205
Si	-4.62088665158307	-6.03468209102387	1.06886954273309
Si	8.06439331166038	-0.35600553214222	1.02128975181437
Si	4.28789178339456	-2.17389347926081	1.12448053822914
Si	1.17696063767878	-3.84982430109777	1.08168019412341
Si	-2.26023681520549	-5.91336885432735	1.04821971186558
Si	9.30081115933750	-2.36816114619525	0.99995962426963
Si	5.59180780417852	-4.12293265475648	1.01319577191614
Si	2.16038548676226	-5.98620240911919	1.01289246856824
Si	-1.28249536594775	-8.06328424755784	1.02553296714316
Si	7.95100494557222	-4.33843081572024	0.99064306466037
Si	4.51330768432314	-6.22507309838045	0.99357212219592
Si	1.09831130560965	-8.09566759415165	1.00546181226120
H	-1.47590975731877	9.15802349031065	2.03755822843013
H	-1.50580926383909	9.21928963222090	-2.03404122304485
H	5.59871225004619	7.03564180536581	-2.16942715313343
H	8.94446646214841	4.79014362359632	-2.17812972618470
H	8.48989435982548	-5.41982882049299	-2.26270214054803
H	5.06249590392360	-7.23611653712876	-2.33417381288102
H	1.68192065938643	-9.13525997756928	-2.27289349385842
H	-1.95057854440053	-9.08203884875078	-2.24519723602760
H	-5.29533094069524	-7.00916211495009	-2.24383039086714
H	-8.60041553002949	-5.05082935192578	-2.12147158770594
H	-8.63889797457581	5.17467132028199	-2.04319736222938
H	-5.21398837117887	7.26875088441192	-2.07934519860757
H	-5.17363288720261	7.21000224451450	2.08733739929091
H	-8.59135394648077	5.13238631551893	2.05857251453886
H	-8.55531551390185	-5.08029280494397	1.95416224767501
H	-5.25772885579415	-7.04605078214194	1.97238818220949
H	-1.91813974339992	-9.11107494213290	1.88792749901938
H	1.71627265060581	-9.16486134335508	1.85441185551648
H	5.09139260563934	-7.27953127991447	1.88777594556246
H	8.51294065155146	-5.45371760650590	1.81917655912603
H	8.95655547142596	4.74766318544360	1.92109322317534
H	5.62056016551537	6.98419990659157	1.99763296955099
H	2.00224016458122	9.13787323364770	-2.06490701627689
H	2.03919440499776	9.07280308836967	2.01273266400224
H	10.60052691404522	1.62085179165824	1.87665479221687
H	10.57868553648914	1.66744813634824	-2.22090890355648
H	10.51833172860053	-2.46731435678892	1.86745771121079
H	10.49579558497510	-2.43909442049992	-2.28619282086529
H	-10.35331906195107	2.05509653330910	2.04375991439651
H	-10.40040904424650	2.10430624965051	-2.05254665845589

H	-10.41440646281130	-1.99515986440079	2.03508888351237
H	-10.45464735042165	-1.97060706489419	-2.12565598356617
C	-0.72867958430644	1.70708103067100	4.11437459706931
O	-2.05305406962413	1.54145717115995	3.58397646049018
H	-0.51534973899103	2.78670241220905	4.09460504500757
H	-2.26205152414546	0.58176218203218	3.58009771564039
H	0.02455196162391	1.18070741807711	3.49512946319405
H	-0.67476705969792	1.34166522051449	5.15534984866207

• **2Si-CH₃OH + H₂**

Si	0.86981394889119	8.11385411816088	0.31323982024869
Si	-1.50822527093788	7.97665272847505	0.04498230140271
Si	-2.51760912831368	5.89412588514367	-0.44928069087892
Si	-4.85647488235087	5.81207332809940	-0.71747157358505
Si	-5.54210506887572	3.60766695750486	-1.26325319255165
Si	-7.88947610249521	3.78484332417526	-1.43364316380573
Si	-9.08262030599509	1.78583595635372	-1.93147747516328
Si	2.12812421315886	6.12274213229025	0.05740055041490
Si	-1.29004085953768	3.90630990658696	-0.70990112885622
Si	-4.32078346151417	2.11764172808338	-2.55107700246025
Si	-7.69632363136555	-0.11316446580152	-2.16708758996148
Si	4.47927621500168	6.32954632436017	0.31777137549217
Si	1.03384428755737	4.07811403681945	-0.42985815543400
Si	-2.43558739892592	1.93841244540201	-1.24266854438681
Si	-5.37421779113880	0.15654654437966	-1.94033980387359
Si	-8.93190526049388	-2.06956107326484	-2.63776165906711
Si	-7.64444486389739	-4.05868475296445	-2.86774725613615
Si	-4.11146764354846	-1.82949285549099	-2.17132400749907
Si	-1.10032417200838	-0.00193125941100	-1.48968648101856
Si	2.18835934397951	2.06080470542324	-0.73311463272544
Si	5.59246584314665	4.24704611476006	0.05589061570314
Si	4.50634546096681	2.20698818815539	-0.43959106221594
Si	1.25264970005265	-0.01882331420617	-1.25832345035291
Si	-1.94349784030149	-1.60992759938070	-2.90332685265927
Si	-5.31641414896519	-3.79408619987920	-2.59161135981152
Si	7.94360932343742	4.33196306515853	0.31728936271430
Si	9.16628812351229	2.29134499213589	0.06396564139779
Si	5.66034572787610	0.19059639139014	-0.72354898705737
Si	2.42750916718586	-1.53355147413957	-2.56932369897895
Si	-0.90823872795195	-3.52635980632716	-2.15741465782062
Si	-4.17927678880339	-5.84589213373669	-2.84866140969463
Si	7.99393521997677	0.29195467593883	-0.42788777232594
Si	4.42185197918199	-1.65748142339221	-1.44494372314943

Si	1.43296161862184	-3.50585094670996	-1.86045569382872
Si	-1.84560428833751	-5.62892656084704	-2.57560379293040
Si	9.34267183445304	-1.63498946549216	-0.64852452962464
Si	5.79668692173723	-3.55634988479353	-1.37460855719571
Si	2.53603624633859	-5.57337452378454	-2.09287579557944
Si	-0.76386656189188	-7.71156065247820	-2.83016333387302
Si	8.15295535397536	-3.64521756574543	-1.14196637520078
Si	4.88494793110946	-5.68294908965755	-1.86274466544254
Si	1.60363386641512	-7.68742048290989	-2.58127222784343
Si	0.63211923563684	7.66451643989883	2.66378913939489
Si	-1.74636405528806	7.53056491549599	2.40078954436657
Si	-2.75495830489665	5.44856689337380	1.90402308354142
Si	-5.09247324862262	5.36213384863732	1.64182573985910
Si	-5.78589445053759	3.15336548563114	1.16021978628680
Si	-8.12507417897256	3.34600803784619	0.91151427839085
Si	-9.30729108162939	1.34376925662641	0.41685488659574
Si	1.89841789138677	5.67870421816561	2.41057908376801
Si	-1.50830592741381	3.47109335626197	1.66458748411644
Si	-4.79084740388414	1.24005435040342	1.97482517680141
Si	-7.91659224922238	-0.55087519354948	0.19006597269085
Si	4.24459771587990	5.88576949418087	2.69243418814908
Si	0.81281358451043	3.63553887559678	1.91794323377872
Si	-2.60220462266445	1.44576883167315	1.29816116812963
Si	-5.60406278994809	-0.32914672177284	0.51011369800733
Si	-9.15917062951308	-2.49870232228982	-0.28545025624093
Si	-7.87127617418666	-4.48622415609403	-0.51575223296025
Si	-4.30785134844579	-2.29403829882492	0.29314426292797
Si	-1.34223655709642	-0.50167771919962	0.87675896325986
Si	1.94609110931945	1.60547797519055	1.62531193871487
Si	5.34927027236292	3.80325507106503	2.40228189764877
Si	4.26453804820085	1.76267502959338	1.90478067609867
Si	1.00257223870216	-0.48337500141267	1.15679481606129
Si	-2.39975269801199	-2.43342101070277	1.59719283741565
Si	-5.54253803772054	-4.22435602851312	-0.22095508701923
Si	7.69865585861421	3.88679799334906	2.67227171885544
Si	8.92444377294958	1.84997119680260	2.41616552607498
Si	5.41324743004442	-0.26184296233156	1.67464475853087
Si	1.93255377375448	-2.39571965202306	2.08426492430399
Si	-1.18936237775216	-3.95063391877069	0.33432825184954
Si	-4.41692910611123	-6.28061344343579	-0.49899601082184
Si	7.75078617790921	-0.14801619929030	1.91915745974499
Si	4.12164684861462	-2.19752274476646	1.43270997559308
Si	1.16581260779086	-3.95240614810195	0.54567256983122
Si	-2.08603244151884	-6.05232870212099	-0.20077279178905

Si	9.10129087315621	-2.07376393474750	1.70251892343241
Si	5.55387559051588	-3.99870720641225	0.98567955297441
Si	2.28485512803531	-6.00453996573720	0.25453366931387
Si	-1.00823417663313	-8.13629014131564	-0.47879123941698
Si	7.91223116425881	-4.08366622809614	1.20407875229168
Si	4.63498768590852	-6.11863221009469	0.48692885141550
Si	1.35874245369725	-8.12141172366493	-0.22934566598310
H	-2.46181123998991	8.42650967598109	3.36663339691862
H	-2.05949841933641	9.18567310400735	-0.64896489396747
H	5.14061973179678	7.53279570583083	-0.28230835040854
H	8.67717815960715	5.50792279416377	-0.25226529757691
H	8.87014274213321	-4.55156690381573	-2.09519043137471
H	5.65197203080567	-6.49406288454188	-2.86178942281534
H	2.34492604641626	-8.55463429101378	-3.55242043396872
H	-1.27419174500322	-8.60047648215506	-3.92297608373095
H	-4.62391636785365	-6.71760519963917	-3.98321106099895
H	-8.09187614026694	-4.98108318646735	-3.96033775407614
H	-8.42006456977100	5.01799237120731	-2.09793057403831
H	-5.53919199956386	6.91890104219743	-1.46030714158454
H	-5.96463293210783	6.12467027121984	2.59073537492185
H	-8.81550190884042	4.27646899441502	1.86063022907345
H	-8.49225921106014	-5.71369322255613	0.07818038780131
H	-5.04860616116226	-7.48361876161098	0.13251616196392
H	-1.70057494874589	-9.32694335728448	0.11096322001918
H	1.92476756632541	-9.30121178866902	0.50034576524710
H	5.20381307654841	-7.26668983648574	1.26339583375475
H	8.45958980610308	-5.29672845325574	1.89199751814150
H	8.24866254124552	4.75550421725617	3.76231943001319
H	4.73551238381176	6.77052031197432	3.79775706166986
H	1.44195659676897	9.37774689325695	-0.25319206235092
H	1.04118229639311	8.61116980113956	3.75106259720049
H	10.06929710748696	1.73413114289958	3.37633096505944
H	10.48188046999426	2.48680877626853	-0.62683144868592
H	10.21911574805029	-2.25706207866898	2.68280397163997
H	10.63790347272486	-1.50355512486474	-1.38967493758541
H	-10.59290548077172	1.16011301383651	1.16471194859080
H	-10.20627874493301	1.94304033800085	-2.91054980149581
H	-10.45506132183754	-2.67167259928668	0.44685425344556
H	-10.06128679418216	-1.94315901652114	-3.61445894129141
C	-0.70426949023980	0.48953675977549	4.35680689277932
O	-2.02494108184287	0.62050381589168	3.82875999925808
H	-0.21204934992020	1.46558232083238	4.21966880920418
H	-2.43229333119162	-0.26732083052035	3.76827871708949
H	-0.11803738345367	-0.28043790274756	3.81735233487257

H	-0.72125051472036	0.24283159373187	5.43590868519412
H	-3.37563906127807	3.47206103102311	4.63489528264318
H	-3.14478730824308	2.76915029028668	4.45881692907859

• **2Si-CH₃OH-H₂**

Si	1.25634479351750	7.97873296114835	-1.21131572063468
Si	-1.14444921799578	7.99224655457274	-1.22284660955512
Si	-2.32897589686497	5.94229896923481	-1.25150609879685
Si	-4.68683463708777	5.89785275797342	-1.24190188034777
Si	-5.43950990111164	3.63722056504758	-1.23447752044371
Si	-7.78522039422483	4.01434502196272	-1.27992381208799
Si	-9.15787782963948	2.06920220128711	-1.33768861178605
Si	2.39416066669950	5.89697830061627	-1.22251450052934
Si	-1.21307390636102	3.86923390768733	-1.23631367112601
Si	-4.49580930642163	1.96311722353740	-2.63265294440807
Si	-7.88153686350838	0.07847639913240	-1.34342859149728
Si	4.76701647282390	5.99956419407413	-1.22763858589091
Si	1.13908949920691	3.88727068009356	-1.25129048175774
Si	-2.56028754673217	1.92490785025185	-1.29447671107643
Si	-5.52288017969397	0.29586824953645	-1.32933427093167
Si	-9.25466477396498	-1.84319670551423	-1.41547385423083
Si	-8.14098607398105	-3.94884913309264	-1.42427417627292
Si	-4.53036091487988	-1.84991266939451	-1.38914291732772
Si	-1.22218647942893	-0.02758200046316	-1.26939370360492
Si	2.20530400450193	1.80080897728832	-1.27595261695975
Si	5.75755592196344	3.84043544113123	-1.21773716593408
Si	4.54475764360575	1.81338540160494	-1.23970656149125
Si	1.12388314850531	-0.27050707777595	-1.33653770802220
Si	-2.30957726640356	-1.91137445477316	-1.95985595407231
Si	-5.78085138584129	-3.84505190014001	-1.39659491240178
Si	8.12493694114676	3.81171733246839	-1.20623350550580
Si	9.23707144895380	1.69247698016768	-1.20950668976949
Si	5.60084036945992	-0.27196846910963	-1.26176009440285
Si	2.11301941132748	-2.04929681526960	-2.44433167663210
Si	-1.24704228047179	-3.86519362874302	-1.34966962985200
Si	-4.77734067509653	-5.98419974102285	-1.41362690643054
Si	7.95467612731918	-0.29944232545588	-1.22784013223267
Si	4.16780564586564	-2.12164879320811	-1.37713126266275
Si	1.10865814433771	-3.82113579117603	-1.35939366691297
Si	-2.41559299169360	-5.90966255046040	-1.36621549957924
Si	9.19104003590682	-2.31146826632502	-1.23652646475690
Si	5.47559300325804	-4.07216894822429	-1.28217514461843
Si	2.07143681597453	-5.96656106686915	-1.32148109556377

Si -1.40067524024616	-8.04229433728023	-1.38450770639613
Si 7.83674819561255	-4.27766097662686	-1.26038082640431
Si 4.42571693057414	-6.18873239883223	-1.30475679087898
Si 0.98213608016245	-8.06305779595904	-1.35533851680567
Si 1.24732255734686	7.96148621590092	1.19203294482978
Si -1.15210080604610	7.97756470107390	1.18441075132850
Si -2.33731800062293	5.92805429929189	1.15949375062389
Si -4.69322426583924	5.94444996140658	1.17031658331258
Si -5.53672500013831	3.73812001785992	1.19792345531229
Si -7.87701829903674	4.01509551035693	1.11200850318219
Si -9.20072813735043	2.03938908475296	1.06511508692814
Si 2.39006068342515	5.88393214851914	1.18055542451425
Si -1.20032441822939	3.86926288210489	1.16194576978300
Si -4.53382916690608	1.90596538384435	2.22527966705395
Si -7.94743027170114	0.03536743906299	1.05134447949290
Si 4.76034483888132	5.98808720600434	1.19960700878680
Si 1.14836961817325	3.86984095876264	1.14909563588911
Si -2.46893465216269	1.89450877277569	1.13973616791074
Si -5.59987922031112	0.15089549592170	1.11981050273603
Si -9.31279847317332	-1.88801779975474	0.98835222841798
Si -8.16900568505676	-3.97626478653449	0.97719496809873
Si -4.48593028300266	-1.91658609953282	1.06361176409141
Si -1.22794812540387	-0.10096628865409	1.20306956490348
Si 2.19445429548315	1.77443746658254	1.14247817734285
Si 5.74354194825148	3.82596015257449	1.18287560710827
Si 4.53373439987863	1.79650495242209	1.16053602982139
Si 1.12158742196830	-0.30413096399219	1.16290207172176
Si -2.34072795459497	-2.00150839895732	1.98335231706756
Si -5.80577101585519	-3.86562951327218	1.00848872357903
Si 8.11033876707514	3.79570602081057	1.20361820542874
Si 9.22199155450030	1.67632037276802	1.19623642102989
Si 5.58443809820238	-0.29109102544530	1.17218906616320
Si 2.07804839438371	-2.09286517468642	2.28584044182309
Si -1.28034111180037	-3.87189539001865	1.07504161101466
Si -4.80483240438153	-6.00748379186669	1.00048215247184
Si 7.93922612557316	-0.31599199846665	1.17344718400252
Si 4.14528392129812	-2.14258644032428	1.23673570183456
Si 1.07983818245928	-3.84314243523298	1.14566569221751
Si -2.43903346337056	-5.92798819219051	1.03163099217694
Si 9.17268598357430	-2.32982172088713	1.16772080333309
Si 5.45519165879241	-4.09104362916497	1.12506435372911
Si 2.04813297528294	-5.98764967876372	1.07935146390655
Si -1.42816305581839	-8.06324557419043	1.02180244478147
Si 7.81669299065562	-4.29568111889050	1.13974345938435

Si	4.40359635526743	-6.20837813613768	1.10039948320071
Si	0.95610379435845	-8.08362256726124	1.04817515131255
H	-1.69719173604251	9.07778787306743	2.04488303944452
H	-1.68049521458545	9.11319731903525	-2.06130346897866
H	5.41572969609224	7.03893201282339	-2.09043471854204
H	8.84360597500341	4.82719447678085	-2.04177308014311
H	8.39985798743866	-5.38142725211046	-2.10320014359084
H	5.01920354025319	-7.21664298576281	-2.21938441512130
H	1.59864191164381	-9.12260755627852	-2.21675761147722
H	-2.01717068257188	-9.08550262141015	-2.26569990170870
H	-5.39123712662161	-6.99884272336160	-2.33012986377961
H	-8.76045329765749	-4.99252643406675	-2.30301823997542
H	-8.27137064031348	5.14423425973806	-2.13579980219520
H	-5.43393547140849	6.85157235652992	-2.12352848803177
H	-5.41599582464539	6.92600868422146	2.04204789240662
H	-8.43231271324962	5.12375792230223	1.95379158568486
H	-8.79366809843734	-5.04526433758042	1.82142469546029
H	-5.44868747109420	-7.04252631293465	1.87272492307735
H	-2.06078039336966	-9.12616483068267	1.86742098031183
H	1.54913738007541	-9.16205272672628	1.90272416380015
H	4.98639925588070	-7.24838720759878	2.00833542732342
H	8.36808478869852	-5.41132550405830	1.97475241728701
H	8.81600133867250	4.80110207197905	2.06228542963377
H	5.40045387760576	7.01948070906495	2.07848878332874
H	1.83786610702867	9.08297749201462	-2.04122727579483
H	1.82115738786335	9.05028040814305	2.04756992818138
H	10.45558088186073	1.67520110126914	2.04765130852047
H	10.48144421296955	1.70093052005405	-2.04484412582982
H	10.37563115559886	-2.43345010057741	2.05443822279804
H	10.40709788331287	-2.39717239691730	-2.10698424251089
H	-10.42215368467148	2.07178916750134	1.93458845918767
H	-10.36495036430147	2.14076711431585	-2.22383877964313
H	-10.55054944080298	-1.88478414668952	1.83363764657372
H	-10.45815827420801	-1.80077384221231	-2.30745119010258
H	-4.47979495074128	1.82632613517832	3.72239726166207
C	-0.03906741836068	1.28604186657188	4.21061137961657
O	-1.12323492553032	0.43603185568063	3.82643116723084
H	0.87452808145153	0.67345936596272	4.15010489707488
H	-2.39437942156951	-2.06069401448653	3.47482984158529
H	-0.16025299044426	1.64776589691337	5.24913505844209
H	0.06621146474997	2.15229524508072	3.52712700610180
H	-1.94947107867586	0.95737869755384	3.85344721163626

• 2Si-CH₃-H-H₂O

Si	1.17741998757180	7.96510015472424	-1.14451782615544
Si	-1.21395368336155	7.92081771652973	-1.20345663898740
Si	-2.34526145827331	5.84581876611307	-1.27650545237411
Si	-4.69666188425590	5.87866459592976	-1.33032862999073
Si	-5.48085875757246	3.64771228811592	-1.36030021416733
Si	-7.82934063930353	3.96897776664825	-1.39135001013184
Si	-9.18035845895429	2.01049654504182	-1.44906698125766
Si	2.25241232596177	5.85860708562016	-1.14960436675255
Si	-1.32350575616151	3.73126301715214	-1.34079602125024
Si	-4.58554104651569	1.89794039738110	-2.64734490501994
Si	-7.92792179233420	0.00824454534454	-1.45225915955595
Si	4.62520868040309	5.94016792216843	-1.08266589031717
Si	1.02386390348183	3.83226814130552	-1.21741975920371
Si	-2.47546180819478	1.81945320065834	-1.88130037673273
Si	-5.56923359151162	0.14955475561014	-1.43502729311943
Si	-9.33207604452749	-1.88808262346643	-1.51945760732965
Si	-8.21880227676522	-3.99187389516274	-1.53901890602360
Si	-4.52210999078909	-1.95681390266358	-1.52288773627386
Si	-1.35876653340894	-0.16308465618454	-1.35473028753562
Si	2.04145437659677	1.72415675600284	-1.19816195471574
Si	5.61689696338437	3.78603501854475	-1.05571235442755
Si	4.38626766839136	1.77326649450281	-1.10572137952608
Si	1.00171235505821	-0.38136050879353	-1.32521331414186
Si	-2.39726723307653	-1.97249631500816	-2.35163401689505
Si	-5.86017924201709	-3.87110125937349	-1.52873360996490
Si	7.98167953533343	3.78945728508522	-0.99555072626770
Si	9.07988113139571	1.66500974049887	-0.99128635081616
Si	5.41813942852764	-0.33022066960626	-1.09166284757408
Si	1.98941578693656	-2.08655810929159	-2.59460496383816
Si	-1.33786841539917	-3.83743614093331	-1.55884667838537
Si	-4.83113862306485	-5.99388694672750	-1.55897180304046
Si	7.77406253810244	-0.31224809059008	-1.02969759356449
Si	3.97338764097493	-2.15543915902212	-1.41000997412924
Si	1.01806678120115	-3.85131655151056	-1.41424173833491
Si	-2.46933851742309	-5.88621124216100	-1.53238546412657
Si	9.01958381272779	-2.31664439270615	-1.03689696206967
Si	5.30782800511326	-4.07693687116956	-1.14978455717238
Si	1.96390656526649	-6.01903640232208	-1.37627545182828
Si	-1.50371573789285	-8.04051925790072	-1.51432668979401
Si	7.67130854078182	-4.28422642560668	-1.10409475382308
Si	4.31680403959202	-6.22002567138849	-1.26542948292870
Si	0.87767745835615	-8.11337817920631	-1.45575727231733

Si	1.11848855225333	7.92771548005786	1.25983737440628
Si	-1.27044660274478	7.86985566825234	1.20378411891005
Si	-2.38727363705497	5.78382395718754	1.12753304369122
Si	-4.73881850748894	5.86013154394759	1.07629191507891
Si	-5.54128890269747	3.64075012614101	1.05193028733651
Si	-7.88295753525701	3.93397802024618	1.00439615961552
Si	-9.22343369106436	1.97285051223937	0.95347964104792
Si	2.18316708837056	5.81745393919158	1.25355153174192
Si	-1.41010274953990	3.64201933476856	1.10574104974598
Si	-4.61410100480031	1.81309300174560	2.18159669942339
Si	-7.96504897816649	-0.02610008394025	0.94669819976546
Si	4.55459969445607	5.91051821006788	1.34425841522045
Si	0.93542230870098	3.80848802466046	1.16939583990007
Si	-2.25562925072467	1.72845888862024	2.15443505858987
Si	-5.60836323851975	0.06718667520131	0.97541990077159
Si	-9.36113289419550	-1.92878236362271	0.88479624953115
Si	-8.23707856619724	-4.02703470461476	0.85967669672649
Si	-4.49128764723740	-2.01183161210337	1.01074933811834
Si	-1.47033338213991	-0.21480973116558	1.06711136237408
Si	1.97396046802853	1.70899497037337	1.20317199254109
Si	5.55383843783531	3.76120111850737	1.34845764719246
Si	4.31803311538104	1.74859661927100	1.28494938008267
Si	0.89456872971151	-0.36587084455150	1.12364658131830
Si	-2.46709554483896	-2.04860759139759	2.11539776713214
Si	-5.87824379376630	-3.90167928904515	0.88822516673618
Si	7.92003987585246	3.75599552915596	1.41266106734507
Si	9.03731461563434	1.63838467725006	1.41211866083191
Si	5.38022827224179	-0.34375528977184	1.33942886591716
Si	1.79997219534752	-2.18232395495303	2.22499203336096
Si	-1.46089504554178	-3.79874428036316	0.98892085697745
Si	-4.86786288254214	-6.03506060243419	0.84051985742748
Si	7.73664281911487	-0.33983669696194	1.37326805531056
Si	3.98219876539577	-2.21687762288996	1.51606319613480
Si	0.89406374573850	-3.93682463205333	1.03199533314506
Si	-2.50911452119795	-5.89398942212836	0.88818093282387
Si	8.96315367974251	-2.35929626655137	1.36502395453322
Si	5.27402519027033	-4.15995030360265	1.26117259997561
Si	1.88651253042193	-6.06552907405597	1.01913020242324
Si	-1.56246878470477	-8.06071367756939	0.88563924412240
Si	7.63287970135088	-4.34362845121634	1.29467058311020
Si	4.23659093724984	-6.27839619546149	1.13654743334898
Si	0.81312524596812	-8.16466295143970	0.94820821493670
H	-1.90396186599397	8.92594327562511	2.05826329294612
H	-1.79442870813301	9.02267841436434	-2.03730502103400

H	5.29843342200067	6.98557301946785	-1.91932035438896
H	8.70943036467744	4.81326159072259	-1.81278933503029
H	8.23445188811434	-5.37983772516773	-1.95705255868617
H	4.99999840862754	-7.20118204794681	-2.16823799582568
H	1.48019974289427	-9.17307629495258	-2.32697299126209
H	-2.14068202537776	-9.06857794879291	-2.39885977624694
H	-5.42216068070122	-6.99693144392487	-2.50181462854081
H	-8.83281386002174	-5.03461505888739	-2.42215301956967
H	-8.33850807043388	5.10248202980734	-2.22875551963643
H	-5.38305855715462	6.85558856540329	-2.23375593240818
H	-5.45541423000395	6.82938600793117	1.96476620313216
H	-8.40923076783450	5.04968879670531	1.85407838761837
H	-8.86411534734260	-5.09573343586184	1.70198231320957
H	-5.47141559324007	-7.09009571397156	1.71625444734892
H	-2.27006266033435	-9.08299760150103	1.72179913749819
H	1.37569112697711	-9.25343897794350	1.81010931464362
H	4.77511193328719	-7.33917998386081	2.04744090134115
H	8.19706784673868	-5.46332824027298	2.11514812833203
H	8.59911968215110	4.76027660877707	2.29385665918823
H	5.14769940942063	6.95199358620598	2.24429403836142
H	1.76883947158445	9.06688741668728	-1.96989233370825
H	1.67217021275847	9.00048341739949	2.14728362276143
H	10.25973654930949	1.63667349066633	2.27938772873169
H	10.33266073978018	1.65405463575063	-1.81378838941746
H	10.15460861273428	-2.46647719547682	2.26711924035341
H	10.24869851680135	-2.38512653351594	-1.89042772334205
H	-10.44941745996342	2.01419605570273	1.81511503683267
H	-10.38220507235723	2.08673656526111	-2.34145958310247
H	-10.59280438513544	-1.90174357630396	1.73839397081029
H	-10.53967300802536	-1.82505300120209	-2.40458397205565
H	-5.07810519988058	1.77123350389059	3.60709019659332
C	-1.56598580680073	1.62538988723617	3.93775377476649
H	-0.46035141994873	1.60265289979910	3.89962971363972
H	-1.87580241184018	2.49601840623143	4.54202101590096
H	-1.93034234438181	0.70631658294829	4.43184027068779
H	0.15419707211808	-1.15330036850149	4.26364528839770
O	0.31438176762740	-2.11508475028476	4.16960193026776
H	-0.54142213569836	-2.43754043538839	3.78726001402993

- **2Si-CH₃-H**

Si	1.18386027580372	7.96044575084296	-1.12512708741252
Si	-1.20615445434991	7.91757763442778	-1.19130441896335
Si	-2.33422523594318	5.84133938218809	-1.27431629379044

Si -4.68501090235331	5.87696061497383	-1.33327177721470
Si -5.47381306044551	3.64728756541081	-1.36591455963517
Si -7.82093222654186	3.97130544219917	-1.41285277230398
Si -9.16834593497680	2.01096043379905	-1.47882335821155
Si 2.25507091140796	5.85218503092510	-1.12765285766608
Si -1.32066884461854	3.72271874096184	-1.33059754422023
Si -4.57258471072807	1.89092409399087	-2.63773897530661
Si -7.91857722942752	0.00633582267229	-1.47085055553032
Si 4.62547730908654	5.94295359936593	-1.06908407193914
Si 1.02323049985350	3.82923230446724	-1.19428107162885
Si -2.46850748127981	1.80831716558641	-1.86246208050981
Si -5.55934924996925	0.13284482487319	-1.44037894959546
Si -9.32248963159511	-1.88879239968603	-1.54650105081554
Si -8.19466443648964	-3.98452039721614	-1.56096957807477
Si -4.47218584685113	-1.95729128390291	-1.52568745150646
Si -1.39352422334565	-0.19058576064659	-1.31155546531397
Si 2.03425037860737	1.72210671606995	-1.19448179577352
Si 5.61267466041003	3.78814546390696	-1.05911644798915
Si 4.37600894275840	1.77830610357535	-1.12341656297249
Si 0.96900470287603	-0.35284927580225	-1.29139083720882
Si -2.37373579194836	-1.96553983975620	-2.43851456789008
Si -5.83540554488666	-3.85621539963601	-1.53813406982355
Si 7.97822021913496	3.79416915915751	-1.00257883191917
Si 9.09076903634869	1.67882386707800	-1.00601059447450
Si 5.42977616700563	-0.31112287083557	-1.15171442605301
Si 1.97039268825135	-2.09961582600104	-2.45546988224225
Si -1.37732095663734	-3.80085783701858	-1.47875120451619
Si -4.82355960418458	-5.98852727865326	-1.53908854628493
Si 7.78328179237858	-0.29520504672135	-1.07420227464712
Si 4.04418222391376	-2.16633989920676	-1.47557536559687
Si 0.97685905796824	-3.88784286334654	-1.36563742149521
Si -2.46281843125343	-5.87618907180560	-1.49803787075489
Si 9.02235653621469	-2.30525139982449	-1.08031807274083
Si 5.33822201812712	-4.10640311054535	-1.22138047148540
Si 1.95343368441238	-6.02868939031365	-1.34934897435886
Si -1.50682824220885	-8.03619393673894	-1.49122248883127
Si 7.70007926033023	-4.29158402882958	-1.15410358929757
Si 4.30763086091645	-6.23198629206697	-1.28770929018818
Si 0.87250799658790	-8.12505250714804	-1.42720986605110
Si 1.12010617828244	7.91981173435816	1.27934972060565
Si -1.26843460524743	7.86080325875838	1.21571316323794
Si -2.38074513087095	5.77340501549152	1.12927986124327
Si -4.73322510704387	5.85701249221533	1.07390277957022
Si -5.54732291247131	3.64257389240191	1.04523327071808

Si	-7.88857551534629	3.93720439429917	0.98286941268559
Si	-9.22874175002027	1.97530291501828	0.92323769314183
Si	2.18379950472240	5.80826115492551	1.27448575071725
Si	-1.40811267031122	3.62834367637977	1.11610497770771
Si	-4.62546178551463	1.81373186602520	2.17550611277068
Si	-7.97304919127974	-0.02519530938513	0.92801900757306
Si	4.55328907125039	5.89949664705034	1.35898661465480
Si	0.93862675168826	3.79501679895917	1.19287838643264
Si	-2.26635637041236	1.73180920598202	2.18419787450826
Si	-5.61684647438686	0.06739755447595	0.96824019944890
Si	-9.36606732934692	-1.93031530843173	0.85719663057724
Si	-8.23431932177849	-4.02441056705667	0.83639476187164
Si	-4.49763530635786	-2.00626614239766	1.03066689901063
Si	-1.46301420287241	-0.21583705923726	1.11714644263744
Si	1.96299790036236	1.68740626078910	1.22421176178930
Si	5.54799178443001	3.74845094982827	1.34156652787818
Si	4.30770275720178	1.73953939020959	1.27235993370698
Si	0.90083010308409	-0.39833912942269	1.18500626199179
Si	-2.47525995357315	-2.05708415969353	2.11816641407372
Si	-5.87734684352154	-3.89153210107179	0.88565602497351
Si	7.91363468427269	3.75355026413139	1.40675504040608
Si	9.02567970677012	1.63688333225253	1.39780646925782
Si	5.36412294961923	-0.35165016678962	1.29054489180273
Si	1.84448137850056	-2.19766234324239	2.31286065754023
Si	-1.44951028664903	-3.82730693373452	1.06544445468204
Si	-4.87431876141331	-6.02818957665166	0.85889903700191
Si	7.71964323075487	-0.33781442026202	1.32466064511439
Si	3.97002657522987	-2.22164006578663	1.45719196577770
Si	0.90866220389327	-3.93303503505758	1.09322435716642
Si	-2.51529894629740	-5.90937237551053	0.92296991863761
Si	8.95529685769700	-2.35085893872058	1.32274939327265
Si	5.27395267502221	-4.15266938480295	1.18891557034595
Si	1.88659812359795	-6.07452548929588	1.04928580146616
Si	-1.56926772676428	-8.07404992878446	0.90919877703148
Si	7.63485653060306	-4.33854933095098	1.24309353847387
Si	4.24057983456624	-6.27779934628039	1.11376214651421
Si	0.80851295199189	-8.17355351264305	0.97544324594033
H	-1.90282302515610	8.91462164135542	2.07226274935736
H	-1.78262463576190	9.02103582281771	-2.02569680036928
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H	8.69840249773486	4.82583684598038	-1.81647045006352
H	8.29189076874030	-5.37810602052260	-1.99890329805102
H	4.94655603226914	-7.23419175245726	-2.19972310015535
H	1.48379640260963	-9.17862219861507	-2.29965246555741

H	-2.14653827880670	-9.05393554316047	-2.38558550958773
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H	-8.79545595054520	-5.03121858333321	-2.44859548636991
H	-8.32447197601012	5.10429249146755	-2.25435347036098
H	-5.36547442141347	6.85659301925687	-2.23828412307935
H	-5.44346289153344	6.83169504971192	1.96156511744541
H	-8.42137871563302	5.05269521698547	1.82877649971140
H	-8.86202604008940	-5.09902429603386	1.67057959011124
H	-5.50165291266955	-7.06810304835745	1.73593301100556
H	-2.26814118226776	-9.10989908782279	1.73596582629030
H	1.36888971699609	-9.26492843920088	1.83553077202247
H	4.82978617319044	-7.31544216650590	2.01970521931283
H	8.18271130481941	-5.45710738042076	2.07590531687456
H	8.59220603602783	4.75424561726868	2.29214242709338
H	5.15970489578929	6.92762804837729	2.26529686738361
H	1.78464347860482	9.05834544445297	-1.94876108116635
H	1.67182812672640	8.99143055958743	2.16936096315275
H	10.23859237552609	1.61431843091869	2.27784147949625
H	10.34974413908582	1.68258841345926	-1.81877508309106
H	10.14080237153536	-2.44930014800436	2.23340819432934
H	10.25664181239073	-2.36603147371744	-1.92704328049551
H	-10.46146430826025	2.01993497353734	1.77505554925107
H	-10.36456756082805	2.08648672312024	-2.37888246199527
H	-10.60164964085625	-1.90817645496475	1.70528648889290
H	-10.52427091781150	-1.82996135913117	-2.43978820256352
H	-5.10122239972877	1.76951800793281	3.59710011616805
C	-1.61035296575423	1.68039994706505	3.97800659650671
H	-0.50530824842679	1.65717980752843	3.96655393782065
H	-1.93982224520878	2.56878606866234	4.54519973633657
H	-1.97700440654381	0.77419769167488	4.49135238982439

• **2Si...CH₄**

Si	1.05261059373387	7.85754097705899	-1.20279829756214
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Si	-2.19620757740568	5.57472279498353	-1.67071115009029
Si	-4.55585198961978	5.86426029897676	-1.76658285342327
Si	-5.68692751058857	3.89014384635203	-2.27103012316441
Si	-7.97259339513161	3.96063812195265	-1.68159808289669
Si	-9.28139629791622	1.99479797227018	-1.59322127975616
Si	2.09101105930708	5.73232773895119	-1.16905155708504
Si	-1.24925095872114	3.70133697129871	-2.79606926904300
Si	-4.53364783972204	2.25944424692458	-1.13628891441238
Si	-7.92299979244972	0.08733580447370	-1.33611158441035

Si	4.43934279485780	5.94527092629862	-0.95285887472931
Si	0.69558336075846	3.83276736620128	-1.43057592434324
Si	-2.16029810584342	2.35109031523703	-1.05302814266001
Si	-5.62063254566759	0.20553281078023	-0.94218880580293
Si	-9.31279118378442	-1.80385687880767	-1.63206920038229
Si	-8.17822469511711	-3.88378631990625	-1.63769725906797
Si	-4.45621325648376	-1.80565131061068	-1.18874414611449
Si	-1.49255193658750	0.05490493002411	-1.01041922590625
Si	1.92225318945789	1.83673932159883	-1.20329559672655
Si	5.50627506784997	3.83295062752197	-0.92914581506319
Si	4.25808285613469	1.84278403864332	-1.08795701780966
Si	0.86085264289800	-0.23354591018944	-1.11918417755885
Si	-2.42828760648885	-1.68996134747267	-2.24339676215029
Si	-5.84616567701151	-3.68241734010456	-1.36671849059262
Si	7.86599284283080	3.86876888386762	-0.81530658390438
Si	8.98925288497264	1.76194471224926	-0.81844383518587
Si	5.32568595452831	-0.23401180162690	-1.08305319473244
Si	1.81595937105542	-1.98782898086020	-2.31083971965373
Si	-1.48828538780063	-3.59231702449331	-1.28897713977623
Si	-4.87808817647546	-5.82638396400416	-1.54876318108660
Si	7.67750929591002	-0.20725484024470	-0.94851503849987
Si	3.92551367671973	-2.08105042451045	-1.39432491298881
Si	0.85812533443511	-3.76970223467114	-1.19977040074498
Si	-2.52979615731604	-5.69838580312048	-1.46113804924960
Si	8.91708346440183	-2.21663702401949	-0.94786877864185
Si	5.23453728347612	-4.02275523331843	-1.16718918257534
Si	1.84040531047335	-5.89933158476953	-1.27066514830130
Si	-1.58333003015464	-7.86537151417370	-1.58932327168301
Si	7.59605483282108	-4.20010506662972	-1.07997228403124
Si	4.19061643041451	-6.13669279876443	-1.24587939695800
Si	0.78567414045541	-7.99618880353772	-1.45854333054521
Si	0.88169896601443	7.80675917343323	1.19124438213656
Si	-1.47857572513639	7.63963244010391	0.99229681798027
Si	-2.40275070055968	5.48959789068497	0.73338428782900
Si	-4.72699429611229	5.54001952881171	0.62571039396725
Si	-5.42236196526257	3.29659272949429	0.87651056810831
Si	-7.73031188691945	3.70873378475369	0.68040659413606
Si	-9.36652367680864	1.99600138030810	0.80875062279983
Si	1.89033069531431	5.67288786697205	1.22015238976748
Si	-1.67229525613475	3.34745893145845	1.18976897326817
Si	-4.97270445530287	1.80988175079042	2.65189492486915
Si	-8.24661948348415	-0.06390932175614	1.04252819603725
Si	4.24749645129333	5.83972643127376	1.46355981721342
Si	0.60512267511402	3.69635453881910	0.99365163267199

Si	-2.76499309244069	1.56400394996296	2.06621690178987
Si	-5.89637670036835	-0.00638720815715	1.43263935781163
Si	-9.60873312804261	-1.96223762000588	0.74975204105115
Si	-8.42033870292625	-4.03473202459228	0.74610123895687
Si	-4.72096972253094	-2.04855161814044	1.35441710628080
Si	-1.59260982138369	-0.34146884127713	1.40113182747441
Si	1.80023634372537	1.72283105723985	1.24587086915406
Si	5.37481718085463	3.76187936722330	1.46641575716425
Si	4.13403420066126	1.76613298355593	1.32159650795511
Si	0.77863189457662	-0.38119805419004	1.33717257853721
Si	-2.63891040282825	-2.17249987267372	2.33162788375442
Si	-6.07352790913119	-3.93649329741459	1.02596237322149
Si	7.73856079960861	3.80135473444678	1.59184516488659
Si	8.86163364980231	1.69077677222308	1.58246236572635
Si	5.20044318964241	-0.31634908631701	1.35813302379808
Si	1.74575493855143	-2.16126404521819	2.49323128640251
Si	-1.56940946169361	-3.87096415433494	1.22985109095086
Si	-5.03205349074950	-6.04555154569535	0.83625907172902
Si	7.55305315409248	-0.27787746106097	1.44633064729459
Si	3.82324416352539	-2.19282669447655	1.52353862877013
Si	0.79349123099060	-3.89220032506077	1.25017996165777
Si	-2.66997769804010	-5.91032705750060	0.94064714456544
Si	8.78891255670609	-2.29258971845227	1.45126101551047
Si	5.13126408670132	-4.11552336671922	1.23823335457721
Si	1.75474154809890	-6.04758448351877	1.12434345676201
Si	-1.71933346606008	-8.06209750783855	0.80092406011778
Si	7.49142483847935	-4.29307063058678	1.31583994169000
Si	4.11070989624865	-6.24847328212868	1.15353597426683
Si	0.65973420381985	-8.13641609241907	0.93878032773506
H	-2.29799414678951	8.54320655748055	1.86116400283889
H	-1.91714945664863	8.88214943458230	-2.20622770678866
H	5.10999893685975	7.03975357495803	-1.72628448376076
H	8.59050939594363	4.91995411355561	-1.59945025089492
H	8.19839113086556	-5.27150584846955	-1.93673079728146
H	4.77733612139776	-7.14451608447662	-2.18644687896663
H	1.42565922833634	-9.01090175454907	-2.35589828545044
H	-2.22322867322234	-8.80016965764909	-2.57008440447806
H	-5.49769248707760	-6.71031699797321	-2.58781103891979
H	-8.65590043328454	-4.89577106342588	-2.63294314764108
H	-8.62622283912655	5.19771167797364	-2.21011165263989
H	-5.18856906560603	7.08324499301984	-2.36322622310570
H	-5.51345415297753	6.49680320315629	1.46837172196165
H	-8.06824925118947	4.90556711789068	1.51658957144606
H	-9.13730453680367	-5.14025725449410	1.45928836589638

H	-5.62906235958326	-7.17938552592749	1.61248274687009
H	-2.41798168629060	-9.16558822455330	1.53553361842851
H	1.18913674263366	-9.26650979287092	1.76839026875288
H	4.73851876253324	-7.28315410199347	2.03691298052816
H	8.04336943876303	-5.41899013124264	2.13611901320826
H	8.38519236517471	4.79216817390294	2.51154651620651
H	4.71537926575497	6.88450550769566	2.43136354472550
H	1.70761971143018	8.95093901887345	-1.99060244403047
H	1.37118378096698	8.84826882534807	2.15110730629835
H	10.04997967252743	1.65692398580595	2.49498480234534
H	10.26931874381660	1.77192469829444	-1.59728214819823
H	9.95252323142850	-2.39220546231587	2.38959635288217
H	10.17326801775174	-2.26688215070681	-1.76259204982240
H	-10.53769813104268	2.40949332007984	1.64861179574274
H	-10.42134115610490	1.84477577160052	-2.55119514741753
H	-10.92480171782170	-2.03776788851489	1.46246106225457
H	-10.40921997405948	-1.63724054488729	-2.63925209259287
H	-1.31582038958910	1.01236907843977	4.83562393936555
C	-0.24191971402460	1.15367379753920	4.62941785270967
H	-0.11643689796941	1.86023194582766	3.79093817926460
H	0.25562650366360	1.55675658289720	5.52619863489355
H	0.20714013600693	0.18441571844152	4.35676759721512

Transition states

- TS 2Si...CO₂ → 2Si-CO₂

Si	1.17941613082911	8.08380649722668	-1.25430629140518
Si	-1.22402455860672	8.09134898652245	-1.25682942279441
Si	-2.43838722385297	6.05383712670830	-1.26032527488796
Si	-4.80675807844458	6.25990157441704	-1.27129831474197
Si	-5.88725586778120	4.13954275627847	-1.26340920259327
Si	-8.26307105563553	4.11842140695338	-1.29222003821536
Si	-9.41863494935017	2.01605904691894	-1.29920917856258
Si	2.38164410300859	6.04067517704797	-1.25809006648656
Si	-1.20481064996094	4.03602102034785	-1.24992598681816
Si	-4.72981778496759	2.08138790121385	-1.23843402094787
Si	-8.17743324013053	-0.00164799490166	-1.28404716862652
Si	4.75596328704506	6.22509125718134	-1.27238807585546
Si	1.16050757981364	4.01782146259195	-1.26201472933868
Si	-2.37615293451949	1.99078243976146	-1.30670406090918
Si	-5.82915114700993	-0.00105019558688	-1.26168417178614

Si	-9.41746701657810	-2.02006955024470	-1.29943131617494
Si	-8.26069345024877	-4.12177408935001	-1.29269257046477
Si	-4.72857878219475	-2.08281826523955	-1.23870003055836
Si	-1.15862728482999	0.00013627674351	-1.23471745627578
Si	2.39905247077459	2.02000314718865	-1.26666669166210
Si	5.87526806303346	4.12371962720344	-1.27290276674108
Si	4.75063860569237	2.04810979730989	-1.27154461747499
Si	1.18181856987277	-0.00016431537318	-1.23092006903455
Si	-2.37495789720503	-1.99131928083774	-1.30667762465107
Si	-5.88487834151953	-4.14159957976287	-1.26392628177183
Si	8.24948438461229	4.12840994728984	-1.28996380719885
Si	9.46400635538429	2.05271865573505	-1.29692067812503
Si	5.92254834918919	0.00103276817726	-1.28167588328372
Si	2.40034701945391	-2.01958098483734	-1.26718157024211
Si	-1.20262178257972	-4.03604813137956	-1.25053768382579
Si	-4.80345331379909	-6.26148477681269	-1.27210156607564
Si	8.27526147991526	0.00165563759680	-1.29037934114777
Si	4.75196266625082	-2.04679858467437	-1.27195724835602
Si	1.16270314338261	-4.01794329881795	-1.26267008600504
Si	-2.43518903520905	-6.05446879012454	-1.26117253465348
Si	9.46516268496176	-2.04874685593341	-1.29733761704493
Si	5.87766698596906	-4.12183810924799	-1.27372887005124
Si	2.38481365532242	-6.04022935603765	-1.25914982948186
Si	-1.22025173200067	-8.09164231480222	-1.25804749810459
Si	8.25189852220463	-4.12518408564767	-1.29078315734272
Si	4.75923798458394	-6.22368657326359	-1.27355734405268
Si	1.18319407702960	-8.08373070186752	-1.25561644948226
Si	1.17922889211585	8.07562732814470	1.14974498381815
Si	-1.22647577439823	8.08808802865375	1.14794065860185
Si	-2.44452984008170	6.05305430767227	1.14516689540975
Si	-4.81606630341750	6.26438128031747	1.14876884180037
Si	-5.91814895803724	4.15530084307957	1.14070091287816
Si	-8.29060691357809	4.13000656004117	1.10757326832957
Si	-9.43740895304591	2.01924291839731	1.10682112439883
Si	2.38401451032745	6.03239882937607	1.14403526388405
Si	-1.21113195557847	4.03569650365160	1.15401847184974
Si	-4.76516898791695	2.09918654309707	1.17141530612064
Si	-8.19646903062134	-0.00178979963382	1.12239201439130
Si	4.76121152020417	6.21917120051776	1.14973838916444
Si	1.15989035753802	4.00691485555562	1.15416754018311
Si	-2.41796252087796	2.01420986671194	1.10062311506223
Si	-5.84470555367248	-0.00119995334596	1.14787184589450
Si	-9.43621470545475	-2.02354174395446	1.10659786265924
Si	-8.28817486540817	-4.13364037051289	1.10710900010858

Si	-4.76385860874966	-2.10093173373167	1.17112275912320
Si	-1.24307279029942	-0.00003616648931	1.30404856795743
Si	2.42050831797504	2.01669124421631	1.12766584633836
Si	5.89163711607362	4.12331083748636	1.12828463734956
Si	4.76927450084109	2.04999878061895	1.13739474899022
Si	1.20715436195556	-0.00048654700866	1.18110042040506
Si	-2.41665541258399	-2.01507376972189	1.10050729257146
Si	-5.91571195224609	-4.15767846714496	1.14019072327094
Si	8.26558023422297	4.13090175352865	1.11198284332552
Si	9.47767361272346	2.05296192496609	1.10690813320612
Si	5.93529876292996	0.00081135240774	1.13234113453113
Si	2.42189860297072	-2.01673268385494	1.12716440208593
Si	-1.20887468549292	-4.03607970567106	1.15345049105560
Si	-4.81270522092231	-6.26628708736126	1.14795177949649
Si	8.28802733354599	0.00142659757800	1.11382150487259
Si	4.77064398999237	-2.04912963696760	1.13696057881626
Si	1.16216400995965	-4.00746387691626	1.15347384167792
Si	-2.44127380920243	-6.05404434849211	1.14432204749473
Si	9.47884860677185	-2.04944358575761	1.10649223309948
Si	5.89406752944377	-4.12185581164338	1.12745268351971
Si	2.38727220912924	-6.03234291114953	1.14299319625823
Si	-1.22263288214229	-8.08873299503957	1.14672323611559
Si	8.26801384668509	-4.12811503096781	1.11115688336727
Si	4.76455577072064	-6.21820760078513	1.14857569789616
Si	1.18307040138877	-8.07590360754984	1.14843761188902
H	-1.76829821742748	9.20926462603508	1.98276233631510
H	-1.77128597664368	9.20951626421830	-2.09198285901653
H	5.33820767570442	7.30780806905566	-2.12919218476986
H	8.93029016871434	5.16732231248641	-2.12906172687077
H	8.93332022288638	-5.16353349102839	-2.13007640137162
H	5.34188915848214	-7.30607273370863	-2.13050553566747
H	1.73454989671958	-9.19895738329145	-2.09198230420234
H	-1.76734726123788	-9.20981205919537	-2.09330954842683
H	-5.39754065275787	-7.33393174851277	-2.13332325473155
H	-8.94609758185722	-5.14651537105446	-2.14477465028924
H	-8.94899670775150	5.14289786205848	-2.14419871190178
H	-5.40126379233756	7.33226006130507	-2.13234268128198
H	-5.40336108397709	7.34838693428446	2.00007502982500
H	-9.00961425716486	5.15445756305346	1.93167886851591
H	-9.00664832016392	-5.15854504901402	1.93111815929903
H	-5.39954367482252	-7.35060420500275	1.99917263489095
H	-1.76419158771472	-9.21018699500146	1.98134542645004
H	1.72897222903052	-9.18920136566489	1.99102919784273
H	5.35186458184314	-7.29757746601200	2.00618022357349

H	8.96333248391153	-5.16830230674335	1.93658293768730
H	8.96032432784314	5.17131509480155	1.93761057028683
H	5.34805706596999	7.29857539973286	2.00761596721253
H	1.73059300774022	9.19929818249542	-2.09043897469201
H	1.72489478382751	9.18893671600518	1.99247754540043
C	0.28467211030819	-0.00096226541472	3.39062091469899
O	1.25147249031801	-0.00201579772581	4.09027222175231
O	-0.95784795651383	0.00002097219601	3.38636929892083
H	-10.64974335981598	-2.05983701218154	-2.15200802817012
H	-10.68323765149666	-2.07082241668526	1.93722351861276
H	-10.68447456466540	2.06569457946862	1.93742894526504
H	-10.65093289056522	2.05522558524029	-2.15178166673550
H	10.72413131631648	-2.13032598788075	1.93691086140505
H	10.72288865335407	2.13441296356016	1.93737235855195
H	10.70049876256933	-2.13073591578816	-2.14246609744281
H	10.69928384568205	2.13560158591905	-2.14204658695185

• **TS 2Si-CO₂ + H₂ → 2Si-COOH**

Si	-1.14220000	-7.97290000	1.06930000
Si	1.25000000	-8.01310000	1.06770000
Si	2.44110000	-5.96700000	1.08740000
Si	4.79960000	-6.22080000	1.20660000
Si	5.93520000	-4.13350000	1.27190000
Si	8.30700000	-4.11270000	1.46060000
Si	9.50000000	-2.02930000	1.51460000
Si	-2.31860000	-5.91890000	1.14090000
Si	1.22080000	-3.95090000	1.00350000
Si	4.81920000	-2.04590000	1.15300000
Si	8.30490000	0.01410000	1.41590000
Si	-4.68690000	-6.12310000	1.23920000
Si	-1.12700000	-3.89270000	1.14620000
Si	2.46330000	-1.96320000	0.98400000
Si	5.96930000	-0.00110000	1.23840000
Si	9.47900000	2.06870000	1.50550000
Si	8.25980000	4.13640000	1.44750000
Si	4.80260000	2.02940000	1.13570000
Si	1.12430000	-0.03200000	0.69200000
Si	-2.51640000	-2.06040000	1.00440000
Si	-5.91830000	-4.08460000	1.28380000
Si	-4.82800000	-1.98300000	1.26730000
Si	-1.19740000	-0.11480000	0.81590000
Si	2.44470000	1.91750000	0.96220000
Si	5.88940000	4.12890000	1.25180000

Si	-8.28580000	-4.06170000	1.49110000
Si	-9.53550000	-2.00400000	1.53910000
Si	-6.04520000	0.03690000	1.23530000
Si	-2.43010000	1.90370000	0.97500000
Si	1.19510000	3.89940000	1.00550000
Si	4.73780000	6.20740000	1.19220000
Si	-8.38620000	0.06370000	1.42460000
Si	-4.77910000	2.00880000	1.13610000
Si	-1.15160000	3.86710000	1.01510000
Si	2.38390000	5.93510000	1.07870000
Si	-9.52410000	2.14200000	1.49720000
Si	-5.87110000	4.10440000	1.22580000
Si	-2.34990000	5.90040000	1.06400000
Si	1.20020000	7.98680000	1.07840000
Si	-8.23860000	4.16740000	1.41250000
Si	-4.70500000	6.16980000	1.16050000
Si	-1.18920000	7.96510000	1.07090000
Si	-1.15140000	-7.87340000	-1.33170000
Si	1.26440000	-7.96160000	-1.33710000
Si	2.53760000	-5.96470000	-1.31290000
Si	4.91420000	-6.23550000	-1.20480000
Si	6.12440000	-4.18540000	-1.12580000
Si	8.48850000	-4.15250000	-0.93270000
Si	9.66000000	-2.04540000	-0.88420000
Si	-2.38820000	-5.84690000	-1.24950000
Si	1.24260000	-3.95760000	-1.41400000
Si	5.02870000	-2.11050000	-1.24890000
Si	8.46790000	0.00980000	-0.98190000
Si	-4.77600000	-6.10970000	-1.18310000
Si	-1.15870000	-3.79950000	-1.28900000
Si	2.69180000	-2.07280000	-1.38780000
Si	6.11840000	-0.00980000	-1.16840000
Si	9.63320000	2.08020000	-0.89450000
Si	8.44190000	4.17700000	-0.94610000
Si	5.02500000	2.08660000	-1.25980000
Si	1.67910000	-0.00410000	-1.66890000
Si	-2.78800000	-2.10670000	-1.61840000
Si	-6.10900000	-4.13230000	-1.09640000
Si	-5.06570000	-2.02900000	-1.13560000
Si	-1.64040000	-0.10000000	-1.50870000
Si	2.68740000	2.05910000	-1.42020000
Si	6.07770000	4.18230000	-1.14210000
Si	-8.47100000	-4.11490000	-0.90310000
Si	-9.70610000	-2.03850000	-0.86220000

Si	-6.21730000	0.02820000	-1.16690000
Si	-2.62610000	2.00900000	-1.41870000
Si	1.22840000	3.92490000	-1.40920000
Si	4.84540000	6.22200000	-1.22630000
Si	-8.56270000	0.04190000	-0.96940000
Si	-4.97570000	2.03410000	-1.26990000
Si	-1.17320000	3.88430000	-1.40870000
Si	2.46880000	5.95660000	-1.32340000
Si	-9.68330000	2.13390000	-0.89900000
Si	-6.04060000	4.12970000	-1.16660000
Si	-2.41920000	5.91430000	-1.33520000
Si	1.21900000	7.97220000	-1.32530000
Si	-8.40950000	4.18100000	-0.98580000
Si	-4.79920000	6.16420000	-1.25890000
Si	-1.19550000	7.94740000	-1.33240000
H	1.73300000	-9.10070000	-2.19360000
H	1.83580000	-9.12240000	1.88870000
H	-5.20090000	-7.24670000	2.08830000
H	-8.90790000	-5.08920000	2.38860000
H	-8.81470000	5.23630000	2.29150000
H	-5.20080000	7.27840000	2.03780000
H	-1.78970000	9.04960000	1.91290000
H	1.77980000	9.08060000	1.92320000
H	5.23380000	7.31310000	2.07290000
H	8.86210000	5.17040000	2.34990000
H	8.92830000	-5.13250000	2.36640000
H	5.30070000	-7.32260000	2.08900000
H	5.50450000	-7.34340000	-2.02250000
H	9.26810000	-5.18320000	-1.69180000
H	9.21230000	5.21660000	-1.70240000
H	5.42680000	7.33260000	-2.04710000
H	1.72220000	9.10610000	-2.16780000
H	-1.71240000	9.07160000	-2.17970000
H	-5.37240000	7.26460000	-2.09950000
H	-9.14520000	5.23750000	-1.75400000
H	-9.24170000	-5.16970000	-1.63850000
H	-5.32130000	-7.23860000	-2.00560000
H	-1.73920000	-9.09800000	1.86010000
H	-1.69310000	-8.96570000	-2.20580000
C	-0.57560000	-0.36100000	-3.09540000
O	-1.13190000	-0.81650000	-4.14240000
O	0.70560000	-0.09310000	-3.15730000
H	-2.14790000	-1.47920000	-3.76080000
H	-2.84720000	-2.07510000	-3.34400000

H	-11.01010000	-2.15840000	-1.59260000
H	-10.72620000	-2.08690000	2.44630000
H	-10.97470000	2.26660000	-1.64810000
H	-10.70530000	2.25770000	2.41180000
H	10.95540000	-2.13100000	-1.63410000
H	10.68620000	-2.08320000	2.42930000
H	10.66660000	2.14320000	2.41680000
H	10.92600000	2.17990000	-1.64710000

• **TS 2Si-CO₂ + H₂* → 2Si-CO-OH**

Si	1.15531134480354	8.07522164415367	-1.32843049443186
Si	-1.23701516890163	8.04614931426062	-1.34183736624089
Si	-2.36919479165206	5.96531953495523	-1.32715398383789
Si	-4.72852436976701	6.15879289187151	-1.36850308269545
Si	-5.71681106457410	4.00907872448626	-1.35028104595511
Si	-8.08558239953691	4.02278557970585	-1.40217683050504
Si	-9.24489088298084	1.93047240961538	-1.41787080007004
Si	2.35715033325279	6.03440146953308	-1.29010383977373
Si	-1.13984481792827	3.94409130605846	-1.27420660533318
Si	-4.50773079993111	1.97478035559238	-1.29288845440148
Si	-7.99096695122425	-0.07658559736735	-1.36456863174593
Si	4.71336576947205	6.27433661229443	-1.31516386762551
Si	1.20506813874534	3.96983503456013	-1.24145803221694
Si	-2.15057057181485	1.80606951631008	-1.31116623187729
Si	-5.63626512369761	-0.08020648057479	-1.28000037870374
Si	-9.26641526194762	-2.06149178088160	-1.40765852774584
Si	-7.94582454017884	-4.05048252447221	-1.39090380251516
Si	-4.20906036140738	-1.96019601534095	-1.26303583250958
Si	-1.01813357484642	-0.18096247138909	-1.77104414433584
Si	2.11912099389424	1.79468529332467	-1.22718855185379
Si	5.66836316682433	4.10596592448990	-1.32102852516331
Si	4.47524935647981	2.05589322602570	-1.26622841939548
Si	1.15718809587073	0.02895136125109	-2.42441686531623
Si	-2.24813821167033	-1.98686709229291	-2.53638100984261
Si	-5.57938067988148	-3.90016584827158	-1.28351964568409
Si	8.04036806436807	4.08632120962202	-1.37611741103987
Si	9.23017549360196	2.00628707992582	-1.39586851771363
Si	5.62940933289393	0.01218359871529	-1.34671835231267
Si	2.14203488504694	-1.77237603363848	-1.28812156355243
Si	-1.24599674436170	-3.69973207467834	-1.28752718087765
Si	-4.60483667372778	-6.05494866185171	-1.32658992519191
Si	7.98189808797464	-0.00071686838525	-1.37803794986933
Si	4.49315040471096	-2.04227145576438	-1.30552792213883

Si	1.10684169727384	-3.88731050649388	-1.24150326953109
Si	-2.24948374884864	-5.85143005874793	-1.29476639838639
Si	9.23689702275442	-2.00453951151199	-1.41205063080719
Si	5.68504001698635	-4.08417031555730	-1.36657746940849
Si	2.28468474433490	-5.94444416408790	-1.33782517072633
Si	-1.20090058972995	-7.97219212122759	-1.36058218042246
Si	8.05610078625161	-4.08982141639563	-1.40622427940094
Si	4.64097262147549	-6.20629207100472	-1.38409765856408
Si	1.18169289448707	-8.03604947410567	-1.36702151321587
Si	1.14973798509499	8.10972649925585	1.07625768857269
Si	-1.24893774700917	8.06989498307063	1.06532180175896
Si	-2.40432856765780	6.00291736776592	1.07752774254737
Si	-4.76812801817978	6.19483408727077	1.05891812284717
Si	-5.77053440144779	4.04922399072655	1.05235031840708
Si	-8.13910070522928	4.03685302337649	1.00186542421394
Si	-9.31464244929806	1.94651348348292	0.98662088437786
Si	2.37152174548684	6.07941853337624	1.11500218246943
Si	-1.15848715548796	3.99348385790365	1.12002880532562
Si	-4.57567878536197	2.00924568986351	1.09816166244991
Si	-8.07852371537891	-0.07131315909827	1.04073670075520
Si	4.73499117941624	6.29213899066712	1.10396555773054
Si	1.19292054321214	4.02649249861314	1.15624828873931
Si	-2.22859441038958	1.89696569357586	1.11134650954678
Si	-5.72457275587233	-0.03815603115025	1.11533917726412
Si	-9.32880916052834	-2.07574421278403	0.99770819141420
Si	-8.04158336505861	-4.09264873768964	1.00986351260900
Si	-4.43898131926495	-1.99774805907453	1.20461092062280
Si	-1.09329367388229	0.02341333148421	1.86492988739791
Si	2.23437789247777	1.92057882648627	1.19604822083392
Si	5.72492858409647	4.13636372425289	1.07948403989972
Si	4.57421533610212	2.07151488692773	1.13689086154550
Si	1.23801585177178	0.00669726811097	2.04810517060232
Si	-2.28510536701874	-2.02259915464875	2.02208444326897
Si	-5.67933586250602	-3.98701913180377	1.10721945109419
Si	8.09536930246438	4.10168145254661	1.02409630106147
Si	9.26843860254713	2.00716498909270	1.01051971532330
Si	5.67895210677024	-0.00024933556166	1.06785126775114
Si	2.23860396783735	-1.87327181830905	1.13432157462100
Si	-1.17986692806334	-3.86836085807592	1.18625298379222
Si	-4.64296901475649	-6.10966435586319	1.08901337845114
Si	8.03154345682130	-0.00876995188179	1.02803231919903
Si	4.57497596746808	-2.07290128868151	1.09865703301617
Si	1.15983584335121	-3.95071662302434	1.16057594065407
Si	-2.28341099983149	-5.94037444597621	1.09914150969236

Si	9.27731282709976	-2.01935088747094	0.99371846877800
Si	5.73277724221603	-4.12963066647685	1.03554130467804
Si	2.32778078686422	-6.00733086345935	1.05941138641293
Si	-1.19630412041398	-8.03798423890743	1.04461971485095
Si	8.10278111817908	-4.11218286244581	0.99465648824441
Si	4.68672085322975	-6.25415628629606	1.03506753521284
Si	1.19195760575999	-8.08097210980752	1.03804943474592
H	-1.82651911311713	9.17569071081212	1.89615134508037
H	-1.82030962292940	9.12886830130507	-2.19832290159744
H	5.30932224859273	7.32652917685090	-2.19947461551735
H	8.69621478394040	5.12102421735196	-2.23960196977149
H	8.71594531428440	-5.12001159762486	-2.27171456642877
H	5.19171569131537	-7.27084235945696	-2.28308563188738
H	1.76404492958762	-9.10685457522791	-2.23831067740787
H	-1.84133446043356	-9.00546340446483	-2.23648889873976
H	-5.21029188006212	-7.07673999908122	-2.24095014979186
H	-8.49403740310649	-5.13137742916569	-2.27231850433998
H	-8.74653488268942	5.05269167386889	-2.26704273811365
H	-5.32909807201009	7.19773177837058	-2.26569392992477
H	-5.38647479925104	7.25470108280412	1.91916692746534
H	-8.84696861384377	5.06828363074389	1.82724197453723
H	-8.68503019825312	-5.17862730192992	1.81837971415292
H	-5.23733276509455	-7.15736485872308	1.98205566584765
H	-1.80287753809692	-9.12700007146084	1.87694688394556
H	1.75942437029000	-9.18636676732761	1.87603213213753
H	5.27289014885024	-7.33664545429993	1.88949500666825
H	8.80729297294105	-5.14731610793299	1.81829234283406
H	8.81196248884526	5.13008385686309	1.84606050235006
H	5.35414537331694	7.34248456327506	1.97485346228355
H	1.71985077865081	9.16969847881846	-2.18224858957056
H	1.67461938980100	9.24407457048450	1.90360407673848
C	0.59997394253546	-0.11541593559193	3.89889412302224
O	1.04706922538449	-0.29590815266636	4.99043189112491
O	-0.85324118057420	-0.02114235919384	3.70958164173064
H	-10.46742007872786	-2.12574515313647	-2.30083908028278
H	-10.56769798929178	-2.16177779915936	1.83637595121103
H	-10.57099836905092	2.00727441305853	1.80164798400898
H	-10.45656542787846	1.94682173792770	-2.29946097563238
H	10.52158025334115	-2.07585495619144	1.82770121228258
H	10.51200726999161	2.05844758561267	1.84601760633657
H	10.45588593028972	-2.03996308380089	-2.28354129585665
H	10.44941012159825	2.05553872702970	-2.26646329099469
H	-2.17674087565383	-1.88636132127374	3.79465221244391
H	-1.61266816201611	-1.10231345954088	3.95278559981117

• TS 2Si-CO-OH → 2Si-CO-H₂O

Si	1.18518362367747	8.07797845318921	-1.31203162171124
Si	-1.20887800211675	8.08425137052934	-1.32217694037444
Si	-2.35474240925322	6.01172258726100	-1.29096781494911
Si	-4.71738023734314	6.16718646197786	-1.31483758199087
Si	-5.66722987866168	3.99944617890615	-1.27575260960441
Si	-8.03809862337094	4.02019688884006	-1.29180923800648
Si	-9.21129859371595	1.93676553051487	-1.28384417920595
Si	2.36694516070437	6.02409752765629	-1.26582155021625
Si	-1.14191205184326	3.97591003804919	-1.25287839245062
Si	-4.46870884030552	1.95902579942314	-1.22974128573629
Si	-7.96496187023917	-0.07225306423963	-1.25892080951944
Si	4.72473308485708	6.24819655726790	-1.27479748751852
Si	1.20589671565188	3.96009510855739	-1.23799134784154
Si	-2.10626869446038	1.81679137593690	-1.29006413641942
Si	-5.61311063817487	-0.08517001164365	-1.21305629183129
Si	-9.25948881871483	-2.04437911111824	-1.28790220857923
Si	-7.96639989581490	-4.05133466831051	-1.29877843094310
Si	-4.23173003480821	-1.99015553827536	-1.22616357612222
Si	-0.96668197633968	-0.18127110658356	-1.68387409545728
Si	2.08626801736912	1.76612164940497	-1.27640503607543
Si	5.66095147292107	4.07307284698548	-1.25746087207355
Si	4.44170616858684	2.03867120526154	-1.21751470397247
Si	1.17062325389448	0.02337751692250	-2.56184884470568
Si	-2.22245818517095	-1.95401352014985	-2.39400749540534
Si	-5.59733305498684	-3.92299117865754	-1.25775731719468
Si	8.03263208270779	4.05223533560742	-1.28047098277155
Si	9.21825283649900	1.97064783233858	-1.28424833772118
Si	5.60050359936628	-0.00567135395303	-1.28192560794922
Si	2.10484962316039	-1.75499696066169	-1.32923924441661
Si	-1.24981392281905	-3.75611800101921	-1.28072339894285
Si	-4.63220860404219	-6.08029788421023	-1.29951628482638
Si	7.95528427748466	-0.02550401092832	-1.28043489205997
Si	4.45383283653372	-2.05439300667837	-1.25349506748158
Si	1.10039405143062	-3.89206503600834	-1.24609241140615
Si	-2.27356755515401	-5.89298634096216	-1.29035153618682
Si	9.21235897399765	-2.02703021317019	-1.29586066643380
Si	5.65479876568408	-4.09139651269714	-1.28857177635923
Si	2.26655417426589	-5.95714395859706	-1.29369836063162
Si	-1.21881585448160	-8.00771347770899	-1.34292954519866
Si	8.02453611719324	-4.10714471569431	-1.29894695824234
Si	4.62205007310487	-6.21760465784176	-1.31573289617182
Si	1.16540566060663	-8.05140751256159	-1.34093355629655

Si	1.17988624534249	8.12699181329450	1.09246361730836
Si	-1.21663353697008	8.12876429323955	1.08231105729218
Si	-2.37454649046741	6.06510370005378	1.11391410377026
Si	-4.73746555833058	6.21049833645701	1.11204952446101
Si	-5.69061010156894	4.04186309598066	1.12958866486161
Si	-8.05810246118808	4.03627582703878	1.11282478369666
Si	-9.23220793306628	1.94682227744156	1.12119713701241
Si	2.37385945485210	6.08024269823321	1.13823419653921
Si	-1.16192898919373	4.03580065551704	1.14436819169147
Si	-4.51616772234042	1.99072206188020	1.15992795952918
Si	-7.99857076848501	-0.07430559614275	1.14763632800455
Si	4.73393600994825	6.28039942851201	1.14186400178378
Si	1.18270147389705	4.03749163274076	1.16409437009156
Si	-2.15769652773115	1.90465120688236	1.10403097562437
Si	-5.63849040210213	-0.07839387678666	1.18362616603892
Si	-9.27964541680615	-2.06144022870191	1.11787746073449
Si	-8.00414724243768	-4.08508385499053	1.10210711267292
Si	-4.30532845701861	-2.02640551716127	1.21742624372799
Si	-1.27173279555352	-0.04176762782577	2.02238645746565
Si	2.17909667713917	1.91693860746398	1.15233959781796
Si	5.68833401819924	4.11080183898540	1.14249318030575
Si	4.51734060549159	2.05199481236448	1.19211309688484
Si	1.09541099762827	-0.00758274501995	1.97120613294415
Si	-2.28568401452580	-2.14224093958309	2.37790272312300
Si	-5.63984438715382	-3.97105396356857	1.14079233120492
Si	8.05772291759112	4.06843585288495	1.12040587723208
Si	9.22646338321293	1.97371794602523	1.12255217187579
Si	5.62262945527697	-0.01597279621211	1.13055076120387
Si	2.16821640473646	-1.91197754603619	1.10128317422359
Si	-1.24423248390248	-3.83826377185249	1.17385628077482
Si	-4.64436738610383	-6.11698952239518	1.11501520710978
Si	7.97657889431268	-0.03214629514875	1.12594089009866
Si	4.50505957663793	-2.07680883072781	1.15575758072977
Si	1.09351100794774	-3.98182898552069	1.16606408008247
Si	-2.28312333425406	-5.95240184915932	1.10709898399978
Si	9.22473619601575	-2.03899791129040	1.11041949514539
Si	5.67017280580845	-4.13317168691167	1.11312074854371
Si	2.28512463940384	-6.02421404468506	1.10270251652536
Si	-1.22016072953702	-8.06243024102121	1.06307513910332
Si	8.03973403785474	-4.12375501142359	1.10229771166312
Si	4.64142924838556	-6.26384134990793	1.10136397493388
Si	1.16615348155220	-8.10720496158522	1.06311960479405
H	-1.78388103208361	9.24307152449629	1.90865273679866
H	-1.77499816134956	9.16837381997828	-2.18814411628192

H	5.33959053930607	7.28345471417196	-2.16586944117994
H	8.69925018704266	5.08754945705657	-2.13475156076943
H	8.68987691415352	-5.14239209885786	-2.15399262662464
H	5.18999618820339	-7.27426347197380	-2.21320762998342
H	1.76256711501160	-9.11240317881786	-2.21495015993052
H	-1.83576882185243	-9.05404505652271	-2.22069537447528
H	-5.24609426418858	-7.10121170166898	-2.21031900621535
H	-8.55333271993784	-5.12318156473199	-2.16690875201670
H	-8.70243788759497	5.05575361421676	-2.14776900170926
H	-5.34442412178797	7.19361185973187	-2.20879159418133
H	-5.36848322041809	7.26396132492778	1.97152814643274
H	-8.74916699428805	5.07425016992089	1.94488651651074
H	-8.63474652563733	-5.16768130307188	1.92566427165643
H	-5.24363242438306	-7.16852617544817	2.00092974642225
H	-1.83147008364175	-9.14706375763499	1.89772726358317
H	1.75009322296909	-9.20951506584316	1.89405315206328
H	5.22585996835788	-7.33618183627453	1.96955785429443
H	8.72544619693786	-5.16007391438368	1.94018808641956
H	8.76169025766089	5.09688439116092	1.95318631449110
H	5.35490550878158	7.32533264415521	2.01786899961907
H	1.76405871096556	9.16318508817305	-2.16844609352068
H	1.73743066147495	9.25164646122052	1.91169585613393
C	1.52900104981311	-0.03253881874555	3.76296560750879
O	1.88767250011535	-0.05114816111022	4.86279373051821
O	-1.52615814790361	0.17353820330008	3.88722983841322
H	-10.47497816699848	-2.08551776634005	-2.16337610373724
H	-10.50737677544752	-2.13391807466058	1.97483796937349
H	-10.47218789358561	2.01225130968205	1.96126725214089
H	-10.43959050958937	1.96397494840066	-2.14209002034499
H	10.45718997376925	-2.09184089908072	1.96199095993521
H	10.45743549478508	2.01765834664172	1.97690814669656
H	10.44001754546541	-2.06325813550754	-2.15485749763555
H	10.44656503079938	2.01236749442493	-2.14215334833983
H	-1.99703815003471	-1.00354314551545	3.86935683096219
H	-2.22445978526769	0.82940640023369	4.10923182534670

• **TS 2Si-COOH → 2Si-HCOOH**

Si	1.23043678522948	7.97903296000883	-1.14547680528940
Si	-1.16356521198183	8.05343399591186	-1.14640343900286
Si	-2.41413697351529	6.04028998938742	-1.16967093902108
Si	-4.77245273319557	6.27220603627383	-1.26384452668348
Si	-5.85720368514846	4.15450502827127	-1.31395823900415
Si	-8.22989078828295	4.14338420450855	-1.49649888995961

Si	-9.44224772316130	2.07237106169331	-1.54529904284471
Si	2.36989920744205	5.90217349954669	-1.17448608109056
Si	-1.22437809626777	4.00522838864665	-1.12447981224110
Si	-4.73214889987650	2.06973305351605	-1.19616625175062
Si	-8.24593017581201	0.03156409176190	-1.44956243633245
Si	4.73633162636287	6.05532585139801	-1.25776522631843
Si	1.12056124570087	3.90412304018438	-1.17972951628267
Si	-2.37017348831571	1.96767890186611	-1.04340035041579
Si	-5.90910684007735	0.04279967363494	-1.27951078271274
Si	-9.41569226752778	-2.02469321221018	-1.53808717253306
Si	-8.15609788793273	-4.06618188884952	-1.48596332763414
Si	-4.67034521694108	-1.94419587125217	-1.17026095696938
Si	-0.96453293429225	0.07441469960091	-0.77506240657006
Si	2.37697915277144	1.93460316629240	-1.32088544180047
Si	5.84653974286326	3.95605433606737	-1.29638886320805
Si	4.71803882641533	1.87962919183716	-1.24381252752614
Si	1.32337594296272	-0.18141883568627	-1.17295369765378
Si	-2.31200209976322	-1.86563731244335	-0.98960498271679
Si	-5.78799080474934	-4.02368408416959	-1.29200258304726
Si	8.20522384169058	3.93378953997368	-1.49675328255458
Si	9.31985806306401	1.81435203139459	-1.57512299560987
Si	5.75879972774718	-0.22330484593077	-1.20899989607843
Si	2.28576459472162	-1.94244687092972	-2.45607892971690
Si	-1.05029874064196	-3.84119004839004	-1.08653175389732
Si	-4.64189324093331	-6.10125557986838	-1.25264217431977
Si	8.10563610025589	-0.21932995186312	-1.45169435600722
Si	4.23440916582069	-2.03111372518040	-1.14659485508027
Si	1.29894975662127	-3.65092979827832	-1.18737845739042
Si	-2.28598560597136	-5.85540348252940	-1.16455040216516
Si	9.36331748993139	-2.21141207348446	-1.55865361490462
Si	5.63005570505629	-3.94322546917128	-1.14977772216891
Si	2.25917390340056	-5.81633966277324	-1.19055792615493
Si	-1.21144781681505	-7.96145524315635	-1.18981128846503
Si	7.97699982399422	-4.15085347374121	-1.48305736474367
Si	4.60299859634666	-6.07881161797485	-1.22026412487585
Si	1.17088061151918	-7.91798228621071	-1.19104551024796
Si	1.23922663019704	7.92267466856981	1.25809208534050
Si	-1.17650781004757	8.01351338683542	1.25761654486852
Si	-2.48397559003120	6.03394402235018	1.23102916471949
Si	-4.86167717274613	6.27979697384656	1.15364687687818
Si	-6.03331921191466	4.20669776595467	1.08133282930121
Si	-8.39904301524111	4.18373881717695	0.89872852456815
Si	-9.59343166443821	2.08946519291788	0.85440502393511
Si	2.43044503641413	5.86757258903103	1.21914317685467

Si	-1.25148410728827	3.99808948092078	1.29337944273655
Si	-4.94273336432833	2.12779411923835	1.19668896355747
Si	-8.40544352113846	0.03380009053111	0.95125892549706
Si	4.82184177181948	6.05061469651470	1.16747045412338
Si	1.12813485509403	3.87788067904612	1.25401255598363
Si	-2.60717781457239	2.06340573406340	1.33724366610427
Si	-6.05522819732205	0.04551308266904	1.12856201337697
Si	-9.56113433784244	-2.04061915090341	0.86154379730893
Si	-8.33314995339081	-4.11614108714290	0.90950148374599
Si	-4.88577383712451	-2.00988002559648	1.22797418575406
Si	-1.50105628152879	0.04196099032021	1.61508686151875
Si	2.60935872980994	2.06575930448814	1.05887051713006
Si	6.03975605784525	4.00105071289475	1.09693678977060
Si	4.92508408542229	1.93821731160470	1.16076512375609
Si	1.78361612735581	-0.11969895441838	1.17379359600853
Si	-2.54330635437219	-2.00735892108173	1.38384614479303
Si	-5.97038394766037	-4.08717470305787	1.10256052772543
Si	8.40121102408829	3.95263091197929	0.89888859257208
Si	9.53302848754005	1.82730576303675	0.82020323710917
Si	5.98002972966191	-0.17699313819715	1.18763216273211
Si	2.56566921713444	-2.03503085934397	2.22498659333263
Si	-1.09596870786345	-3.87219326659810	1.31033237003154
Si	-4.72868865247085	-6.11770339375029	1.17027771695824
Si	8.32388292268273	-0.21252542464230	0.94113071463765
Si	4.72744336677622	-2.15875077929288	1.42957796497955
Si	1.27872552516043	-3.73487036698627	1.27936285996203
Si	-2.34693828045736	-5.89730610600398	1.23440095535782
Si	9.54063733379797	-2.24505533230530	0.83636761008790
Si	5.92848013309791	-4.14183838315957	1.23920895231438
Si	2.32814767130391	-5.84897763850958	1.20676169854143
Si	-1.22386288438916	-7.97830527278147	1.21547770641549
Si	8.26304653465351	-4.27633886168489	0.89514887671892
Si	4.68937120489201	-6.16208612639447	1.18159597763332
Si	1.17674898130250	-7.91922142970026	1.21334361231462
H	-1.64685359437224	9.15368433447174	2.11100001930343
H	-1.70872799669172	9.18121233406348	-1.96951253648723
H	5.30386549983685	7.13504379058973	-2.12821884708760
H	8.83599174360835	4.94244961140029	-2.40792499714776
H	8.37457278476134	-5.24044373785586	-2.43171100370923
H	5.21877581441536	-7.07135886797069	-2.15900545181840
H	1.80043552554171	-8.98080666754926	-2.03948957620622
H	-1.81701765781054	-9.02181778263509	-2.05827146385430
H	-5.16520169757668	-7.19544594072665	-2.13256651949738
H	-8.73942347293631	-5.11004087947725	-2.38958630439093

H	-8.84574232874328	5.17302764597714	-2.39493361480298
H	-5.31417855270108	7.35940346578965	-2.14037842492103
H	-5.45577897737247	7.37764823735703	1.98248934224267
H	-9.16641595593775	5.22325334139274	1.65841564464948
H	-9.08934120129503	-5.16555211912522	1.66690808486844
H	-5.30289104449024	-7.22556411929140	2.00084439559745
H	-1.75301007215056	-9.09485066894677	2.06483118739944
H	1.75928223115974	-9.01046141940533	2.06084929452951
H	5.20055280796460	-7.28264729829654	2.03610431340153
H	8.99235702816425	-5.38127957493882	1.59753057957417
H	9.19259935452379	4.96588498904003	1.66904799548065
H	5.40398825608335	7.15005269100694	2.00408309667494
H	1.83745172393373	9.07817881149362	-1.96413702676045
H	1.78922835469413	9.02609310365663	2.11202715369792
C	0.82870132492376	0.06852117465404	2.92602144905085
O	1.41563813893446	0.88058691632663	3.85180951738110
O	-0.48709034828590	0.11036086882912	3.05657853085086
H	2.38412086637356	0.86701404729478	3.69468141421084
H	1.37215459004059	-1.27558156925364	3.37803689688092
H	10.48930394143662	1.82506616400301	-2.51281005593393
H	10.84379506503086	1.89249347205987	1.54543365702496
H	10.82170315768783	-2.34165713932476	1.60778370447276
H	10.51452354409480	-2.30402268500340	-2.51210198391656
H	-10.84633241940306	-2.15573367856720	1.62450078132279
H	-10.88418325333503	2.18933324453495	1.61022349768800
H	-10.63134511507638	2.13250866939343	-2.45546819843112
H	-10.60102046362769	-2.10854524508824	-2.45118247540344

• **TS 2Si-HCOOH → 2Si...HCOOH**

Si	-1.03287312382818	-7.96709703218677	-1.19865698988844
Si	1.36726537556958	-8.03528993423733	-1.21683850511615
Si	2.60323865887910	-6.01619336132483	-1.32185007936511
Si	4.96879160591636	-6.24195076537179	-1.32973069296743
Si	6.01071378179957	-4.11579309955886	-1.33840323548480
Si	8.38915206662242	-4.06889490877265	-1.33345945552079
Si	9.48285197859787	-1.94324629882639	-1.34459792523905
Si	-2.21129275821881	-5.90769120610908	-1.23092576627967
Si	1.34030950568178	-4.01917085400577	-1.41290150363900
Si	4.77749914950552	-2.09724180878389	-1.26063915270787
Si	8.15950578142447	0.02276628857186	-1.31094093456883
Si	-4.58588458997333	-6.07756155484022	-1.21961547832902
Si	-1.01499768222802	-3.87250867516021	-1.30411030994106
Si	2.43881780423983	-1.96903500859723	-1.58070245177056

Si	5.80635256926495	0.01524210031621	-1.26784914964265
Si	9.34582290992031	2.07102040826604	-1.32412170857188
Si	8.09736164032480	4.11333944258303	-1.30858677487178
Si	4.58070888907886	2.02094028744342	-1.19378406549888
Si	1.15747467194886	-0.07812630846374	-1.75531804121122
Si	-2.31916947118498	-1.92700548235254	-1.43292294418634
Si	-5.75425412746127	-4.00470532595654	-1.24839302363619
Si	-4.66155008370681	-1.91027105568630	-1.32975490970958
Si	-1.13133092064339	0.09501115477045	-1.46267640315314
Si	2.24488141177948	1.87158964580113	-1.10278122554255
Si	5.72023912254290	4.08789837195663	-1.24700451002892
Si	-8.12827601011093	-4.09611950773062	-1.22858792775717
Si	-9.43856027362051	-2.07994638029642	-1.25778976613824
Si	-5.96495865292775	0.06552496661787	-1.34033177300458
Si	-2.46460977733479	2.06381930961105	-1.37905252324818
Si	1.12375404494290	3.94409267611287	-1.22231948598116
Si	4.68087212266547	6.22002403377460	-1.26315113921745
Si	-8.32301061473799	0.01206493679270	-1.30158224780931
Si	-4.81956806758553	2.12010642649216	-1.35216549412246
Si	-1.23856300705672	4.05139037525427	-1.29643862736558
Si	2.32120765481340	5.98701421744587	-1.26315546900057
Si	-9.56881551162584	2.03263016346660	-1.29931977391705
Si	-6.02055530721295	4.15578547963125	-1.34954043597295
Si	-2.51200509430760	6.04224156884742	-1.32494386543502
Si	1.09631545691815	8.02359153055857	-1.32489986345493
Si	-8.39644023302161	4.13102722038346	-1.32227534643030
Si	-4.88969255542089	6.24377368582635	-1.36079075461707
Si	-1.30460392569690	8.07965573436202	-1.33001470394811
Si	-1.01360372287120	-7.90853178083718	1.20778067496140
Si	1.38288710825733	-7.93482575459074	1.18720735092459
Si	2.61721027958974	-5.91122428984668	1.07580423821153
Si	4.97675592344013	-6.22115990303130	1.09017705523354
Si	6.02917085425608	-4.10733185759036	1.06334711940141
Si	8.40636857419032	-4.06037353452745	1.06472333321514
Si	9.52402028756664	-1.94665941968787	1.06116151871497
Si	-2.18501661326820	-5.84769763953281	1.16556124676004
Si	1.38462105043750	-3.88981250991646	0.99587978346720
Si	4.78399564835866	-2.09653080309467	1.14256726605885
Si	8.19940884556952	0.02060149442348	1.10380407943145
Si	-4.56220370641029	-6.01626541422630	1.20375361412433
Si	-0.98431346436792	-3.81854550555078	1.11798857163470
Si	2.47050098194166	-1.80234334483720	0.89052851076497
Si	5.84458121695861	-0.00611310549026	1.13711660752739
Si	9.37530026176004	2.07721832419158	1.08011674619958

Si	8.14956208745216	4.13952488441766	1.09039137260579
Si	4.64258588880463	2.03446423173530	1.20284306955373
Si	1.18449419152358	-0.01561539846041	1.70779485888498
Si	-2.28712989906204	-1.88602315320486	0.95109677057280
Si	-5.73248606742425	-3.94960923123655	1.15168225943876
Si	-4.62278944843821	-1.87029658738346	1.07895567344381
Si	-1.04129907208069	0.12554678355194	0.95855680033088
Si	2.29854963502809	1.98548853921944	1.31342440637387
Si	5.77259368892556	4.11061694630791	1.15614191476291
Si	-8.11025891837336	-4.05198473185492	1.17238156899978
Si	-9.42809678433722	-2.04552521926793	1.14358405266675
Si	-5.94389918152901	0.08574262826781	1.07550568602689
Si	-2.44802793981906	2.04253617337845	1.00999464660813
Si	1.09974038303548	4.01017407541298	1.18041889373584
Si	4.68379914138210	6.22608046302147	1.15587898679151
Si	-8.29754224832581	0.03435585567590	1.10649765272955
Si	-4.79721300493076	2.12658140205575	1.05099673615397
Si	-1.27072517459800	4.05921098672925	1.10970155735971
Si	2.31380090095028	6.03764080697920	1.13399065166647
Si	-9.54681166502756	2.05111819610488	1.10233470932135
Si	-5.99763390585169	4.16150339656354	1.05467246999992
Si	-2.52796910671144	6.05915232158553	1.08019908911584
Si	1.09754813150152	8.07691667462617	1.08031579189651
Si	-8.37395375062102	4.14406122762623	1.07747286462385
Si	-4.90124675346224	6.26719349074177	1.06220863785447
Si	-1.30664317588828	8.09185273520900	1.07577217367986
H	1.95068860139281	-9.00984360186924	2.06501998231851
H	1.87836784326664	-9.20187335243938	-2.00816176404096
H	-5.16689953145717	-7.18329093732043	-2.04807216096444
H	-8.78323106078281	-5.17736422073452	-2.03475268591455
H	-9.10977843810224	5.15534108506918	-2.15210891529294
H	-5.44997682113955	7.33328145155227	-2.22415442666414
H	-1.82674999579493	9.20074627912427	-2.17748856643526
H	1.67567746971604	9.11231514111617	-2.17769508785246
H	5.28495519521958	7.27430822060004	-2.13971376425086
H	8.72724733185258	5.16322511266889	-2.17320991978828
H	9.09597814490509	-5.08672638519611	-2.17580326046878
H	5.57104289236188	-7.31629083303629	-2.18271017478223
H	5.52199033394311	-7.31000986005354	1.96354993429435
H	9.10458558760106	-5.08664056170447	1.90407042160982
H	8.85043397601206	5.18735260214423	1.90154029985655
H	5.27304753123657	7.29940275572593	2.01992606826311
H	1.64492585544690	9.22011556819889	1.88169971261807
H	-1.84917076069368	9.21515267441503	1.90747775173906

H	-5.50700599839656	7.35055845530932	1.90213876496345
H	-9.05868938622666	5.18610871995301	1.90926182916438
H	-8.73572805045285	-5.11350607718517	2.02667726080463
H	-5.12426738864577	-7.08146198448700	2.09647561086961
H	-1.61537513153156	-9.09269346524669	-1.99965434382381
H	-1.57249264312040	-8.99664885127480	2.07497064653435
C	-0.47818066954406	-0.60981484466049	3.66471893201837
O	-1.01844715623093	-1.77747298100054	3.98459301482146
O	0.80077284229823	-0.52128602303096	3.43354262383984
H	-1.11163681415258	0.26175790757821	3.87758866939099
H	-0.41493279849566	-2.50086789972356	3.68933828529407
H	-10.65422197981851	-2.15544699747762	1.99860206993174
H	-10.67156846663419	-2.23261637584330	-2.09641404962360
H	-10.78139663139792	2.10093940920077	1.95072987109131
H	-10.81874847736051	2.08492414850862	-2.12502179383156
H	10.77864470625818	-1.96787235192051	1.88092481166267
H	10.70728514380859	-1.93099983823674	-2.20877727536606
H	10.61646962501526	2.15980541614754	1.91656895719666
H	10.56170422758080	2.15607958484732	-2.19650690672111

• **TS 2Si-CO + H₂ → 2Si-OCH**

Si	1.28823625627511	8.06968131966934	-1.26126493492622
Si	-1.11289718537965	8.10193543072755	-1.25460920163230
Si	-2.31676731465299	6.06168911642481	-1.25320235558677
Si	-4.68986427437175	6.22142859511986	-1.25201788104329
Si	-5.74788407708726	4.09232114730656	-1.23690189681839
Si	-8.12051685479643	4.11719066926037	-1.23337475105665
Si	-9.36210833932082	2.05933799214163	-1.23118959015489
Si	2.46672465223046	6.01006746146214	-1.26373598141561
Si	-1.11320919463679	4.02955373942878	-1.25915765054377
Si	-4.61202305355721	2.01765982721689	-1.24513785039106
Si	-8.17551513267066	0.00994930529707	-1.23629672869540
Si	4.83306675911849	6.16248947953379	-1.28161808740840
Si	1.23952225117706	3.98549199835188	-1.25686522419410
Si	-2.25058065805409	1.97440639420703	-1.24201208570417
Si	-5.82275764328680	0.00000070027766	-1.24265906749009
Si	-9.39618734955312	-2.02102088158960	-1.22906169263166
Si	-8.18552096615947	-4.09628412541065	-1.23137683873900
Si	-4.63213207488841	-2.03475588973968	-1.24986574675165
Si	-1.00613135139507	-0.03160260738071	-1.32772122829557
Si	2.25714597037245	1.85326618397188	-1.33423025652232
Si	5.80167123902233	3.99662720726971	-1.27439609788804
Si	4.60581023137357	1.95787037510745	-1.27170394383662

Si	1.26092068784174	-0.19946617400323	-1.72963393819100
Si	-2.27865497263786	-2.00880020779414	-1.25229950510032
Si	-5.81282483047427	-4.08047346923032	-1.24043833406367
Si	8.17100911494503	3.97572234358395	-1.27548750332185
Si	9.30044180114661	1.86383585938515	-1.27607220910228
Si	5.67655241409834	-0.13329883690281	-1.27645797568815
Si	2.28116739314380	-2.05648634075804	-2.50085191851403
Si	-1.10148740060395	-4.03606326101013	-1.26061623908562
Si	-4.72511547015511	-6.19227848693940	-1.25390666541118
Si	8.03301478170510	-0.13582884511964	-1.27608975151117
Si	4.28792623286555	-2.03864488985339	-1.30328402901133
Si	1.24142674398324	-3.77499865569717	-1.29990662944596
Si	-2.34977869652437	-6.04568559267211	-1.25267753572669
Si	9.30063943544140	-2.12882824391952	-1.27270871754553
Si	5.62895266024281	-3.98341818061087	-1.26249340278172
Si	2.25705225814766	-5.90809605888144	-1.25568152553822
Si	-1.22419628202620	-8.12590253852203	-1.25091369771918
Si	7.99369600028685	-4.13014933615491	-1.26638848580083
Si	4.61540453005348	-6.12241029236438	-1.26303422602279
Si	1.16566723847477	-8.01136970475177	-1.25422028197020
Si	1.29502687733640	8.07014613403379	1.14304021525919
Si	-1.10559003515362	8.09931518134640	1.15164528249079
Si	-2.30627033745178	6.05645444948363	1.15247036427097
Si	-4.67965935722504	6.21894071044903	1.17146238670131
Si	-5.74131828676774	4.09184080830612	1.16255987792096
Si	-8.11406384232135	4.11740861626384	1.16930587511931
Si	-9.35559184626169	2.05969369030436	1.17377297826870
Si	2.47171580252702	6.01083673274102	1.13820207274560
Si	-1.10357524738016	4.02262747516101	1.14125888118274
Si	-4.60517979899984	2.01807069747883	1.15912370532666
Si	-8.16883475537968	0.01075807174926	1.17117600495215
Si	4.83781434164031	6.16359531041882	1.14314270742172
Si	1.24782776038827	3.98678171522727	1.15274393920098
Si	-2.24573502647962	1.97161398225292	1.16134028880205
Si	-5.81622763880919	0.00035478975759	1.16575694861538
Si	-9.38982185005885	-2.01964261793942	1.17410173323659
Si	-8.17831640475321	-4.09404815375345	1.17258218305241
Si	-4.62429968793925	-2.03301335591352	1.15782800870433
Si	-0.99998568115690	-0.02706211025097	1.08435656654675
Si	2.26097211592198	1.86024047454618	1.07486978832279
Si	5.80331140020537	3.99717819216434	1.12950222968633
Si	4.60804894209293	1.95867665038548	1.11903124955804
Si	1.20417672532598	-0.07991720645492	1.87825910311696
Si	-2.27023779756149	-2.00454039870696	1.13937413689799

Si	-5.80566394275159	-4.07887322735392	1.16502897428642
Si	8.17246030389253	3.97597812073930	1.13048229237962
Si	9.30214663028904	1.86536791030222	1.12942501440870
Si	5.67721096832068	-0.13057244727317	1.12463385896716
Si	2.29520212326793	-2.06512726925353	2.37849472352460
Si	-1.09615098540762	-4.03154719607807	1.13611635063322
Si	-4.71898093271891	-6.19050596703342	1.16819681111516
Si	8.03284890190860	-0.13256079057227	1.12886805559531
Si	4.28705098767121	-2.03140403897012	1.16623518381598
Si	1.24377589719440	-3.76652919916443	1.17310644022135
Si	-2.34444937964081	-6.04017202679709	1.14918005289328
Si	9.30140665473965	-2.12409920080604	1.13331641712673
Si	5.62697331858329	-3.97458010764769	1.13553121316314
Si	2.25791950223595	-5.89836738353718	1.14361197443831
Si	-1.22087892574732	-8.12067395540765	1.15439475767117
Si	7.99259348660888	-4.12325803311434	1.13555301719317
Si	4.61489342206690	-6.11304735014286	1.14722076927785
Si	1.16798758884049	-8.00354550951207	1.15072588114855
H	-1.64547213395639	9.21638530065498	1.99260112704235
H	-1.65471632658545	9.22254895441613	-2.08964024085890
H	5.45370230412316	7.20717566277626	-2.15815555058255
H	8.86961430281689	4.99745653290934	-2.12067486114219
H	8.59271530639533	-5.21733347867084	-2.10671759839008
H	5.21054424029485	-7.16728205483631	-2.15844485798639
H	1.79273696316774	-9.08426168547572	-2.09275470209798
H	-1.77140861167180	-9.22929113596432	-2.10490960292745
H	-5.33223271903085	-7.25999505666055	-2.11241663287704
H	-8.87263989731507	-5.13582503758982	-2.06437855773317
H	-8.79371093413491	5.16582965254174	-2.06651865501509
H	-5.30157362250515	7.28293608639444	-2.11459854394783
H	-5.28205842052613	7.28045639086247	2.04053427705020
H	-8.78293754986820	5.16641980714086	2.00542248086463
H	-8.85873199656655	-5.13252009610036	2.01235080236292
H	-5.31560977671010	-7.25993290274502	2.03191619299023
H	-1.76692125204820	-9.21823623671391	2.01658879957099
H	1.80198989585643	-9.06867587799974	1.99401785242909
H	5.21051225124937	-7.15065454421482	2.05074784794139
H	8.58642867236086	-5.20894839160255	1.98157713292686
H	8.86891688900035	4.99874428725193	1.97609346029398
H	5.46629264131695	7.20604319228539	2.01682642450822
H	1.85504822434865	9.17379577518712	-2.10160639933583
H	1.86876956649747	9.17391469194118	1.97905107545259
C	0.78837712929294	0.64154568040696	3.70039834731440
O	0.27687903019250	1.53020597800542	4.25721205477543

H	1.50450396975377	-0.63004048257082	4.60299660900823
H	1.90600199831051	-1.35454549696975	4.29010780524836
H	10.53967742740848	1.88650019819499	1.97490816599244
H	10.53723979472169	1.88829508681207	-2.12256778343183
H	10.52045507692070	-2.19079910872857	2.00244719505561
H	10.52026704597972	-2.20048297091869	-2.14063888777617
H	-10.60046278061025	2.15218264873974	-2.07040050535982
H	-10.58935982906380	2.15116024282316	2.01985428741013
H	-10.63455735200902	-2.08977402111253	-2.07029284358226
H	-10.62366804821220	-2.08705028433574	2.02207063282379

• **TS 2Si-HCOOH → 2Si-(OH)₂CH**

Si	-1.41953618032092	-8.03558455081117	-1.18978507992627
Si	0.97081781655007	-7.96535686912033	-1.15077993413367
Si	2.14406167911363	-5.90648586735114	-1.12378875854682
Si	4.49403934480573	-6.17398358918966	-1.18856849157390
Si	5.64015566490783	-4.10217405882500	-1.24299658647383
Si	7.99217108092587	-4.23889004611381	-1.44487164270750
Si	9.23955535401568	-2.20508027158772	-1.58659085534133
Si	-2.61583472376474	-5.99004989234198	-1.21325527929404
Si	0.97833549648698	-3.85862534066778	-1.10027041907056
Si	4.58000917515827	-1.99858818828784	-1.15224285691279
Si	8.10632353553084	-0.12333457943453	-1.49527160490491
Si	-4.98201953429441	-6.13362160019745	-1.37886376437019
Si	-1.35814973209845	-4.00184842214803	-1.11372321757045
Si	2.25342753161687	-1.89084087149587	-1.00485381220207
Si	5.77368451960612	0.00911108968247	-1.21165734669064
Si	9.43054484627794	1.81529684722665	-1.71083038537976
Si	8.17558450431317	3.84920729731306	-1.68963039679252
Si	4.37488386117945	1.92505226196397	-1.14694773533259
Si	1.29182540830162	0.27860230728842	-0.96265444531168
Si	-2.46763116640770	-1.95036219821758	-1.06594514981730
Si	-6.01879419277094	-3.98966947631143	-1.42233146488771
Si	-4.82833675255889	-1.93988529398328	-1.26307564257513
Si	-1.01217680207053	-0.09920830606137	-0.70046937799844
Si	2.35249372483798	1.86339149504792	-2.36876465967915
Si	5.82215538150587	3.80925796599936	-1.32449117839256
Si	-8.38562101063025	-3.85000741627146	-1.65411453702206
Si	-9.49242978472556	-1.71667763852050	-1.66856767450555
Si	-5.88822150602404	0.15521968295712	-1.30833274282164
Si	-2.20483229493850	1.92788781537715	-0.97909753470785
Si	1.50585965163397	3.66203313789823	-1.12681616645964
Si	4.85888842991052	5.98172459922228	-1.35061025497382

Si	-8.22198584903340	0.27383182388875	-1.50420295998021
Si	-4.54964034061954	2.07066396996022	-1.15197958581082
Si	-0.84489291950640	3.83592616024636	-1.01600075866867
Si	2.50546107707774	5.80986827714689	-1.22007544826171
Si	-9.29821258393765	2.38223995507815	-1.55630291172395
Si	-5.58253070059716	4.19142419991142	-1.23880400336859
Si	-2.01128092144199	5.88383818182203	-1.09488665970370
Si	1.45179112955667	7.93335686777462	-1.20824566310852
Si	-7.93946712133544	4.35387072883353	-1.45104996653308
Si	-4.35409207801514	6.21378822067597	-1.16838270111720
Si	-0.92639146831688	7.98054452951843	-1.14306300533264
Si	-1.46752055434033	-8.01644147643934	1.21274838479269
Si	0.95104359714655	-7.94894041492851	1.25337302239235
Si	2.19500003212133	-5.92294065719722	1.27329118690304
Si	4.57728126241635	-6.16660801143231	1.23382967887065
Si	5.81394155372384	-4.12909105605681	1.15162568640546
Si	8.17854443947496	-4.21098568382923	0.95096649328731
Si	9.46349346787297	-2.17239255108795	0.80719146937875
Si	-2.74729751182281	-6.02020085556149	1.18684630246721
Si	0.95331403754697	-3.89516597677497	1.31872871662271
Si	4.75634693939537	-2.02065074866526	1.25239515529580
Si	8.38369817239091	-0.06553170540617	0.89206318004885
Si	-5.13344075681998	-6.18180538087802	1.03838626560757
Si	-1.44734652074313	-4.03346291429945	1.29648474896027
Si	2.40024088942192	-1.99796622272152	1.38528101078383
Si	6.04465615732450	-0.03062054167061	1.17841088594490
Si	9.67663838871865	1.91550439164443	0.67774063701365
Si	8.51413181153556	4.01665468447002	0.68251602821658
Si	4.97190473513530	2.04802283113521	1.31493986595562
Si	1.69589156533234	0.23598133156334	1.41793302367031
Si	-2.79748984256973	-2.10105519324888	1.29650554729910
Si	-6.25722715303956	-4.08069323641059	0.96461804820969
Si	-5.11570214379311	-2.03799457985042	1.12052505784068
Si	-1.60464144572523	-0.15955071349837	1.65110476852375
Si	2.87476552132583	2.09256989139973	2.18276121761142
Si	6.18046789693675	4.01347784619558	1.04196130514651
Si	-8.61291746637681	-3.93991449824822	0.73424202439051
Si	-9.68924093839552	-1.78072101314334	0.72624891654893
Si	-6.07048601038868	0.12158615109727	1.10239672446260
Si	-2.42114274639889	2.01654393540313	1.39426915697466
Si	1.52751183457618	3.79134052582104	1.33606557557333
Si	5.00882093659602	6.07378398485340	1.05558250056998
Si	-8.41599474650689	0.22284993433355	0.89095372691303
Si	-4.77125387947778	2.10362617764909	1.25219210346440

Si	-0.87173276012045	3.83433178646338	1.38981654736269
Si	2.63543897892781	5.86785139111905	1.16986163376790
Si	-9.45866288594017	2.35511125299878	0.84127543868785
Si	-5.76447797221249	4.22943413747634	1.15563958134187
Si	-2.05201593273505	5.91302693761796	1.30344080118798
Si	1.50727847787372	7.94475758773878	1.19589645318151
Si	-8.12389613855138	4.36632800817351	0.94572815373465
Si	-4.43191460213788	6.20583482211539	1.25284159323338
Si	-0.89567145929836	7.98327023287521	1.26201812010225
H	1.46327523809774	-9.08022727940965	2.09473005846791
H	1.60075521181749	-9.04901577028114	-1.97264254941588
H	-5.52138555616051	-7.20495720951683	-2.27660084424572
H	-9.03759044971378	-4.81920600268462	-2.59333159957074
H	-8.45510596705030	5.44667341543798	-2.33778198057395
H	-4.82573648828762	7.33939898580662	-2.03767153126024
H	-1.56572511519467	9.03859074084315	-1.98984853801354
H	2.06937621749482	8.98560499211183	-2.07810566412447
H	5.45267961107352	6.98405104574225	-2.29335272001047
H	8.66842801218747	4.86266976619178	-2.67773196503006
H	8.53572713369508	-5.32444396321562	-2.32308131220062
H	5.01983099049396	-7.26954917092071	-2.06498598796075
H	5.12934130814112	-7.26422536071091	2.09255420758705
H	8.91968651173570	-5.23887407649058	1.75223561372196
H	9.30889318339386	5.09844803027705	1.34933326238841
H	5.61031038292032	7.16815225931503	1.88590917475976
H	2.09836094159290	9.04192729970983	2.02993782570080
H	-1.39201035403839	9.10696829172690	2.12277915229461
H	-4.96975824354128	7.31729902710040	2.10314193231833
H	-8.84636894578150	5.42819028602202	1.71943111150928
H	-9.44685195924696	-4.96024322212424	1.44812931572559
H	-5.78546622554749	-7.28077088912441	1.82122493142140
H	-1.96640627530789	-9.14448077754081	-2.03651588646310
H	-1.95522084128257	-9.16039775619953	2.05066568664734
C	-0.50786294977273	-0.21409885266014	3.24742291997188
O	-0.12104824246972	-1.41910311483693	3.80008793898575
O	0.64273297323720	0.61136747991341	2.83130767574803
H	-0.98371755356923	0.37416284035630	4.05059321482540
H	0.04547903193496	-2.06722377012227	3.08016170585355
H	-10.99993625882280	-1.83284188459196	1.45214342050810
H	-10.66990599381474	-1.70657392829192	-2.59588168002493
H	-10.74136963509369	2.52652556496976	1.59806857790398
H	-10.47041529138832	2.53769986558664	-2.47678252836827
H	10.76630276964984	-2.32423586860463	1.53373902226365
H	10.39420670672181	-2.28757836729342	-2.53834611217466

H	10.98448482144519	1.98557145786501	1.40660413021842
H	10.57055018264719	1.80433615824216	-2.68244031415430
H	2.30717599829900	1.77058491693004	3.85037573119655
H	1.49850834120104	1.24334249178150	3.62240452481320

• TS 2Si-OCH → 2Si...OCH₂

Si	-1.24516039942406	-8.08626512069225	-1.24313135354588
Si	1.15394172050730	-8.10087454985164	-1.24213335676584
Si	2.32594844090040	-6.04444119198785	-1.24698565171368
Si	4.69795762171751	-6.20491449695336	-1.25225726272898
Si	5.75642625342713	-4.07826271137244	-1.24005352047566
Si	8.129566111114399	-4.10808339364613	-1.22807452612110
Si	9.38488669221416	-2.05779624737717	-1.22127488455701
Si	-2.44884508915035	-6.04197065814060	-1.23081329374007
Si	1.10508620855245	-4.02320882169985	-1.24298023500869
Si	4.60956040518298	-2.00959059940885	-1.25346632005575
Si	8.19936604789536	-0.00830109098071	-1.23057679889787
Si	-4.80850313060860	-6.25363997053154	-1.23148729369710
Si	-1.24571312352771	-4.00023256862227	-1.24417254794011
Si	2.24730130080505	-1.97437570267915	-1.26800829139177
Si	5.84730321327275	-0.00884949364456	-1.24484220853795
Si	9.39177252446469	2.03895211611990	-1.21798769268809
Si	8.14445385700871	4.09261812428718	-1.22409294045764
Si	4.61535433658757	1.99662320296493	-1.24848452074572
Si	0.95329265209515	-0.00330739255823	-1.30630082999082
Si	-2.24078621399279	-1.86153716608620	-1.26182237701567
Si	-5.77198565530801	-4.08986061186470	-1.21876704415470
Si	-4.57309040752132	-2.05511237586578	-1.22201209003248
Si	-1.24838306558516	0.10019544576960	-1.94265753319512
Si	2.26313746729733	1.94054509598277	-1.25990463827434
Si	5.77190285184127	4.05600841056134	-1.23837534273101
Si	-8.14003489992202	-4.08481959682490	-1.23760877814724
Si	-9.31064194721633	-1.99700332209128	-1.26350634587128
Si	-5.69798605648711	0.00422490050147	-1.24195340738173
Si	-2.32233565938171	1.99619118967802	-2.48284888403638
Si	1.11324464440641	3.98050473167821	-1.29456057120545
Si	4.70036777086571	6.17555975564256	-1.26399006769713
Si	-8.05686530709069	0.01095240437019	-1.26893003120483
Si	-4.32283271444080	1.92185859867246	-1.27428472036239
Si	-1.23412102208113	3.73804768175533	-1.35084111330880
Si	2.32804082220565	6.01181101016692	-1.28679038606222
Si	-9.32046187423686	2.00547748321280	-1.28346930333349
Si	-5.65622986247817	3.87891704813327	-1.23292323485711

Si	-2.29857869581382	5.85578607506776	-1.28415976596612
Si	1.17268328738900	8.07590133018808	-1.28224032312821
Si	-8.02284410463042	4.01325800388217	-1.28032552560637
Si	-4.66033375704783	6.02856674449524	-1.29138616637607
Si	-1.21926110172463	7.96420980660971	-1.28833582449290
Si	-1.24908429230449	-8.09204278109690	1.16084343612280
Si	1.15028016890831	-8.09508819210349	1.16522109969727
Si	2.31879610992567	-6.03555581389464	1.15934238195347
Si	4.68971702415442	-6.20215588107844	1.17241952179017
Si	5.74329356089021	-4.07332437721118	1.15967023787524
Si	8.11573520118663	-4.10625075231247	1.17475205978153
Si	9.37044016609154	-2.05668264715780	1.18352077422903
Si	-2.44374538717811	-6.04342526092724	1.17114145779838
Si	1.10203364042454	-4.00991625124842	1.16147617166790
Si	4.59419358395996	-2.00827938517518	1.15260057494258
Si	8.18232024837262	-0.00822311064035	1.17701383685508
Si	-4.80623881352002	-6.24396516289563	1.19108301815735
Si	-1.25290213335601	-3.99996645426482	1.15855327655305
Si	2.23627145438885	-1.95258168687246	1.12929873681865
Si	5.83004416413766	-0.00787864905918	1.16139040084427
Si	9.37653705376645	2.03758593617647	1.18500478667229
Si	8.13040525549784	4.09182602645525	1.17976562246346
Si	4.59186167864366	1.99694553840554	1.15824865267860
Si	0.88940376097210	-0.01225961206326	1.15672266562438
Si	-2.21215428631345	-1.84078598328181	1.21179661568283
Si	-5.78274155127307	-4.08193892871754	1.18395655263720
Si	-4.56011854183472	-2.05080272877912	1.17206274354456
Si	-1.07990683083238	-0.15541011307250	2.39708771550914
Si	2.23337735663353	1.92072252244258	1.13776392557479
Si	5.75729495531414	4.05369712947666	1.16484045736519
Si	-8.15437287825830	-4.07512401744755	1.16659288638270
Si	-9.32821612013645	-1.98743462396621	1.14223082539262
Si	-5.72314256108495	-0.00450347394337	1.15428794211243
Si	-2.21785757641416	1.82105381804424	1.88231053177851
Si	1.10359149856556	3.96813448004364	1.10391773051770
Si	4.67826833025814	6.16806294472034	1.15947058460461
Si	-8.07611030883309	0.01893666110310	1.13713997222440
Si	-4.42692342516442	1.94965651351683	1.19577367384015
Si	-1.22791325315091	3.76838050653139	1.09115467033989
Si	2.30668662990114	6.00001675701107	1.11601757513914
Si	-9.33858351215751	2.01439457009275	1.12312126864068
Si	-5.69267980718724	3.93217260997949	1.16581979410149
Si	-2.31491662496639	5.85595835235389	1.11807987240412
Si	1.16735319192987	8.07039861880267	1.12378249861743

Si	-8.05910577876861	4.03364401261291	1.12177240991915
Si	-4.66988068309024	6.06252278071944	1.11962879098232
Si	-1.22135249069513	7.95942707032701	1.11743131592332
H	1.70586686861073	-9.20107891558519	2.01084874534146
H	1.70346252280427	-9.21461840023228	-2.08154993148110
H	-5.43328363762784	-7.29494504633388	-2.10933835773163
H	-8.81363440119639	-5.12519250322919	-2.08012827583049
H	-8.61168616328207	5.09039849601532	-2.13996907160664
H	-5.29076048620033	7.04092226870112	-2.19922303431985
H	-1.84254652699594	9.03918005277065	-2.12675088485382
H	1.70660532487728	9.18846849917049	-2.13268990596699
H	5.31786068560009	7.23800266024598	-2.12170689643340
H	8.81728779764834	5.14454697378320	-2.05354627310024
H	8.80347266104915	-5.15887898875077	-2.05827648185912
H	5.30143732823294	-7.26760390489553	-2.11945368504907
H	5.29555869419969	-7.25945903967791	2.04449443213713
H	8.77640337961512	-5.15937162508021	2.01253941523503
H	8.79494857416730	5.14198379065749	2.01809197965463
H	5.25533378074202	7.24037780516519	2.03285305886110
H	1.70294294791406	9.17110636929862	1.98829667663548
H	-1.85964900703037	9.02245977982558	1.96009039917833
H	-5.25416225796319	7.11656959988875	2.01058703267205
H	-8.68187112108993	5.11807426742561	1.94821573517427
H	-8.84981176359324	-5.09978069841982	2.01094059908819
H	-5.41391184586526	-7.29321186368311	2.07161903963526
H	-1.80847023151449	-9.19002467729528	-2.08671275053413
H	-1.81068361482277	-9.20493864722789	1.99343402333335
C	-1.12110229474342	1.56080186459631	4.21408523710150
O	-0.08466547928807	2.17533979750522	4.31278339273252
H	-1.70425765315968	1.01506827548777	4.98003377696814
H	-2.11705466873669	2.18509687225745	3.53810275753226
H	10.60764904189773	2.12487196006090	2.03524203885512
H	10.63287937517684	2.13078057739923	-2.05313857794078
H	10.60019775217529	-2.15281232235217	2.03494916612490
H	10.62476240961222	-2.15642348824617	-2.05768039266102
H	-10.56309902088759	2.08787877755934	1.98386312499539
H	-10.53558150657893	2.07703183071429	-2.15727971554453
H	-10.56830507268335	-2.01722726420845	1.98352847289041
H	-10.53803647057774	-2.04122471177682	-2.12248029149281

• **TS 2Si-(OH)₂CH → 2Si-CHO + H₂O**

Si	1.14143552947159	8.05907197544006	-1.14044129860302
Si	-1.24344871499551	7.91250026549866	-1.10071516292526

Si	-2.35053165441052	5.81574948185658	-1.09099883061999
Si	-4.70912415758765	6.02661510557139	-1.17544969723497
Si	-5.80435142714612	3.92858413136431	-1.25415163452807
Si	-8.16254727385035	3.94999808265148	-1.47565307883797
Si	-9.32365484186631	1.86058018843161	-1.60246185588962
Si	2.39740526519333	6.05081779632975	-1.17873596609768
Si	-1.11833237702101	3.80918242129083	-1.06372969673118
Si	-4.67252859531964	1.85773268298363	-1.17155826660653
Si	-8.10509150890569	-0.17102100532604	-1.52734038756634
Si	4.75304056809344	6.27858012289839	-1.36928740638635
Si	1.21068563237299	4.02058541701700	-1.09515471612024
Si	-2.34274697702730	1.81570552081674	-0.97320499225875
Si	-5.76750967038582	-0.20191620215305	-1.27675755208364
Si	-9.34716524895700	-2.16854500896168	-1.72302540941663
Si	-8.01757042182023	-4.15683162876259	-1.68984111404253
Si	-4.30085289656692	-2.06829922300668	-1.21288627929136
Si	-1.30297964375820	-0.31398251642615	-0.83824700639749
Si	2.39768960395504	2.01315351175272	-1.08443524664386
Si	5.87023488078506	4.17559987323235	-1.43692983602368
Si	4.76007981658777	2.07933852207039	-1.28328694941945
Si	1.00214524920729	0.10999086310314	-0.72193330061728
Si	-2.21798469404093	-1.89889382077347	-2.34657224833970
Si	-5.66268691173004	-4.02518105867722	-1.38751563383865
Si	8.23751524270243	4.11525179891227	-1.69725704721490
Si	9.41724610227099	2.02115281247740	-1.72944283852438
Si	5.88756777650975	0.01932045384806	-1.33154651590632
Si	2.26398971505889	-1.88156906326406	-0.97389943025175
Si	-1.38230333278046	-3.67611183560054	-1.05031323756331
Si	-4.62676044006806	-6.15872351229382	-1.34339756622238
Si	8.22261995493001	-0.01544423701205	-1.55485228875431
Si	4.61233021506209	-1.93852065562493	-1.16298779109882
Si	0.96731655939397	-3.83215846832337	-0.97445763463977
Si	-2.29130412268463	-5.85840809596409	-1.16521482698196
Si	9.36935083615038	-2.08634214093224	-1.62419063315607
Si	5.71910817880113	-4.02232215207247	-1.25916146077108
Si	2.20827767512079	-5.83501432833051	-1.07790095361131
Si	-1.18179465474389	-7.95399806956269	-1.16370973347882
Si	8.07761309805487	-4.10182529322471	-1.50485844189004
Si	4.55882509727947	-6.08474873292006	-1.17792748389422
Si	1.19446818414592	-7.96711726744574	-1.11607764087979
Si	1.19490598446528	8.02350920476885	1.26119297270716
Si	-1.22148991359786	7.88033377347095	1.30243118735875
Si	-2.41193246989069	5.82263036628595	1.30656022375206
Si	-4.80351561666282	6.00613014720590	1.24578004975542

Si	-6.00131181009449	3.94959439855262	1.13709067829283
Si	-8.36251055830118	3.93297634802853	0.91881763636767
Si	-9.52284581846560	1.82102710154411	0.79361762874074
Si	2.54941392023807	6.07590783995383	1.21970577632486
Si	-1.11535463259042	3.82530794602307	1.35249680122849
Si	-4.89951876938225	1.86973374814008	1.23554632782578
Si	-8.34856411972686	-0.23934818891460	0.86404065287523
Si	4.92713176656074	6.32334561118578	1.04526858049236
Si	1.30821108501131	4.04530551746827	1.30999986114229
Si	-2.55491794255642	1.91966344304968	1.40495387288398
Si	-6.00504379527460	-0.21257137883303	1.12151416431528
Si	-9.58086706585753	-2.25652362240567	0.66656518019187
Si	-8.29510366115097	-4.28186892637627	0.69544846949454
Si	-4.71772143871236	-2.18441698840082	1.18202791552064
Si	-1.72216990379808	-0.26823082092633	1.58768967931900
Si	2.76557092841456	2.17046972784039	1.26666358626666
Si	6.13272629472943	4.26906339001398	0.94786104607678
Si	5.08263845986733	2.18126343862104	1.09856162472802
Si	1.67278916353705	0.15553949858941	1.58068989886005
Si	-2.76626392353793	-2.17399990358561	2.41312609341848
Si	-5.95245575115174	-4.15822517145023	0.98836958900930
Si	8.48931815384101	4.20861648834833	0.68881545428565
Si	9.64096806858453	2.08772872750091	0.66309479282453
Si	6.09949209333592	0.05363485049013	1.07688661307685
Si	2.51911236115373	-2.00389132114667	1.39615036333479
Si	-1.40264644629642	-3.79660299161848	1.40401232762232
Si	-4.78480632541565	-6.21768308402549	1.06758187745392
Si	8.44489329500960	0.03761482851374	0.83793557750080
Si	4.87194339578513	-1.97232875531525	1.23499810883279
Si	1.00168566357767	-3.84779149130865	1.42706067632373
Si	-2.42208859398630	-5.92926942845607	1.22347513871552
Si	9.56018163792577	-2.05787167249822	0.77126433995895
Si	5.93581100680788	-4.06142630112564	1.13244588970209
Si	2.27654848382459	-5.86857300809028	1.32192198415347
Si	-1.22752319554010	-7.96959198827196	1.24032055947712
Si	8.29581644625323	-4.11353618689271	0.88883077981234
Si	4.66447144722929	-6.07860078090830	1.24193698095295
Si	1.17717331177901	-7.96816970737563	1.28915379087244
H	-1.76053868371500	8.99184371166150	2.15346141993095
H	-1.90998298606068	8.98043652396747	-1.91411775410332
H	5.23945378764236	7.37575905771680	-2.26573212606212
H	8.84600625220113	5.10717352006448	-2.64182189359048
H	8.61740552053671	-5.17447081019062	-2.40165657816189
H	5.06060555138075	-7.19190612194093	-2.05394030959751

H	1.85868760745889	-9.00480789130591	-1.96891676947722
H	-1.79386553709635	-9.01247007902201	-2.03019635965941
H	-5.12063556623466	-7.22622761656074	-2.27329464897579
H	-8.51680631840446	-5.19764304826911	-2.64673790511750
H	-8.74910930676414	5.00360530211648	-2.36546289775389
H	-5.23316946812193	7.12734767682309	-2.04646039702741
H	-5.38791215818942	7.08791843471703	2.10344281340012
H	-9.15687928612512	4.93172725867376	1.70575732402612
H	-9.00810738764523	-5.39340223363336	1.40562006262658
H	-5.38991968686654	-7.30767020459460	1.90249495370095
H	-1.77825875340233	-9.08884969572923	2.07322319443109
H	1.70523077855710	-9.08018875311846	2.14621213987259
H	5.25293903762386	-7.17181070789931	2.08241418979971
H	9.06571273876698	-5.15190682672212	1.64838997486648
H	9.29535457720955	5.25657667265290	1.39452605873809
H	5.54805395852648	7.44045254543331	1.82744801213295
H	1.66176215627322	9.18749945436550	-1.97792789500807
H	1.64474427573215	9.17799833021540	2.10611311905688
C	0.67740683542001	0.25516580084007	3.22869332155916
O	0.31053380332762	1.61300837787264	3.77696805952469
O	-0.68966387529823	-0.17796886942076	3.15512701183603
H	1.16965719564010	-0.25995359990041	4.06898359154273
H	0.40001303546793	2.29904187450562	3.05115173155104
H	10.95754165056162	2.18688734430258	1.37323929332542
H	10.58375159752475	2.05505057274787	-2.66977573646088
H	10.85781328889130	-2.18299942758892	1.51131104169687
H	10.53436451943444	-2.19966761259748	-2.55967807253783
H	-10.82604038714063	1.89928666986562	1.53139043083599
H	-10.49164046882101	1.91105205058676	-2.54052500514322
H	-10.88083765771613	-2.37578161492944	1.40337813464878
H	-10.48980573599968	-2.20437907468349	-2.69159001404635
H	-2.86597133631882	-2.17691057599997	3.90583738924264
H	-0.75863239967832	1.00758819641974	3.64545643388798

• TS 2Si-CHO → 2Si-OCH₂

Si	1.12549416418312	8.01586044847055	-1.08201193958685
Si	-1.26551896657251	8.03267922421274	-1.11757694889921
Si	-2.46465904755409	5.98572737050350	-1.15940601488180
Si	-4.82666538100374	6.15587026558263	-1.33118937679095
Si	-5.88652511692692	4.02579123105472	-1.39820000559364
Si	-8.24423382102509	3.90304440144014	-1.65637220131761
Si	-9.29079598546057	1.74354529149874	-1.68162155487155
Si	2.30668690303586	5.96251781281236	-1.08444819561799

Si	-1.24060123668088	3.98385274202482	-1.06737923639134
Si	-4.73854846049022	1.94525315448777	-1.26072436580571
Si	-8.02697026148270	-0.25090204212599	-1.50399947574049
Si	4.66242228293460	6.16388142641594	-1.17609832883894
Si	1.08943446376737	3.95110221726879	-1.04029787959125
Si	-2.38924961174055	1.95593922489696	-1.08963589213951
Si	-5.68632291172097	-0.19847967398065	-1.27609561379777
Si	-9.24467693658442	-2.27245040168239	-1.57464159136224
Si	-7.86089840746152	-4.21418233644616	-1.45284907751257
Si	-4.17951312464795	-2.02311437123413	-1.11301775919664
Si	-1.20247793556988	-0.07123946111774	-0.76039742368721
Si	2.27377352543675	1.94324745635749	-1.06545106185641
Si	5.73440121367035	4.04886515046575	-1.25249035153721
Si	4.61172097136386	1.96840505950328	-1.15826864347715
Si	1.14139704603641	-0.10594438702705	-0.79928929619635
Si	-2.07040769910247	-1.78680063444464	-2.16600168780993
Si	-5.51164156290622	-3.99509858800949	-1.20101370106521
Si	8.09152420504475	4.07060568659698	-1.48778660963540
Si	9.27199166310606	1.99329486636631	-1.60736387536709
Si	5.73912195770115	-0.07677084720445	-1.28142883647066
Si	2.15899912978606	-1.82832486834080	-2.01025055745437
Si	-1.15719670863498	-3.61808682284237	-1.00612975607528
Si	-4.45509354265266	-6.10349689292760	-1.11179152157519
Si	8.07629313955972	-0.05057711354813	-1.52393522703860
Si	4.35297151034615	-1.97919611765645	-1.26708991102880
Si	1.18442617121459	-3.71547053150989	-1.14820140406072
Si	-2.12300858044535	-5.77326888589814	-1.04983726273934
Si	9.33051555146615	-2.04049154127129	-1.70354019308460
Si	5.67103194382373	-3.93285999897675	-1.39775151577323
Si	2.24601536458328	-5.80133900953261	-1.19838271881763
Si	-1.11503853697596	-7.90736293736630	-1.06511331825657
Si	8.02979409298473	-4.04590402562490	-1.66736483173202
Si	4.58750637022284	-6.03514068202198	-1.32128252087332
Si	1.25235124128910	-7.94236146290955	-1.10767371709009
Si	1.11057189834251	7.96632167733381	1.32091433222678
Si	-1.31166520237987	7.98845689259705	1.28353658169299
Si	-2.59059208394854	5.98851933828963	1.23937123423771
Si	-4.97863460142869	6.19103390992422	1.08833008280280
Si	-6.15331868413529	4.12283470184506	0.99073494226111
Si	-8.50149010320472	3.99385010676166	0.72980380950221
Si	-9.51789772460044	1.80969735377389	0.71352266267045
Si	2.36789029446031	5.94672597308937	1.31216408507533
Si	-1.30213845220766	3.98751776525943	1.35292654644355
Si	-5.05131498455008	2.06166556155651	1.12885441506414

Si	-8.25227814862675	-0.19672911260501	0.89068928655071
Si	4.75632739755071	6.14943804583915	1.24567256026237
Si	1.09695287838544	3.92897997862969	1.38701375102356
Si	-2.74228784709833	2.12003165122725	1.26184160617701
Si	-5.90551621051643	-0.12237245421890	1.12336467745255
Si	-9.43364557710527	-2.24424626389844	0.81928348605812
Si	-8.08343860123585	-4.22612815596149	0.94158273851909
Si	-4.51131797173005	-2.04127585751302	1.29327091451859
Si	-1.72822263628389	0.07081063938277	1.60907360638180
Si	2.53233403184443	2.03221145858901	1.30373288198042
Si	5.95277403760641	4.08666978280516	1.14491042798043
Si	4.87193390461647	2.00121881957274	1.23531766916250
Si	1.75376626454796	-0.17353128411293	1.55774542728293
Si	-2.46663355024414	-1.98602578613972	2.41735112502879
Si	-5.73447540867392	-4.03822879233797	1.18502707238370
Si	8.31132424950087	4.07278875535752	0.90627390228237
Si	9.47521177305599	1.96465331684455	0.78971336079816
Si	5.95345067613196	-0.08831914290419	1.11417238730646
Si	2.71253724259075	-2.09117774745323	2.43168069812287
Si	-1.09679832566656	-3.64403967222579	1.43329102345107
Si	-4.52513166506933	-6.06840262228503	1.30207699403136
Si	8.30236794788801	-0.09954678827001	0.86846960105801
Si	4.68082690105121	-2.07395703153546	1.23645908385734
Si	1.29023676509261	-3.63615520576814	1.35660131615753
Si	-2.15841732281035	-5.77280199962089	1.34207947460303
Si	9.54582970997693	-2.11106401843024	0.68921061129603
Si	5.93469819081343	-4.01946632372546	0.99150951182798
Si	2.33329954687452	-5.75966165652439	1.21076821520196
Si	-1.09160586140693	-7.88285430311235	1.34091049598903
Si	8.27965548317394	-4.14897733458727	0.71911120263857
Si	4.70253135177093	-6.03474154603412	1.08273843026458
Si	1.29675589953087	-7.88038638509531	1.29216791349925
H	-1.80801763212026	9.12482545813397	2.12721859399616
H	-1.83537320581040	9.14274851788654	-1.94758074514289
H	5.21486747735967	7.24810666884875	-2.04976859186826
H	8.67050448375310	5.11699085058916	-2.39034511334553
H	8.53115119102651	-5.09506374102630	-2.61271814549724
H	5.09248090916869	-7.10473655826296	-2.24087493893033
H	1.89842902816478	-8.98963724895090	-1.96185913831261
H	-1.79209595659655	-8.93863850824679	-1.91507134646374
H	-4.95423352125449	-7.21039078677026	-1.99129813285356
H	-8.32087843270613	-5.32898948677059	-2.34332248229989
H	-8.89235315341554	4.85534148029139	-2.61490338874886
H	-5.34431280919173	7.24243628390886	-2.22387252260270

H	-5.61157683299510	7.29425890107176	1.88160669958860
H	-9.35344825708318	4.99643353848759	1.44691491130357
H	-8.75984010863611	-5.31392811841065	1.72127292557141
H	-5.06442627711563	-7.13788270363020	2.20585238395496
H	-1.64705497868933	-8.96125345883532	2.22232952195446
H	1.92542090465512	-8.91707101243779	2.17333948112927
H	5.25744788136374	-7.12169277216436	1.95294163710921
H	8.97740906299877	-5.25737754473344	1.44698290772415
H	9.11240343051334	5.08112833449009	1.67292515929006
H	5.36559751299057	7.22868500290839	2.08871841212871
H	1.73994977896182	9.11483391725879	-1.89482768384357
H	1.60322905347920	9.09380464846732	2.17899863276243
C	0.57639667000660	0.18138239381608	3.04293630558135
O	-0.66045816806659	0.61613371354785	2.92426580733515
H	1.09778334958716	0.62039087118124	3.91857409542976
H	10.78279284575897	2.03923785682595	1.51944237242212
H	10.43987307355948	2.04877874057141	-2.54483081206504
H	10.84012150917833	-2.22439442676159	1.43577645507725
H	10.47389769093834	-2.07472081382610	-2.67056498298839
H	-10.83875858748718	1.83643088060402	1.42312792254278
H	-10.46067447136502	1.71324236394634	-2.61887550304724
H	-10.71272396036656	-2.36411264099358	1.59124476857704
H	-10.39252456578052	-2.38216052770757	-2.53106939528804
H	-2.52790867351472	-2.04606038899615	3.91072758945107
H	1.33804373687353	-1.83320953224040	3.80101483907789
H	0.64091644405715	-1.21498779264974	3.70545475680369

• TS 2Si-OCH₂ → 2Si-OCH₂*

Si	1.09678722827970	8.01052346548178	-1.08708953289549
Si	-1.29131737299679	8.01650632919510	-1.08766733582612
Si	-2.46316712465956	5.95666307877028	-1.09675660267207
Si	-4.81985118944964	6.14477994126062	-1.25976828983877
Si	-5.86944190104485	4.01691540094703	-1.35464098294565
Si	-8.22552170127945	3.91523775150693	-1.62933598812807
Si	-9.32346938250848	1.78564463265842	-1.70967515455605
Si	2.29576799340889	5.96580077671525	-1.10123510684680
Si	-1.21543996848324	3.96617818818051	-1.00530525366606
Si	-4.71133871947398	1.94998679067087	-1.21459724536757
Si	-8.07543067092254	-0.22332488434597	-1.57745260663655
Si	4.64714480798362	6.20019543660739	-1.25982798436615
Si	1.11123915926898	3.941111188781781	-1.01320096182951
Si	-2.37225710183530	1.94746822964029	-1.01813571409330
Si	-5.74182934243180	-0.14835392540257	-1.32353321627899

Si	-9.26336415357593	-2.25847020761287	-1.71105305475676
Si	-7.92741405372087	-4.24043802376507	-1.62816806268718
Si	-4.36561738061016	-2.06041230551061	-1.23529862634910
Si	-1.13007769664522	-0.01566508532971	-0.59230074126620
Si	2.32264604736506	1.96060910950447	-0.95112248968237
Si	5.75145692156130	4.10064055762149	-1.34597898646452
Si	4.65619859211228	2.00125929879433	-1.19681632693193
Si	1.20202257674259	-0.08963227231625	-0.58940805298939
Si	-2.09308317035856	-1.83589707935614	-1.69305126762696
Si	-5.57270760149710	-4.09343284214539	-1.36609726460563
Si	8.10393617900511	4.07442224441319	-1.65065114965119
Si	9.24861109431866	1.97114562815473	-1.74255601009706
Si	5.71708453120754	-0.07880147656054	-1.29683671030303
Si	2.09343012448868	-1.73735650191459	-2.05390699916403
Si	-1.05209611871256	-3.77246494662431	-1.03578994159015
Si	-4.44104680086873	-6.16420510667576	-1.24729824422825
Si	8.04812126374755	-0.06526357859441	-1.59068068559233
Si	4.28055985094972	-1.95631421165877	-1.16613720162399
Si	1.28150983583542	-3.64653356727148	-0.97851267287367
Si	-2.10967428409671	-5.86021797286829	-1.13042408246987
Si	9.30485677072485	-2.05702365383003	-1.74674889063623
Si	5.63497793991514	-3.91014044758203	-1.32800017218741
Si	2.28417308257463	-5.77761302238322	-1.09266094946153
Si	-1.06755865883413	-7.97799892702153	-1.07200944271480
Si	7.98568504619543	-4.04593750501090	-1.64874874089114
Si	4.62057471394053	-6.04189502609934	-1.22247965709873
Si	1.29867505079716	-7.92424981133909	-1.07414425062111
Si	1.11582507817384	7.96577981994864	1.31467634821651
Si	-1.31047772495384	7.97613580513801	1.31447352377559
Si	-2.57576414483020	5.96486995995681	1.29823710654619
Si	-4.96571573836797	6.15258434559039	1.16002492311894
Si	-6.14226679445914	4.08010696210197	1.04051225975232
Si	-8.49141097684320	3.96616894408514	0.75754965755716
Si	-9.54865597054113	1.79967189783731	0.68648504350576
Si	2.40585980897787	5.96698130837650	1.29254354814729
Si	-1.26245491325510	3.97205089563394	1.41813200669792
Si	-5.02895552413053	2.02010485489749	1.16666691778383
Si	-8.30680482725976	-0.22675561129787	0.81497429680667
Si	4.79545455802371	6.21110968755223	1.16045032740741
Si	1.15648992048040	3.93366817238080	1.41708826711326
Si	-2.70654724418521	2.09413028320169	1.33541838287547
Si	-5.96038103870837	-0.14191161237295	1.06819904071180
Si	-9.47820620965423	-2.28145787349871	0.68266610945005
Si	-8.16115032944273	-4.29071372843418	0.76259388880325

Si	-4.64476571365419	-2.11630129789755	1.18789821276210
Si	-1.74077785808865	0.02772715825678	1.79382779457331
Si	2.65953826895977	2.09287390958308	1.41006337992645
Si	6.03688863430823	4.17773905603732	1.03806118945839
Si	4.97644506285634	2.09096057348758	1.18883594114424
Si	1.70329859317128	0.00569759443881	1.80862626981104
Si	-2.61200301298648	-2.06614825261217	2.30492527035395
Si	-5.81149451534065	-4.13571628332137	1.02081469169109
Si	8.38639676234183	4.13030521088538	0.73522668280082
Si	9.50447961740505	1.99324640072272	0.65053799052120
Si	5.98065916713321	-0.03711847318847	1.09466719995459
Si	2.69317267771101	-2.01225181974564	2.39787353069761
Si	-1.11766274321987	-3.69102240472923	1.43887977863422
Si	-4.54628432852807	-6.13086289582132	1.16299050452277
Si	8.32269800876798	-0.06500547012511	0.79950298105187
Si	4.68759764434078	-2.01620770999843	1.22759628220875
Si	1.28252781912350	-3.66705904332589	1.46539207486762
Si	-2.17663353027437	-5.81765899097952	1.27007713180323
Si	9.55754648564635	-2.08180089828131	0.64227875680826
Si	5.93325930611863	-3.98267896969118	1.04954428352636
Si	2.37225995127679	-5.78038324654786	1.29802642281692
Si	-1.07656048128688	-7.91197671744256	1.32971120318485
Si	8.27701954975088	-4.11106295960826	0.73652909120041
Si	4.74868717679465	-6.02570403560113	1.19210077263936
Si	1.31598009105761	-7.89317692262791	1.33136274156698
H	-1.79418316000546	9.11601442775955	2.16140012050852
H	-1.89533941845498	9.10826427165860	-1.91792061667111
H	5.14016604993487	7.30006751468307	-2.14993676469523
H	8.68512488988474	5.08223376703907	-2.59547059120839
H	8.46166271650536	-5.11707295111378	-2.58341552451384
H	5.11439258660702	-7.13468315354146	-2.12235625212308
H	1.97084841186611	-8.95071115008774	-1.93332428997208
H	-1.72314960378128	-9.03024393220052	-1.91264264014345
H	-4.89937884587878	-7.27568252590288	-2.14125128056817
H	-8.41589425172413	-5.31959381008368	-2.54619583193848
H	-8.84414778433536	4.90328000434491	-2.57056993152403
H	-5.34492808328601	7.23509333340457	-2.14282271799024
H	-5.61861380354219	7.23652078918089	1.96332612621510
H	-9.35097670169955	4.95683045444688	1.48224153124336
H	-8.84611573360982	-5.38903417868134	1.51789925321157
H	-5.09096276198389	-7.21352093851357	2.04539005454766
H	-1.65968733525400	-8.96913641891071	2.21832980685940
H	1.88521689746042	-8.96874038562080	2.20714687144067
H	5.32981117490998	-7.09465670144838	2.07031310822262

H	9.00023966592815	-5.20279339903460	1.46676597510779
H	9.22646328630322	5.14129557984699	1.45581605703704
H	5.39735642929860	7.31748078094562	1.97375582520675
H	1.69657286374641	9.10993551597773	-1.91044235164023
H	1.59930322461507	9.10603572671935	2.16161319869794
C	0.57460639520505	0.31504486841023	3.37103081975711
O	-0.81694390473114	0.29042490497935	3.17776109873098
H	0.86861615923369	1.30850173963747	3.76711721795496
H	10.83116062852363	2.07032903101757	1.34572391673414
H	10.40235913049160	2.00063737487193	-2.69935582227874
H	10.86162039350064	-2.18967163442933	1.37331771759901
H	10.43466831028717	-2.11350453317223	-2.72897961532376
H	-10.86853751894753	1.82955295223146	1.39723122082382
H	-10.48892927466171	1.79163516354193	-2.65225383207469
H	-10.76978353688912	-2.42512189830057	1.42888561726430
H	-10.40575512162028	-2.34762080329762	-2.67584297488482
H	-2.77378638276864	-2.23579252372551	3.78165590543738
H	2.81580761346453	-2.16229008176337	3.88314894320683
H	0.84146341658120	-0.43921917055467	4.13786447545923

• TS 2Si-OCH₂* → 2Si-OHCH₂*

Si	1.34027404021231	8.04361079075655	-1.15307937155364
Si	-1.05034663589058	8.00562831649003	-1.11326020594547
Si	-2.24085036598131	5.95687108314157	-1.08599195772180
Si	-4.59299571929929	6.20328539792868	-1.17978613107034
Si	-5.68293367857803	4.10061264176066	-1.25579703530564
Si	-8.04291482096433	4.14068956512198	-1.45009139203885
Si	-9.23983333523988	2.07239920494415	-1.56453601657634
Si	2.53666112684064	5.99578184748051	-1.16618542605187
Si	-1.05267649323067	3.92669403437981	-1.04574710737105
Si	-4.58573587699568	2.00541777567912	-1.16717663603042
Si	-8.06294830893685	0.01618559918534	-1.49200637653905
Si	4.90151503608975	6.12909891690251	-1.33965722135126
Si	1.27427387458007	4.01514312819124	-1.06005924584531
Si	-2.25348427841296	1.92419940638456	-0.99899755522667
Si	-5.72230049471704	-0.03487375526845	-1.27596642882966
Si	-9.34850601865741	-1.95300323557231	-1.67627271185043
Si	-8.08637326046872	-3.98438997257868	-1.65783537404614
Si	-4.37409968820854	-1.96975417682623	-1.24660096409162
Si	-1.16915011366729	-0.15907750179696	-0.87366750092510
Si	2.38049977779905	1.96621287290531	-1.02024128668118
Si	5.91363482011731	3.97886156338095	-1.38591848960387
Si	4.72643421211130	1.92323510760342	-1.22798603868505

Si	1.15853982766269	-0.04225503323315	-0.68854956444610
Si	-2.19581208530117	-1.87698264268915	-2.08623853005942
Si	-5.72259134641009	-3.90771371744649	-1.41265024582271
Si	8.27058085437073	3.84303748541340	-1.63978489256791
Si	9.31259809141383	1.68310385733289	-1.65647206930704
Si	5.68917171383640	-0.21420817359362	-1.24681090528780
Si	2.05953748581639	-1.77688854513184	-2.03487933564669
Si	-1.24593200173032	-3.75120862531888	-1.16105952216728
Si	-4.66637884964578	-6.02651059903619	-1.33817364065930
Si	8.02787545774881	-0.29665021258810	-1.47865133970465
Si	4.20584116965165	-2.05134900801292	-1.09791688801369
Si	1.08890905093974	-3.66525027539196	-1.04330540917167
Si	-2.31608521884795	-5.83477022717477	-1.23181298090267
Si	9.23140462784642	-2.32664123718554	-1.54823186647027
Si	5.49577576840000	-4.04203322045741	-1.20391430567894
Si	2.08672537224626	-5.79990663192961	-1.09982320325996
Si	-1.30676749158118	-7.96897043689421	-1.15067541826102
Si	7.84616951977624	-4.26641571884138	-1.43651194911818
Si	4.41679280971100	-6.13784212537603	-1.12728414108414
Si	1.06242722204024	-7.92600847725912	-1.10175587062659
Si	1.39025179317332	8.03213914095307	1.24818114452138
Si	-1.03066664121162	7.99016975273334	1.29041383393645
Si	-2.29352170811855	5.97304484520485	1.31055652037006
Si	-4.67786775232282	6.19014386147530	1.24283611209155
Si	-5.85762284809887	4.12057030697150	1.14082835094221
Si	-8.22192361941902	4.12850259996094	0.94780200193846
Si	-9.42169538070162	2.04069617899424	0.83414833822555
Si	2.66277327183805	6.02835047360600	1.23025647106360
Si	-1.04598934188617	3.94194910902696	1.37963092354334
Si	-4.78235216611055	2.02509922799966	1.22268781988902
Si	-8.27742216206177	-0.03744176807973	0.90062071040139
Si	5.05279908772956	6.18060981550828	1.08007189529806
Si	1.34905430822298	4.04800175610526	1.35735230454213
Si	-2.43471761122946	2.00404776867465	1.39396946092194
Si	-5.92822255292025	-0.03565611964528	1.12360890709520
Si	-9.55211849195848	-2.03041261032580	0.71813265029591
Si	-8.32747638171303	-4.09252942293211	0.73034198095427
Si	-4.71467295634742	-2.04734667840976	1.23079129764351
Si	-1.79617942125690	-0.25552127207319	1.45322779435756
Si	2.72459454029507	2.13405980959358	1.32996273508119
Si	6.17591418755107	4.08372961676634	1.00599337189796
Si	5.03182328256310	2.04245975979865	1.15863939567568
Si	1.65024904523274	0.11231639292471	1.71098555690605
Si	-2.78292076165782	-2.15343330125435	2.46715234143850

Si	-5.97612691554713	-3.99387125693304	0.96874971312311
Si	8.52295614281637	3.93912427350118	0.74714839133722
Si	9.53108597547892	1.75147232580406	0.73872983877876
Si	5.89783780019971	-0.14372443625844	1.15014357845360
Si	2.43299953462387	-1.98951955570174	2.36402249814165
Si	-1.35085514429379	-3.67129878520384	1.37002045230398
Si	-4.76978538566388	-6.02600870758825	1.06912987766737
Si	8.24586086111242	-0.24261312122134	0.91576934601484
Si	4.50813031655001	-2.06740807340300	1.31165940753487
Si	1.03448420013119	-3.64965600054392	1.40767516874318
Si	-2.39276370833974	-5.79229964170744	1.16609236693569
Si	9.40917447246806	-2.30116657489664	0.84765297818630
Si	5.69970078760639	-4.08207205658978	1.18316852133250
Si	2.09934227764433	-5.77697060122702	1.29308380084217
Si	-1.35445239305637	-7.91194885321591	1.25050484021130
Si	8.05065304406130	-4.27905495834146	0.95870853008509
Si	4.46452455319424	-6.09674614162373	1.28694093619249
Si	1.03262877946201	-7.89074958883058	1.30309166518734
H	-1.53143462986043	9.12928930439116	2.12837152957528
H	-1.67141775386358	9.09474495468820	-1.93454814258049
H	5.44592527208980	7.19439001821147	-2.24186314849341
H	8.92016977599627	4.79368113617425	-2.59893952328525
H	8.30621039776418	-5.38135488343349	-2.32648047861134
H	4.92230104784323	-7.24605902208635	-2.00105036467210
H	1.74222348630136	-8.96413704528008	-1.94131016779268
H	-1.93340117158655	-9.02384564774042	-2.00992271553023
H	-5.19168573666635	-7.09218849125405	-2.25154437564717
H	-8.62075869670873	-5.01669400665900	-2.60378851619263
H	-8.63284387028292	5.19596957021922	-2.33537947914088
H	-5.11567931319454	7.30055348163812	-2.05582452866805
H	-5.27975683485415	7.26681334532868	2.09449096719768
H	-8.99659071560753	5.14094314227811	1.73646993572536
H	-9.04122923083495	-5.18985678413101	1.45993542101228
H	-5.33568036493552	-7.10379028765444	1.94463056004316
H	-1.97161266901639	-8.95246262611724	2.13528088449170
H	1.60400775784899	-8.95590303860395	2.19043276190381
H	4.96898265372684	-7.17574895168167	2.19943442646852
H	8.71833526141779	-5.36851344804666	1.74340639810486
H	9.37986663874073	4.93917493721988	1.46211896072365
H	5.71297302621788	7.27486260746821	1.86331724939413
H	1.89961246028050	9.14294447818020	-2.00406489234043
H	1.88410784639380	9.17808205206930	2.08008601802446
C	0.39155598679864	0.48353927204145	3.11372326351420
O	-0.65968333322366	-0.48718410381243	2.85120244001933

H	-0.03533015557132	1.50505105942426	3.12676489459455
H	10.84735556481970	1.77381208986976	1.45687287585489
H	10.48222124657602	1.64174877946031	-2.59340880353858
H	10.68470942250361	-2.43638513708720	1.62307753292578
H	10.38428218162688	-2.43802092709973	-2.49831587424206
H	-10.72081887690749	2.13539870373118	1.57665977626888
H	-10.41393342449282	2.13743451930332	-2.49374767369092
H	-10.84515602046321	-2.11982581742100	1.47041174799411
H	-10.50025721727997	-1.96457703759751	-2.63420306486790
H	-1.59098964808373	-1.15232479675362	3.46369790758938
H	2.46896230882627	-2.10211463719589	3.85803993229840
H	0.83310163317618	0.25175770298275	4.09801198706404

• TS 2Si-OHCH₂* → 2Si-OHCH₂

Si	1.35778571963471	8.03964252834319	-1.17470337599684
Si	-1.03590386699681	8.00905167278954	-1.12359432459613
Si	-2.23688980934115	5.96671549869117	-1.09090590908260
Si	-4.58997788323924	6.21885688264669	-1.13226753740941
Si	-5.67033401646715	4.11014152977902	-1.19187877284826
Si	-8.03457066817015	4.16556830266486	-1.32927655091450
Si	-9.24603418640070	2.10524096252534	-1.43111250313998
Si	2.54930415923129	5.98824956202567	-1.20382776345419
Si	-1.05929338323761	3.92492494300751	-1.06996978771636
Si	-4.57350487450912	2.01774877649937	-1.14064873368309
Si	-8.06393881145139	0.05117905220960	-1.42820627238118
Si	4.91721133599374	6.11025322722271	-1.35366529156580
Si	1.27539531959566	4.00993487079520	-1.11835322738410
Si	-2.24067304305249	1.90129649821361	-1.02727788417368
Si	-5.71719464879810	-0.01495226240921	-1.30462303869651
Si	-9.35756957968430	-1.91613989332453	-1.57953406327571
Si	-8.11058814572654	-3.95916719433697	-1.59514512737461
Si	-4.39088834681742	-1.95847874508529	-1.38854181733249
Si	-1.20595853250920	-0.19624862951630	-0.95843968226010
Si	2.35969847534734	1.94348868077719	-1.15110607115747
Si	5.91452554145129	3.95071978643206	-1.38742468654393
Si	4.71558992007265	1.90106660174849	-1.25856965043584
Si	1.11906095134622	-0.04893642032020	-0.83024037555672
Si	-2.21283605164616	-1.88578214852439	-2.17796492210698
Si	-5.74020249638882	-3.89801011555233	-1.45509273223454
Si	8.27768598807751	3.81852956703100	-1.58084865079191
Si	9.32371107218772	1.65931389469653	-1.57920531776707
Si	5.69047723271616	-0.23349026273795	-1.25350132685087
Si	2.05758578121846	-1.80922091879330	-2.06128993490607

Si	-1.27503529710747	-3.73541645496164	-1.18820650093242
Si	-4.68596478639516	-6.01786899362924	-1.37525251565900
Si	8.03524851785246	-0.32016530328778	-1.42761652924214
Si	4.19782903754745	-2.06072413873110	-1.12223494137158
Si	1.06795512872929	-3.68398527747574	-1.05854902494000
Si	-2.33363181225102	-5.82473234901391	-1.24731956223227
Si	9.23454125187184	-2.35429221958029	-1.46334093947073
Si	5.48176684359779	-4.05208571178633	-1.18426925456959
Si	2.07363379661632	-5.82138011154431	-1.10722282198959
Si	-1.33039127228818	-7.96528523380162	-1.19086002369860
Si	7.83505497531495	-4.28475949743700	-1.36487930791217
Si	4.40741792131784	-6.15031214244383	-1.13378873800734
Si	1.04099950210322	-7.94239460601742	-1.13959428345572
Si	1.41309387982977	8.02477293396609	1.22600786912525
Si	-1.00224410530973	7.99750099814857	1.28020124486063
Si	-2.25160679772352	5.97422862610263	1.31140322797842
Si	-4.63011728863027	6.18711653675054	1.29072391180217
Si	-5.78859671173188	4.10560769002319	1.20966786939589
Si	-8.15563698478920	4.13733670542837	1.07188377371505
Si	-9.34411476028677	2.04717438862669	0.97180434199294
Si	2.66024464104150	6.00724828807001	1.19597077507186
Si	-1.03332160576642	3.93071318608067	1.34534673153113
Si	-4.71590642675344	2.00341303362605	1.25069745393818
Si	-8.18854876530570	-0.02499501363734	0.96986216473834
Si	5.04428876107450	6.15596966184048	1.06825261333707
Si	1.35414983296964	4.02505193580091	1.29287714592273
Si	-2.36137453347075	1.94898073333336	1.36190185008036
Si	-5.83352487449432	-0.06759521385755	1.10519410830887
Si	-9.49603609804838	-1.99520799397913	0.81925548503706
Si	-8.25500677776115	-4.04225450190254	0.80175570260137
Si	-4.55207112216110	-2.03955005784899	1.12315149858492
Si	-1.63410727603367	-0.28117788420709	1.53557689850843
Si	2.65116751660347	2.06283148252497	1.20790644355181
Si	6.12077233556548	4.03785340842015	1.00924437078679
Si	4.96267484624889	2.00197848620180	1.13146372711778
Si	1.47231584478333	0.09705998858188	1.63674022748818
Si	-2.68430826698984	-2.13154490206712	2.45303762288672
Si	-5.89575018271003	-3.94336916249759	0.93944853732518
Si	8.47379580507487	3.90361735288327	0.81325696851898
Si	9.49499600623909	1.72583382849918	0.81964997130424
Si	5.84860931067954	-0.17119343891257	1.14696353522547
Si	2.31994961261673	-1.97617783657088	2.31848931057066
Si	-1.36565509411616	-3.70516642779278	1.34711158039651
Si	-4.78154207198821	-6.02459313923415	1.03100839046117

Si	8.20061217409070	-0.26260324313414	0.97094998244850
Si	4.42192114716326	-2.06765450371211	1.29364222614050
Si	1.01589218343361	-3.70310743499279	1.37227518621500
Si	-2.41172984215905	-5.82162997209602	1.15154698531285
Si	9.36506411221843	-2.31952305301502	0.93558006649037
Si	5.63403671921621	-4.08003906332711	1.20994478195307
Si	2.08655075320861	-5.82554099211624	1.28300828861099
Si	-1.37902015502750	-7.94227449667729	1.21040105207093
Si	7.98978894874434	-4.28361595948781	1.03420606234445
Si	4.44652831451755	-6.12616248857323	1.28163267925055
Si	1.00803391173919	-7.93321801195974	1.26670479855822
H	-1.50562752227205	9.13307018875535	2.12112404924988
H	-1.64721939013385	9.10577412317802	-1.94209094965527
H	5.48080792157209	7.16925650166622	-2.25156442039015
H	8.95550694164371	4.77102066418167	-2.51866332687173
H	8.30881487676409	-5.40819753580738	-2.23688645486852
H	4.92782008522381	-7.24305861950625	-2.01858807288199
H	1.70869276309669	-8.97868796662446	-1.99145200818789
H	-1.95964466546361	-9.00967074425987	-2.06141446639720
H	-5.19570914218756	-7.08104147407941	-2.30077525788027
H	-8.70216918485638	-4.98848541256293	-2.51041656448465
H	-8.63410380789114	5.23310697844058	-2.19321364373267
H	-5.13499486411324	7.31708484279120	-1.99336946341206
H	-5.21653344396914	7.25628031562092	2.16245911913215
H	-8.90756757960219	5.14379698301998	1.88973817121843
H	-8.91829560135237	-5.14450086344171	1.57052946122720
H	-5.40011419707940	-7.07303720493219	1.90601496015459
H	-2.00292578937177	-8.99507805886505	2.07568651980722
H	1.57603483392954	-9.01141053400303	2.14049677605224
H	4.97723706747724	-7.19948065088321	2.18568497763204
H	8.63407022446440	-5.37468296406404	1.83622261022340
H	9.30042612057821	4.91097135881659	1.55329093141203
H	5.70709323453776	7.23790617067917	1.86609577079689
H	1.90351782247719	9.14492004098327	-2.02691925322845
H	1.93263926994714	9.15535055192959	2.06276834158096
C	0.52060774877283	0.70313949915794	3.21214640784662
O	-0.62371772012584	-0.19876757730661	3.32775989727577
H	0.16867820661856	1.74801582484012	3.12661156617899
H	10.79568915745430	1.74736330020621	1.56553737591678
H	10.51029234247093	1.62226916054840	-2.49483181754772
H	10.62399611757949	-2.45039737466315	1.73822860119853
H	10.40218060770724	-2.48098502710994	-2.39336761220163
H	-10.61771825209807	2.11382981957816	1.76020425761940
H	-10.44914303749746	2.19315498353150	-2.32071562891870

H	-10.76521397218507	-2.07770003053863	1.61176169104862
H	-10.53109673535598	-1.92227272684059	-2.51109629602244
H	-1.24663555060487	0.02192193886186	4.05649239955943
H	2.37004701986180	-2.05450626287799	3.81484846492266
H	1.15591121883558	0.58023310048205	4.10726920018600

• TS 2Si-OHCH₂ → 2Si...CH₃OH

Si	1.36651411440191	8.03615455561274	-1.32667502458614
Si	-1.03257851736276	8.06951485526140	-1.32508390096527
Si	-2.23974728116846	6.03189643409008	-1.31867015817167
Si	-4.60350049854000	6.23221336991001	-1.33862924793852
Si	-5.66419741322734	4.10948425376413	-1.32465351688982
Si	-8.03073116610703	4.17470609718301	-1.35092781037012
Si	-9.22301025126330	2.10012062231475	-1.35130559846230
Si	2.53555388982095	5.97015199554135	-1.31287056817067
Si	-1.05991208541790	3.98631643847777	-1.29960518023701
Si	-4.51492395361801	2.04301352831112	-1.29915842651856
Si	-8.00718863409560	0.06750081217248	-1.33428199487756
Si	4.90102571341033	6.08913120276368	-1.32935324534935
Si	1.28818552912946	3.95980397590841	-1.27991130156136
Si	-2.16991327467789	1.92092154516585	-1.28930963123328
Si	-5.65241477120010	-0.00299366170670	-1.32678038363664
Si	-9.30830314115226	-1.90235495536664	-1.34623998236042
Si	-8.03024698529827	-3.91860515540208	-1.33713772194463
Si	-4.30240710730252	-1.89827800045292	-1.58113205086124
Si	-1.14245220164893	-0.20302288502912	-1.34853687597783
Si	2.21712630052830	1.78985385929216	-1.38003749697601
Si	5.80108274400230	3.89578773617898	-1.32021002409741
Si	4.56667937227653	1.87441912093322	-1.32512960204987
Si	1.16081646147015	-0.23119497630618	-1.74014533963892
Si	-2.20390003055306	-1.93606983391653	-2.49142281745547
Si	-5.66375015624846	-3.78884194822730	-1.33450884841046
Si	8.17009873263560	3.83607164435306	-1.30740034791353
Si	9.27858449038709	1.71406030724032	-1.29852135155343
Si	5.62376205161553	-0.22065327737109	-1.32580870563869
Si	2.18068760712440	-2.06073505602776	-2.57631948668993
Si	-1.26337868237525	-3.73300478508474	-1.37559036432048
Si	-4.69226641881885	-5.94211846502822	-1.32914042675273
Si	7.98053874613971	-0.26373993157673	-1.30730416631656
Si	4.17935629263057	-2.07836174142550	-1.36824902403795
Si	1.10125188463794	-3.73759009053430	-1.35515484948711
Si	-2.33251590870021	-5.82771036272621	-1.33085498091670
Si	9.20899204451922	-2.28025487555866	-1.29655736691809

Si	5.49164706464324	-4.04155070515979	-1.31808120863604
Si	2.07648930982266	-5.89162912593734	-1.32176782472932
Si	-1.36034841150654	-7.97962752632308	-1.33384700869633
Si	7.85052754755008	-4.24646796438279	-1.30195322670629
Si	4.42892030225264	-6.15065766935967	-1.31653123123209
Si	1.02004012798986	-8.00411886419117	-1.32936532846949
Si	1.36565124828240	8.05224668321905	1.07759605673972
Si	-1.03491965402729	8.07740214083555	1.08045016338897
Si	-2.24690409380756	6.03907419559202	1.08776557453770
Si	-4.61336820365997	6.24130939612963	1.08973042185027
Si	-5.68603611671648	4.12339485022089	1.07668279552511
Si	-8.05187241980264	4.18504313838721	1.05627190527787
Si	-9.23998337219205	2.10589392860492	1.05399305265027
Si	2.53627603778053	5.99085877216984	1.09040345794397
Si	-1.06395174178902	3.99002274046217	1.10258860942186
Si	-4.54418868937489	2.05589556232824	1.09292990923684
Si	-8.02701424500932	0.07004977208132	1.06694465715330
Si	4.90114849739499	6.09489345251803	1.09631001672880
Si	1.28758838164662	3.98505944846269	1.11688005133929
Si	-2.20397254278646	1.93194431842590	1.11700389609570
Si	-5.67111240668557	0.00099114475122	1.10381850705307
Si	-9.32522454318978	-1.90306692691049	1.05716189115485
Si	-8.04828482732475	-3.92169037489037	1.06088383189644
Si	-4.33136222566129	-1.90371541437460	1.36110480281146
Si	-1.21481337189007	-0.20182108874255	1.08267990722300
Si	2.21439820453957	1.82630370335844	1.05181599713031
Si	5.79089154184221	3.89719173290981	1.08215598531214
Si	4.56085869785372	1.87727253821202	1.06577465771697
Si	1.04437864976703	-0.08272772904325	1.70059147217210
Si	-2.21748542460540	-1.94851606659607	2.23726821407905
Si	-5.68293617091862	-3.79687378486735	1.08909480132386
Si	8.15934803431319	3.83785967165427	1.09920426183412
Si	9.26610623668379	1.71643395741999	1.10643837703486
Si	5.60879044085848	-0.21977233772839	1.08006025049751
Si	2.18592247891066	-2.12333674195338	2.35093482273174
Si	-1.27842847407226	-3.73381551191286	1.10001814970544
Si	-4.70043853367966	-5.94655023133234	1.07036935209861
Si	7.96570643398129	-0.26022730169297	1.09761713259417
Si	4.15486706151947	-2.06556023688374	1.10568545651047
Si	1.08189540851823	-3.73465107718363	1.07897578543551
Si	-2.34020960175706	-5.83054903055299	1.07611126208215
Si	9.19440943932548	-2.27671813130710	1.10825427822803
Si	5.47335270252916	-4.02344952681816	1.08141309452904
Si	2.06335565819967	-5.88641377598478	1.07444533146846

Si	-1.36848558853132	-7.98300333302895	1.06897290825434
Si	7.83327277792426	-4.23969340951956	1.10002679646964
Si	4.41494351526856	-6.13577507567010	1.09262086904679
Si	1.01215151332118	-8.00241367957183	1.07586824000174
H	-1.57459482016424	9.19855757361867	1.91621999416149
H	-1.57651901311691	9.18251059709794	-2.16861094254870
H	5.54232879837199	7.12177016068874	-2.20542787375082
H	8.88467884765711	4.84988034306491	-2.14891904290151
H	8.42862249864124	-5.34774630148105	-2.13852732675018
H	4.99922834514951	-7.21271019707439	-2.20822820971468
H	1.62412840219128	-9.07333867526890	-2.18856631104275
H	-2.00894685738041	-9.01444362307523	-2.20220653500188
H	-5.34056132510110	-6.93669046683115	-2.24234960265613
H	-8.61540623936648	-5.01086226737337	-2.17917481779055
H	-8.69107981964066	5.21113428031717	-2.20856839359009
H	-5.19696251043426	7.29156606501105	-2.21671654054006
H	-5.21260054629237	7.30723371159344	1.95605177820995
H	-8.73443402305501	5.22493889414208	1.89214194360472
H	-8.65037205353883	-5.01367515098034	1.89133332696390
H	-5.34264938301937	-6.95275786406836	1.97534487151412
H	-2.01995830144593	-9.02156414867487	1.93091162167033
H	1.61749275449110	-9.06669684172425	1.94051845905469
H	4.98499450058155	-7.18335752412411	2.00169128942983
H	8.39052668821792	-5.34214510498774	1.94954117349046
H	8.86047822475160	4.85511842819759	1.94795666349124
H	5.56318793341505	7.11565369519906	1.97107290107356
H	1.93904436852350	9.13238931528361	-2.17331441329179
H	1.93327534967313	9.16192570138305	1.91000709240786
C	0.54575286251588	0.50832187099441	3.81600837771029
O	-0.41475412997840	-0.29265432534360	4.43243063789161
H	0.05519066253346	1.42988776009078	3.45301833364906
H	10.49680861081139	1.72279708026102	1.96212078576138
H	10.51960000937433	1.72448412626035	-2.13900126580681
H	10.40324351398396	-2.36814029858758	1.98926923619256
H	10.43059575957649	-2.37587746177440	-2.15924605208887
H	-10.48329016915539	2.15650326277658	1.88951033617008
H	-10.45447030976292	2.14219081125307	-2.20451766032270
H	-10.54418715077502	-1.95607294346757	1.92638476648504
H	-10.51479701208146	-1.94887872266815	-2.23288432999391
H	-0.00436190346716	-1.14956987832401	4.67092300266243
H	1.43833497536450	-0.61169214571683	3.22552100472822
H	1.40488731226618	0.78504940575458	4.46035536493835

• TS 2Si-CH₃OH + H₂ → 2Si-CH₃OH-H₂

Si	1.33119368074380	7.99291996675450	-1.24090782420703
Si	-1.07044295224533	7.99885582435272	-1.22551790836641
Si	-2.24886234506396	5.94469565310501	-1.24289214971425
Si	-4.60582022980438	5.91535574368920	-1.19395209231563
Si	-5.37224040445929	3.65555821646799	-1.18060817272718
Si	-7.72031925926134	4.02068729688413	-1.20218371858968
Si	-9.08970603378581	2.07176839182168	-1.27030717553840
Si	2.46966735204836	5.91235804387637	-1.27227368320709
Si	-1.13958754243083	3.86498965948923	-1.25798789534515
Si	-4.44583832575653	1.99512024363288	-2.57642705192816
Si	-7.81943984479628	0.07688296719101	-1.31784615278474
Si	4.84334187782714	6.00251401663435	-1.29659575806502
Si	1.21295103048040	3.90390084127530	-1.28502978861211
Si	-2.45731325206388	1.89690435860757	-1.32967890055441
Si	-5.45458989324676	0.25680972296128	-1.36375485821662
Si	-9.18354255195377	-1.85406163018920	-1.36045010798149
Si	-8.02942196619354	-3.93792348944251	-1.36553303734350
Si	-4.38150774799816	-1.84541462223429	-1.59528150655862
Si	-1.21102388276451	-0.12533803199096	-1.37077099416335
Si	2.24299145636962	1.79819271242250	-1.31533171546584
Si	5.80982164578892	3.83256565976780	-1.29827207777643
Si	4.58589389154591	1.81100707678817	-1.30578830941199
Si	1.15195118321906	-0.27227209360475	-1.38719396225667
Si	-2.24045138671520	-1.93588537856816	-2.35339732447997
Si	-5.67250046157102	-3.79154060321505	-1.38102567025261
Si	8.17753278388514	3.79934536782944	-1.30799442515859
Si	9.28767300316746	1.67849072327197	-1.32241407336046
Si	5.64583757250708	-0.27600187934615	-1.33788926411501
Si	2.14760169038877	-2.05659219396233	-2.47395589071345
Si	-1.24399523278673	-3.76945531785118	-1.36458769144496
Si	-4.68276893633341	-5.93719186365092	-1.38194317649006
Si	8.00003627185519	-0.30982661849875	-1.32799876423193
Si	4.21420410258620	-2.12719516432854	-1.44330358179034
Si	1.11715669341238	-3.81289456886240	-1.38573559193502
Si	-2.32495307412066	-5.85303838500005	-1.35887221026775
Si	9.22957238214214	-2.32638492462043	-1.34615956083438
Si	5.51340077386902	-4.08024758277180	-1.34660377997590
Si	2.08998467884046	-5.95595664265642	-1.34995910563311
Si	-1.36337376623776	-8.00890073976312	-1.36959899597717
Si	7.87328677630284	-4.29222180682008	-1.35116620970112
Si	4.44361909607982	-6.18714168125571	-1.35879278342997
Si	1.01691104268267	-8.06053449214655	-1.36731413501722

Si	1.34975996315125	7.97213147204854	1.16233410532837
Si	-1.04909528748396	7.98029794234802	1.18239043608705
Si	-2.22657898780891	5.92513663923728	1.16468861336686
Si	-4.57988456523836	5.99011078754094	1.21527522637960
Si	-5.48783681935364	3.81579469741169	1.28765546520086
Si	-7.82799143580420	4.02552901407973	1.18956003022050
Si	-9.11408771888551	2.02935490134940	1.13151205274347
Si	2.48951251215727	5.89453151655188	1.13265335402134
Si	-1.09393194783808	3.86648249707774	1.14156792490516
Si	-4.41560471314852	1.90316511635534	1.98545288224305
Si	-7.85757980191741	0.03139131210552	1.07947409445444
Si	4.86020251949113	5.98794504688755	1.13059927136213
Si	1.24937996160478	3.88106805062414	1.11460904172517
Si	-2.28569947952562	1.85324229070778	1.11111681043425
Si	-5.51345542258192	0.07345296981126	1.09841991157392
Si	-9.21680072992792	-1.89405424080908	1.04273939806445
Si	-8.02913978104724	-3.95415345818440	1.03280125743438
Si	-4.27714823757373	-1.91993785562860	1.25724826249456
Si	-1.19819141419532	-0.23779157961209	1.05208198801585
Si	2.25449133107251	1.76652193104743	1.09941785324229
Si	5.81860103538633	3.81571451020593	1.10314024295704
Si	4.59673904648618	1.79134588658010	1.08866051906744
Si	1.16640610878816	-0.30647372108848	1.11848469461770
Si	-2.19099044343568	-1.97983949023984	2.23672620681077
Si	-5.66678218793756	-3.80186694065439	1.04002883851917
Si	8.18569841110383	3.78274896194474	1.10138213367279
Si	9.29624041044755	1.66287317383729	1.08294430490662
Si	5.65314568105427	-0.29673961967307	1.09292219838419
Si	2.14728197964686	-2.08990015383054	2.22105973065843
Si	-1.24742885177242	-3.77454074559011	1.10336453801739
Si	-4.69361463899665	-5.95503632965825	1.02187896273830
Si	8.00761787110225	-0.32543619119384	1.07390112713812
Si	4.21540944223256	-2.14734044524429	1.18374066282954
Si	1.11801011009617	-3.83475385608538	1.10976613856570
Si	-2.33260139705486	-5.86470865637302	1.04866162250780
Si	9.23702788694825	-2.34165692831217	1.05808503603317
Si	5.51874024192361	-4.09783933592397	1.06202716694590
Si	2.09566882640249	-5.97415809724438	1.05102762911735
Si	-1.36760953875975	-8.02033739057343	1.03536466086016
Si	7.87959427219778	-4.30723570326931	1.04889820210590
Si	4.44993028303863	-6.20644967522655	1.04488556223171
Si	1.01451894730396	-8.07383971044622	1.03588561225879
H	-1.59751007375565	9.07400136702138	2.04903645605346
H	-1.62326835840268	9.12168183089392	-2.05046299548157

H	5.48993289115214	7.03985232053101	-2.16352843672476
H	8.88988495117279	4.81500978466754	-2.14897170733418
H	8.42731297906023	-5.39643910103939	-2.19953621161703
H	5.02137634042433	-7.21769933171171	-2.28062574770779
H	1.62065197906998	-9.12114932498456	-2.23675347873286
H	-2.01640241678373	-9.03966238102614	-2.23915698444923
H	-5.31725690440114	-6.94050628638750	-2.29591218561596
H	-8.64250067913601	-5.00196530568715	-2.22320774756340
H	-8.21190770792324	5.15833148200482	-2.04408505906445
H	-5.38046633798798	6.85634577852344	-2.06511715605979
H	-5.28467935276951	6.98096523842678	2.09009405876245
H	-8.39483776454628	5.13407004245234	2.02223857276666
H	-8.61868064091296	-5.03536656092850	1.88571154232226
H	-5.35520497762349	-6.96414021020224	1.91001553520352
H	-2.01413369885614	-9.06615800237491	1.89206271053484
H	1.61043085800351	-9.14977187688118	1.89198428929741
H	5.03268037498887	-7.25272685619076	1.94571861434093
H	8.44073842556633	-5.42114659388006	1.87984939025438
H	8.89906002714786	4.78906027587440	1.95277258457301
H	5.51052889401057	7.01724689482278	2.00445820167206
H	1.89362581609294	9.10308547999840	-2.07591616175411
H	1.92535613851550	9.06194486600323	2.01517593826803
H	10.53783103953948	1.66129309718788	1.92280798498796
H	10.52349356300347	1.68752875835552	-2.17057834298510
H	10.45063710390949	-2.44448702413649	1.93051225246330
H	10.43726760527939	-2.41809099796017	-2.22790599066640
H	-10.32293809792479	2.03317642954852	2.01782966657261
H	-10.30460421163362	2.16943073302208	-2.14226381815097
H	-10.43905081451988	-1.87933439019860	1.90956389686117
H	-10.39441213463537	-1.82864433008027	-2.24272902299340
C	-1.36599260443932	0.90154336040379	4.63474688890256
O	-2.66902564982791	0.28316718926747	4.58837986315599
H	-1.52135838801125	1.96710186932698	4.86156540932374
H	-2.61818275406743	-0.55864757384340	4.04113085041224
H	-0.84475040926316	0.80466547736994	3.66480280090962
H	-0.76631946176155	0.43358948529735	5.43284960951949
H	-4.36024319533393	1.71385874886260	3.84154593730623
H	-3.69004126992165	1.13058324871619	4.08653914813421

• **TS 2Si-CH₃OH-H₂ → 2Si-CH₃-H-H₂O**

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Si	-1.14973830726087	7.95632256851060	-1.27618629982821
Si	-2.28030351448558	5.88277057061647	-1.35332975593711

Si	-4.63224880924814	5.91746223442698	-1.37793224349884
Si	-5.41987178590080	3.68742391737998	-1.38216447617896
Si	-7.76844030801578	4.01343036364415	-1.38477765205049
Si	-9.11127826066166	2.04825200355438	-1.41404497973542
Si	2.31922427132948	5.88652927799734	-1.23296667399455
Si	-1.25922530828554	3.77516059916991	-1.42245332467882
Si	-4.54887371810318	1.93635832445231	-2.68805442663745
Si	-7.85108829253585	0.05143751087849	-1.41076011156610
Si	4.68894635044542	5.97499138943761	-1.18939216568899
Si	1.07906024649677	3.86755026383536	-1.31489722302214
Si	-2.43368370498434	1.87392689355776	-1.92580318917063
Si	-5.49447106838236	0.19441190021632	-1.43962179565661
Si	-9.26209574147021	-1.84047610298857	-1.45818303870112
Si	-8.16199299739385	-3.95047685587552	-1.47790599461087
Si	-4.46473684400216	-1.92010447557449	-1.50867221950797
Si	-1.33349997369458	-0.09436742492616	-1.32383079392080
Si	2.08716134176785	1.76220734447412	-1.26684620756084
Si	5.66357952177024	3.81500201617813	-1.16122384885585
Si	4.42661133971734	1.80606199165676	-1.20898119014152
Si	1.01844161668480	-0.30612682366198	-1.35713100253872
Si	-2.32307061574314	-1.92443360416780	-2.31715496074768
Si	-5.80248465253853	-3.84055648884023	-1.48141768054923
Si	8.02966839525771	3.81761696857327	-1.12424869878573
Si	9.15275856370303	1.70801899340382	-1.11800139507317
Si	5.50257463084308	-0.26533181990676	-1.22166319107563
Si	2.05448606017180	-2.04642496251981	-2.48824920391092
Si	-1.29251278475243	-3.81337967713655	-1.51262485379113
Si	-4.78564979776239	-5.97032253807267	-1.49965089601490
Si	7.85526435948041	-0.27167489204966	-1.15932678561135
Si	4.08001047198287	-2.11813532061202	-1.36208963470949
Si	1.05779444164569	-3.84528747878630	-1.43558386055315
Si	-2.42352762802521	-5.86889073683856	-1.48401715022313
Si	9.10654810868437	-2.27319813070745	-1.16414556265444
Si	5.40900174959963	-4.05486380705185	-1.26796736843726
Si	2.03329318450261	-5.98562187329111	-1.38862449698170
Si	-1.44284346572056	-8.01721599728962	-1.48131117924382
Si	7.77052072292113	-4.24986299161185	-1.21812272417753
Si	4.38850862575590	-6.18535274157828	-1.33007200491349
Si	0.93955215878771	-8.07743972100373	-1.43888505071857
Si	1.19980378115717	7.96343938264095	1.16851535329281
Si	-1.18880546682341	7.90199895564291	1.13077237463270
Si	-2.29379911662291	5.80931261918121	1.05052077682779
Si	-4.64746820774219	5.90594892180187	1.02867064067553
Si	-5.45567332574739	3.68985169541734	1.03093903874019

Si	-7.79587117281255	3.99320439119616	1.01095468288399
Si	-9.12895367017439	2.02538389994063	0.98766201658505
Si	2.26055448494270	5.85047644720311	1.16819176968319
Si	-1.34531666167979	3.65177588771001	1.04955268514879
Si	-4.47311943947443	1.88852221405188	2.15713248400942
Si	-7.85999174229204	0.03135285086795	0.98980639037816
Si	4.62832831745632	5.94716916512599	1.23933135238085
Si	0.99983544684426	3.84683245013620	1.07286515445499
Si	-2.12075190526318	1.84238061673676	2.28330371722278
Si	-5.49855151606269	0.13210579775233	0.97403915614300
Si	-9.26938980944996	-1.86341737899601	0.94500588417831
Si	-8.15992026780980	-3.97037046813824	0.92109338797850
Si	-4.41082006177400	-1.96124899237874	1.00317362376511
Si	-1.41584867433586	-0.08108897129138	1.11735218021916
Si	2.03119155558448	1.74650528412847	1.17281528818600
Si	5.61730657230504	3.79453851874507	1.23756805399612
Si	4.37496890884475	1.78551194899295	1.19939459415510
Si	0.94953587256014	-0.32530631671910	1.15476651047768
Si	-2.35644266101375	-2.02265208047455	2.06537703165495
Si	-5.79994773364067	-3.85387539816747	0.93786659948276
Si	7.98256043501484	3.79649922409422	1.28607022129951
Si	9.10429415608355	1.68430947824342	1.28707545614366
Si	5.45333208051396	-0.28952431764443	1.21770409165993
Si	1.94072702081216	-2.11967173214969	2.23899391872211
Si	-1.35301656272036	-3.79166825971771	0.97772083908849
Si	-4.80182097991979	-5.99407034341133	0.90326493327729
Si	7.80925889595995	-0.29785356446991	1.24085742714688
Si	4.03119500572999	-2.15174996104426	1.23895995745869
Si	0.99838695444883	-3.86591946837517	1.05206750765560
Si	-2.44021500049672	-5.87435896696965	0.93111144444388
Si	9.05681272139059	-2.30316419381151	1.24020320717015
Si	5.36023979219212	-4.08953119927730	1.13616128977385
Si	1.97757644876368	-6.00557136116535	1.00892724352705
Si	-1.48018001502787	-8.03337794945057	0.92091759066664
Si	7.72063951260078	-4.28095464972137	1.18180837976593
Si	4.33151038951226	-6.21625820605722	1.07461258293558
Si	0.89837687678956	-8.10630689411374	0.96430598725742
H	-1.81520618797247	8.95650045583305	1.99256539768385
H	-1.72726433100168	9.06170399070353	-2.10765217682155
H	5.36158832230784	7.00912059909285	-2.04069163978773
H	8.73966012778628	4.84531163844013	-1.95237097545351
H	8.35419399951526	-5.34228762296012	-2.06196057814304
H	5.01914848329039	-7.19384772896493	-2.24194932568412
H	1.54382875632015	-9.14063800820442	-2.30488400126961

H	-2.07258508712109	-9.05325377045782	-2.36203773956122
H	-5.39256780549576	-6.98003673155699	-2.42564792601785
H	-8.78910058679367	-4.99431963882633	-2.35067613135335
H	-8.29038356663998	5.13899237532205	-2.22548720339545
H	-5.32750447938290	6.88641768186141	-2.28377996004847
H	-5.34712278395290	6.88566003937025	1.91968724803916
H	-8.31956159459250	5.11253225884627	1.85792699747381
H	-8.78443853611163	-5.03223683611601	1.77482744567746
H	-5.41797786264983	-7.03769483321739	1.78541422347136
H	-2.16050731173313	-9.06818353456434	1.76485567490562
H	1.47738169894230	-9.18732846632230	1.82557531101637
H	4.89969526453388	-7.26044046157894	1.98767779028660
H	8.27208586558517	-5.39433673309298	2.02014525220719
H	8.66583788411053	4.80588254051971	2.15826757812993
H	5.23758731073176	6.98066465852360	2.13780143727504
H	1.83380724641018	9.08557631157597	-2.07342334058085
H	1.76546980826174	9.03891035063821	2.04538100889131
H	10.32334401429640	1.67999919842373	2.15917478615054
H	10.40515934064313	1.71402363592653	-1.94110212261004
H	10.24958795300001	-2.39932437603698	2.14185206677194
H	10.33510729977298	-2.33643290834610	-2.01913231486332
H	-10.34867547368402	2.06541750008536	1.85908493631403
H	-10.32062478079360	2.10730095276607	-2.29805976014109
H	-10.49505327787820	-1.83162439334111	1.80800417809696
H	-10.47676296981032	-1.77715997124926	-2.33383629111471
H	-5.04710874533376	1.82157319224611	3.54699847071062
H	-2.07746602398490	-2.01047905507910	4.28427420228103
C	-1.89352248170449	0.10637068196765	4.55625367727811
O	-1.97945937602427	-1.53776028150806	5.21391296507496
H	-0.97193448105592	-0.03561405581143	3.99121787333443
H	-1.83463832333508	0.72495617847098	5.45748109680021
H	-2.83085911839534	0.11657814901249	3.99826272296262
H	-2.86275561335952	-1.65476810580262	5.63041279587536

• TS 2Si-CH₃-H → 2Si[⋯]CH₄

Si	1.11813837129537	7.83871755126941	-1.18566552392434
Si	-1.26492037233890	7.74964361824767	-1.35154282370505
Si	-2.14004805965043	5.56152386702012	-1.62864895496325
Si	-4.50166669201107	5.86002975763312	-1.69813031099001
Si	-5.63130253901255	3.87815665431627	-2.21223274526889
Si	-7.91232853516907	3.96421861433051	-1.58339045286594
Si	-9.21920633298132	1.99706462458922	-1.47344132223512
Si	2.14869770955319	5.70991954810529	-1.15791256594235

Si	-1.19342226458434	3.70807347311853	-2.78812216335276
Si	-4.45931084509784	2.25468444241888	-1.08614835443899
Si	-7.85822253126119	0.08975271166535	-1.23255740993271
Si	4.49932301401129	5.92304783332099	-0.96510435947761
Si	0.74399403064560	3.81291900210498	-1.39647394716012
Si	-2.08533182222161	2.36981321271496	-1.02791947007238
Si	-5.54821266897444	0.20014305982655	-0.88367352303943
Si	-9.25501628600923	-1.79676218050715	-1.52896023755027
Si	-8.13552158672062	-3.88305860944312	-1.56043595274950
Si	-4.40846070475513	-1.81654991317176	-1.16419742167210
Si	-1.42936543507235	0.07044781676864	-0.97080504327962
Si	1.97667610832902	1.81786046470067	-1.18747707709080
Si	5.56476046439669	3.81039181509721	-0.95613948769157
Si	4.31469823885726	1.82178007961628	-1.11422212435006
Si	0.92102511355464	-0.24986355326391	-1.08924986031847
Si	-2.36376941958237	-1.69380452661078	-2.17630935994548
Si	-5.79830734066199	-3.69450124406603	-1.32797032822840
Si	7.92530294976108	3.84614212503337	-0.86843906939745
Si	9.04467614768542	1.73825664511759	-0.89463425991738
Si	5.37477724306560	-0.25585492726716	-1.12941558955723
Si	1.84843479958049	-1.99014148556054	-2.32452840153723
Si	-1.42442504197667	-3.62202183243814	-1.28791436451719
Si	-4.83386663557385	-5.83848575083493	-1.52696057008492
Si	7.72753315662938	-0.22783130321059	-1.01907376732449
Si	3.96742135913842	-2.09958327416143	-1.42112468071553
Si	0.91856075768229	-3.78666226524894	-1.20965319621076
Si	-2.48505882518755	-5.71658532123587	-1.46254384706008
Si	8.97036100654017	-2.23447053672058	-1.04410087826495
Si	5.28618587217648	-4.04089263358070	-1.22684868785031
Si	1.89502122772424	-5.91754726649185	-1.30750989805922
Si	-1.53741770305587	-7.88156804495437	-1.60745450843583
Si	7.64970767996190	-4.21757748017357	-1.17451770844991
Si	4.24479748687808	-6.15696018705859	-1.30537311033138
Si	0.83315956094502	-8.01047131216976	-1.49987093722367
Si	0.98375288647287	7.79682428465814	1.21071764102167
Si	-1.37569806843933	7.62342989666562	1.04317748660445
Si	-2.31028445493908	5.47822096347880	0.78428869219826
Si	-4.62955196105576	5.57225016965536	0.69231411673500
Si	-5.33380896644495	3.33111847626872	0.91406907957559
Si	-7.64629492906941	3.72675169341938	0.77133774240659
Si	-9.26658175873805	2.00137076093375	0.92870889906470
Si	1.97558868450206	5.65417539205592	1.23053712304911
Si	-1.59993825279550	3.31668403352560	1.17854651886856
Si	-4.85435766183304	1.80904254473517	2.62578575036318

Si	-8.14987028886309	-0.06382150944510	1.14674130865156
Si	4.33464097025353	5.80898584624317	1.45324900169913
Si	0.67751732688262	3.68282054173840	1.03923817509289
Si	-2.49687649486025	1.51809810355029	2.27402842829196
Si	-5.79135680761524	-0.04202315630506	1.49627524546396
Si	-9.51863978682518	-1.95888455525058	0.85507113435649
Si	-8.33696159000931	-4.03571966807207	0.82726395733380
Si	-4.60328069999760	-2.07488418108440	1.38261694366642
Si	-1.50484682867790	-0.41894156913366	1.40796629709413
Si	1.87195684915203	1.69728019449926	1.26403932344334
Si	5.45694595402642	3.72882876102011	1.43779265670518
Si	4.20954263524063	1.73486313511168	1.29378604932974
Si	0.86648670060581	-0.41985606429634	1.37765708296678
Si	-2.54101299735550	-2.22168674642411	2.41353438156686
Si	-5.98537201808366	-3.94628323686446	1.06690635059108
Si	7.82230532631379	3.76554536771926	1.53995397847476
Si	8.94438397945052	1.65467962456006	1.50710041003251
Si	5.27683775657556	-0.34710221665766	1.31807132265245
Si	1.85007342049621	-2.21354394422427	2.49143076037870
Si	-1.49433059791633	-3.88645916891768	1.22837660741063
Si	-4.95690558572934	-6.06137039761557	0.86014257095828
Si	7.63055549636883	-0.31037029645634	1.37590709122326
Si	3.91468630251169	-2.23199054136598	1.49474065300987
Si	0.86821741123989	-3.92296735580235	1.23765852445253
Si	-2.59292912228350	-5.93034548686377	0.93876789057094
Si	8.86813042837350	-2.32490722612197	1.35578461390327
Si	5.21718115291162	-4.15240574278603	1.17687447569728
Si	1.83019608785926	-6.07816992047447	1.08559372076216
Si	-1.64856295775689	-8.08459737142093	0.78368332962486
Si	7.57763848530705	-4.32986362025137	1.22171782061120
Si	4.18715864574819	-6.28107249104561	1.09417928902626
Si	0.73170529915925	-8.16536456238374	0.89763470608050
H	-2.19147375330553	8.51680506235642	1.92639985075871
H	-1.86131700621824	8.87623187136690	-2.13974131802047
H	5.16389166304117	7.01884722782293	-1.74224086160250
H	8.64216828793380	4.90105537926916	-1.65472225138760
H	8.24102944018073	-5.28190733394091	-2.04772643947969
H	4.82319350179586	-7.15876656850588	-2.25760878086609
H	1.46357936369803	-9.01971433987329	-2.41018267941369
H	-2.18483110018609	-8.81469968310229	-2.58494042110204
H	-5.46566658479710	-6.71751453810360	-2.56294062273893
H	-8.63573673893447	-4.88945220916383	-2.55009195051356
H	-8.56805029553094	5.19514204098202	-2.12322279105061
H	-5.13069782796254	7.06983977167996	-2.31709780286153

H	-5.41223922767817	6.50925544167159	1.56007741603515
H	-7.96432110005291	4.91772318178954	1.62323041135522
H	-9.04656650341681	-5.13839621424546	1.55228383271963
H	-5.55307836479510	-7.19418534045963	1.63868653216535
H	-2.34271907588372	-9.18857125271146	1.52197783818581
H	1.26576088463747	-9.30302605133809	1.71401377759882
H	4.82045091544391	-7.32152956500030	1.96711268503838
H	8.14570867451557	-5.45944206250895	2.02592724193116
H	8.48022846204271	4.74960697407840	2.45916873395718
H	4.81259835213918	6.84880809748737	2.42183888664516
H	1.76591817436021	8.92783565282586	-1.98548460784580
H	1.48724470655272	8.83912098688659	2.16280294407568
H	10.14257865466220	1.61591395366773	2.40661582321928
H	10.31572553703386	1.74742208644120	-1.68821272059210
H	10.04195443617725	-2.42535907880538	2.28139533194883
H	10.21779936509405	-2.27664993038000	-1.87272413338839
H	-10.42390574214957	2.41179263460594	1.78942614175284
H	-10.37189741232376	1.83595978504803	-2.41430122833543
H	-10.82501078996403	-2.03640907191262	1.58542851318642
H	-10.36126387019053	-1.61456285255765	-2.52254026763523
H	-3.26489519228240	1.72012132924006	3.76162328757039
C	-1.90442049933355	1.51390137411934	4.31107054119247
H	-0.84128924365999	1.61632024916148	4.02022966908947
H	-2.14145504834326	2.34093490179451	5.00233508067169
H	-2.07072529897542	0.53187759089332	4.78006494190885

3.2 Hydrogen absorption on silicene bilflake

- $2\text{Si}\cdots\text{H}_2$

Si	1.23732224811668	8.10533243554521	-1.21733534606177
Si	-1.15728729332012	8.10736306552778	-1.21588738189839
Si	-2.31866246239462	6.04283427380300	-1.21843427029408
Si	-4.67976953936703	6.24608611562479	-1.20221502601716
Si	-5.64645382803291	4.08286568340448	-1.18152207129997
Si	-8.01669756053733	4.08368959745094	-1.15754811791922
Si	-9.19663077161085	1.99829680333464	-1.15456409436992
Si	2.39829197147822	6.04227455332083	-1.21439175295126
Si	-1.13923542533561	3.98806871426589	-1.21924213948781
Si	-4.43053266974311	2.05085168061868	-1.16492485822864
Si	-7.93310134730904	0.00027287839191	-1.16461295087847
Si	4.75698245033831	6.25278847395738	-1.24491959138050
Si	1.20818836273096	4.00225088744397	-1.21223881037646

Si	-2.07634036234554	1.82142950352506	-1.24030242552059
Si	-5.57935321537803	0.00021385595807	-1.19223672423779
Si	-9.19680453405087	-1.99760809285947	-1.15465464506646
Si	-8.01734247815453	-4.08324529380325	-1.15780385320357
Si	-4.43096679307740	-2.05078138459481	-1.16490562039357
Si	-1.20891682890647	0.00003737135603	-2.45809243992235
Si	2.16936393413570	1.86499042577090	-1.24106687580661
Si	5.72154560245429	4.08938203957896	-1.24641156410676
Si	4.51653856678452	2.04743400637885	-1.26816776394944
Si	0.95173638090551	-0.00000411728185	-1.86022072610343
Si	-2.07667738861561	-1.82147345450751	-1.24066616304265
Si	-5.64709419064478	-4.08276126187287	-1.18180994982020
Si	8.09323316575093	4.08215969475973	-1.26581972267377
Si	9.27355807358503	1.99790854313966	-1.27459325012570
Si	5.66024693902244	-0.00007513474922	-1.25387268085299
Si	2.16940748656771	-1.86490692439697	-1.24068863143580
Si	-1.13947029508272	-3.98813833842185	-1.21941879242885
Si	-4.68027465861723	-6.24593756288813	-1.20267074323479
Si	8.01204366799033	-0.00015248593661	-1.26862465398342
Si	4.51645392542599	-2.04742949735886	-1.26820115308857
Si	1.20795915110223	-4.00199802989293	-1.21234203931667
Si	-2.31919310427779	-6.04273935771607	-1.21887091538516
Si	9.27346547372549	-1.99827842254626	-1.27467344447743
Si	5.72129624908100	-4.08943850537024	-1.24646436713921
Si	2.39794266410196	-6.04203968547133	-1.21458833213387
Si	-1.15774721840961	-8.10724500692688	-1.21639109654646
Si	8.09296904676550	-4.08244127013300	-1.26592934345492
Si	4.75662100561084	-6.25278185008524	-1.24498528021512
Si	1.23686414668644	-8.10500712013369	-1.21766668753998
Si	1.24726561378253	8.10641809781796	1.18963888628878
Si	-1.14706688773284	8.10300938225289	1.19122088286951
Si	-2.30553228738202	6.03896293644459	1.18543820049046
Si	-4.66374397480169	6.24988740444388	1.21813315412579
Si	-5.62888960495957	4.08684053656933	1.22123751567092
Si	-8.00022721797392	4.08132260029308	1.24408149109341
Si	-9.18260204855402	1.99862076255344	1.25232194268046
Si	2.40953834578877	6.04257131986513	1.18969834703872
Si	-1.11567523300013	3.99965071360828	1.17892965378651
Si	-4.42402616619131	2.04476547349449	1.23973464838804
Si	-7.92251369159520	0.00023607649576	1.24378842875790
Si	4.77060751997901	6.24702312674709	1.17519379482989
Si	1.23195923731596	3.98674645571959	1.18605447069713
Si	-2.07853300448230	1.86302352133102	1.20429113912438
Si	-5.57158440795658	0.00038166175088	1.22109646100296

Si	-9.18268656816183	-1.99806745117607	1.25223458859426
Si	-8.00095152045073	-4.08106703457199	1.24378700201531
Si	-4.42507567944494	-2.04470935339185	1.23973920692578
Si	-0.85358492961775	-0.00046178680644	1.81657852828950
Si	2.16527357437566	1.81814239269498	1.20670174460592
Si	5.73634272793941	4.08356350842526	1.15676942931643
Si	4.51975735644744	2.05188148577472	1.13583713192356
Si	1.30305604080341	0.00007329390700	2.43369161299629
Si	-2.07936861762250	-1.86352145178113	1.20384169060086
Si	-5.62961101335497	-4.08701109832236	1.22093948432927
Si	8.10672511501268	4.08293152327239	1.13571877437994
Si	9.28481717805037	1.99658872114153	1.13234634293189
Si	5.66605879946846	-0.00021009738713	1.16023525769853
Si	2.16513430234959	-1.81804948467728	1.20704158690798
Si	-1.11581569874369	-3.99993133615851	1.17876846821859
Si	-4.66422481224322	-6.24991469272505	1.21772770027188
Si	8.01926181669671	-0.00019749589446	1.13955536882408
Si	4.51950893992246	-2.05214382789832	1.13583660670399
Si	1.23177935675900	-3.98646664677460	1.18596001101467
Si	-2.30609311939487	-6.03896399024173	1.18501137393584
Si	9.28472174856896	-1.99706823171538	1.13225970121840
Si	5.73610845429798	-4.08379217107104	1.15669045422420
Si	2.40906724502389	-6.04250482878279	1.18950540663440
Si	-1.14765471023150	-8.10305498103284	1.19068308916531
Si	8.10648237342572	-4.08334733046824	1.13559666873362
Si	4.77016083639881	-6.24720883739669	1.17509693920737
Si	1.24669908130094	-8.10629275054834	1.18929143410888
H	-1.71951901861425	9.19916153233171	2.03816252926261
H	-1.72183768855617	9.21341050540285	-2.05526643024688
H	5.35914693215428	7.29736134350588	-2.13442561078180
H	8.76647265549942	5.11646120247129	-2.11636776924533
H	8.76602517096729	-5.11675759464971	-2.11659592160528
H	5.35848625257468	-7.29745828752387	-2.13455908699834
H	1.80836957899176	-9.20324063523508	-2.06239870948161
H	-1.72204461230054	-9.21327336091021	-2.05595713432678
H	-5.30912221510564	-7.28504214961422	-2.07998163606408
H	-8.70536586643743	-5.11999248900422	-1.99329440881432
H	-8.70438213920850	5.12077023659156	-1.99297446980012
H	-5.30850348794961	7.28519878472321	-2.07959441302323
H	-5.26471940302885	7.29399709988892	2.10915007038271
H	-8.67101921058719	5.11552451474456	2.09670027584734
H	-8.67186497786980	-5.11525973634904	2.09630137341422
H	-5.26519113346340	-7.29415830426513	2.10858523028148
H	-1.72013611761822	-9.19924310574423	2.03753763699465

H	1.81119736205845	-9.21131139400363	2.02995365662583
H	5.39732336192005	-7.28662878358675	2.05329069667006
H	8.79286398556196	-5.11952764742249	1.97307982185141
H	8.79308533387250	5.11909522994498	1.97325013503879
H	5.39784385659178	7.28641764533762	2.05338395498074
H	1.80868842196010	9.20362866179219	-2.06208037148940
H	1.81188938202419	9.21132397704745	2.03037639217237
H	10.51967555240288	2.03638418011785	1.98100594542497
H	10.49868695662330	2.03831175767056	-2.13724268652168
H	10.51956600041200	-2.03690248988718	1.98093795973676
H	10.49857473394937	-2.03871334378678	-2.13735229679522
H	-10.40683026233815	2.03752044761564	2.11626475675254
H	-10.43240689639231	2.04090339717976	-2.00169128726342
H	-10.43269246943151	-2.03996890579862	-2.00163308210257
H	-10.40695208868864	-2.03692595504769	2.11613518642337
H	-3.86994617840512	0.00125913316030	3.94656756556489
H	-3.17120478852970	-0.00232938868819	4.24490380288346

- **2Si-H₂**

Si	1.19332742280452	8.10938252889066	-1.21090810860316
Si	-1.19996851988154	8.10699550801378	-1.21585211215382
Si	-2.36182754624658	6.04347966699921	-1.22077762037743
Si	-4.71918663833648	6.26117771084795	-1.22663244785196
Si	-5.66347926248392	4.08741584001972	-1.22132826928397
Si	-8.03340537482654	4.07938732081263	-1.21632239435132
Si	-9.20997876669884	1.99335553035157	-1.22083570833845
Si	2.34813700165073	6.04341547840509	-1.20095449198726
Si	-1.19911918430910	3.98043452588232	-1.21046909299413
Si	-4.44918130101272	2.05352248834382	-1.20430047308805
Si	-7.94159274587698	-0.00005781817729	-1.22336455766132
Si	4.70594886103531	6.25840562525713	-1.21724451099861
Si	1.14865469644057	4.00706106076135	-1.19710566657069
Si	-2.09458193823457	1.79429222843202	-1.23098083734013
Si	-5.58822827081309	-0.00050495511880	-1.23588352140103
Si	-9.20997244739771	-1.99346252889338	-1.22078925073795
Si	-8.03301582965126	-4.07934265188744	-1.21617208835099
Si	-4.44817786642718	-2.05406243084886	-1.20394196960509
Si	-1.23159006279087	0.00043837316250	-2.48425336310657
Si	2.11842196339280	1.86733194142327	-1.21581845799542
Si	5.66910096263774	4.09554646406206	-1.21071806527306
Si	4.47378313840938	2.04877841942639	-1.20320803305860
Si	0.92762278073740	0.00056407623937	-1.87144657430024
Si	-2.09360924875573	-1.79390370391605	-1.23127324569291

Si	-5.66311713475517	-4.08757003396858	-1.22116658971139
Si	8.04108900337201	4.08231071083105	-1.21965657868897
Si	9.22617870083324	2.00129358341659	-1.22332107915419
Si	5.61733435822648	-0.00017212249699	-1.21592947216986
Si	2.11760677849985	-1.86685059361920	-1.21619284060812
Si	-1.19932153635638	-3.98041930769154	-1.21035917978244
Si	-4.71885114133433	-6.26138813576217	-1.22642959639278
Si	7.96903540184429	0.00011752550028	-1.22077524043027
Si	4.47291557770921	-2.04867060509175	-1.20335666429109
Si	1.14844527277975	-4.00686787646094	-1.19715278401577
Si	-2.36146859374210	-6.04377030101097	-1.22087704235213
Si	9.22599819979171	-2.00116804653702	-1.22359731603639
Si	5.66843490476323	-4.09529458008605	-1.21118044092315
Si	2.34753479268928	-6.04339753575012	-1.20126031901981
Si	-1.19997709666883	-8.10747836802392	-1.21586037518701
Si	8.04040693815661	-4.08200631808468	-1.22019583291913
Si	4.70538161280400	-6.25819748648930	-1.21761405905410
Si	1.19326788189248	-8.10972842120963	-1.21100948014319
Si	1.19216821575598	8.11476728895653	1.19630844034295
Si	-1.20147230876003	8.10791947246781	1.18957377087865
Si	-2.36328224911529	6.04512382993275	1.18364057828900
Si	-4.71960334344921	6.26415850133600	1.19130036269892
Si	-5.66155611056069	4.09028130913041	1.18013292592421
Si	-8.03247992614680	4.07737318632122	1.18429683323954
Si	-9.21008528917068	1.99294098686702	1.18646808114250
Si	2.34807124964441	6.04841641123292	1.20286044127716
Si	-1.19497878555873	3.98705861048606	1.18843552843003
Si	-4.45440246796667	2.05120374393364	1.20121879309234
Si	-7.94260257532915	-0.00002138249779	1.18432634853167
Si	4.70759460615919	6.25787313106351	1.20536946383880
Si	1.15564411490339	4.00298508031097	1.19950605657516
Si	-2.10739973310299	1.81706090527796	1.19997742583486
Si	-5.59054049132695	-0.00029982063530	1.18480516141924
Si	-9.21007666403035	-1.99295309047386	1.18650479702542
Si	-8.03207707702633	-4.07719948397587	1.18440674685992
Si	-4.45372639496180	-2.05142164186716	1.20149476208856
Si	-1.16411202093612	0.00039740747611	2.35200032432932
Si	2.12524098930143	1.85277349631196	1.22149082862216
Si	5.67572452332692	4.09667248749927	1.19152933494265
Si	4.47836658005216	2.05455560247217	1.19632967817377
Si	1.20229403402787	0.00043652200609	2.34281279610194
Si	-2.10676103827847	-1.81639836681580	1.19976089542096
Si	-5.66117311425619	-4.09035286658323	1.18022467034395
Si	8.04690057598807	4.08467870682368	1.18246713997079

Si	9.23004882092297	2.00154098583307	1.18399135385515
Si	5.61919632781658	-0.00023563751483	1.19370305563293
Si	2.12438155415572	-1.85238586336696	1.22135177785723
Si	-1.19525630260276	-3.98688233222782	1.18861454369556
Si	-4.71931158345675	-6.26437688817925	1.19144313464981
Si	7.97227369193190	-0.00007922190528	1.18955263658862
Si	4.47751720803728	-2.05456354601606	1.19617112062586
Si	1.15541540749249	-4.00278496767539	1.19948256900559
Si	-2.36289810408940	-6.04533182314836	1.18362208250349
Si	9.22988330117403	-2.00176641626213	1.18374336344806
Si	5.67507098298187	-4.09657537675950	1.19110181792928
Si	2.34762791979668	-6.04829905600164	1.20258888928123
Si	-1.20131487700260	-8.10828636244439	1.18970148113422
Si	8.04622553324113	-4.08469930024936	1.18197213886811
Si	4.70711848827597	-6.25776754179989	1.20501300178741
Si	1.19233609890495	-8.11505309967314	1.19634495716639
H	-1.77654750512151	9.20664379702814	2.03171707589630
H	-1.76563183100749	9.20908470629720	-2.05897298026317
H	5.31780881929778	7.30189106178478	-2.10113286270661
H	8.71921098805944	5.11645163071717	-2.06648523925136
H	8.71826772834398	-5.11634695974470	-2.06726777084648
H	5.31716594642372	-7.30182058432895	-2.10166710633226
H	1.77144876405411	-9.20309815697560	-2.05768719931395
H	-1.76591258367716	-9.20947976823888	-2.05887177255116
H	-5.33364863291895	-7.30256641689323	-2.11116005598829
H	-8.71511752389225	-5.11473395648039	-2.05859735541341
H	-8.71552829858590	5.11456717999463	-2.05891235149747
H	-5.33404521509072	7.30272252562693	-2.11158559006179
H	-5.33378537278383	7.30157124523404	2.08105321510023
H	-8.71007771171928	5.11155573197612	2.03197680262879
H	-8.70964232705180	-5.11163599737829	2.03202556696168
H	-5.33335107511741	-7.30188570416272	2.08140068112142
H	-1.77644342064935	-9.20658684750368	2.03164323154916
H	1.76024152878661	-9.21641858706058	2.03972334786299
H	5.32728193762836	-7.29903550319940	2.08546130793531
H	8.73102214901960	-5.12050362739093	2.02199309164017
H	8.73133958839116	5.11978046145077	2.02234027700807
H	5.32788592186716	7.29954717069605	2.08593153050421
H	1.77123726754585	9.20316078740198	-2.05764489421172
H	1.75972680446472	9.21600003152698	2.03947163787628
H	10.46173874408578	2.04711547307847	2.03637747788995
H	10.45475719277302	2.04513493540879	-2.08077752641869
H	10.46162534356702	-2.04758039281310	2.03632030007961
H	10.45479629119052	-2.04514234926413	-2.08131064207014

H	-10.43719674703905	2.02820171898334	2.04618541748844
H	-10.43900908374631	2.03175691873926	-2.07840674893227
H	-10.43919022914834	-2.03208363367368	-2.07859151399893
H	-10.43726674524333	-2.02834736167469	2.04645336430393
H	-1.61017850134886	0.00008456146378	3.78258319679694
H	1.68225227800901	0.00031954375433	3.76278972979274

• TS 2Si...H₂ → 2Si-H₂

Si	1.19657130291223	8.09073982666745	-1.19268095083819
Si	-1.19664865096683	8.10331833696556	-1.20511092184270
Si	-2.35572592521098	6.03835524806014	-1.21938887022091
Si	-4.71449994794638	6.24143331009142	-1.21486895299461
Si	-5.67036840645977	4.07235299096742	-1.20300816547407
Si	-8.04031416222193	4.07532319350237	-1.20404878931106
Si	-9.21988292911025	1.99141894844434	-1.21061142025554
Si	2.35411148395958	6.02712582947237	-1.18892969360228
Si	-1.17593066791150	3.98148489332316	-1.21754798924264
Si	-4.44200913118999	2.04907113105343	-1.17578493057841
Si	-7.94764499113076	0.00000040725406	-1.20571880243201
Si	4.70895335614558	6.25708985054332	-1.20795539530272
Si	1.17291547164995	3.98050754799303	-1.20365266600463
Si	-2.08532801885151	1.80123404412412	-1.25670009204390
Si	-5.59330368184922	-0.00000107250490	-1.20746101470896
Si	-9.21987832187533	-1.99142041649685	-1.21062061621472
Si	-8.04030452532260	-4.07532204819105	-1.20406072526039
Si	-4.44200235650375	-2.04906930795987	-1.17577554486990
Si	-1.23346106466709	-0.00000435497818	-2.49201772602345
Si	2.11666994708874	1.83853372944707	-1.24899317412679
Si	5.66244404373904	4.09108549800877	-1.21042751385705
Si	4.46277161921884	2.04711549599043	-1.21939761019268
Si	0.96823791337250	0.00000123496276	-2.00415222726873
Si	-2.08532163744176	-1.80123272359369	-1.25668217662072
Si	-5.67035902621683	-4.07235213360150	-1.20301000768058
Si	8.03418385851855	4.07765729574486	-1.22404257202833
Si	9.21883546716770	1.99698870681922	-1.23033173690157
Si	5.60605103547972	0.00000105793487	-1.21767661391906
Si	2.11666805750666	-1.83853336856736	-1.24899558501024
Si	-1.17592934738344	-3.98148474726070	-1.21752962974460
Si	-4.71449448936231	-6.24143413141526	-1.21486806933542
Si	7.95650569875765	0.00000129968622	-1.23011948332991
Si	4.46277022324853	-2.04711239443008	-1.21939968329540
Si	1.17291650925630	-3.98050797047536	-1.20365530720080
Si	-2.35572072714717	-6.03835615107713	-1.21938703375519

Si	9.21883699370407	-1.99698517055510	-1.23033065477815
Si	5.66244487677591	-4.09108128757073	-1.21043156658333
Si	2.35411372483076	-6.02712521297339	-1.18892729595953
Si	-1.19664246354685	-8.10331877084276	-1.20511064669450
Si	8.03418484203886	-4.07765354226070	-1.22404437050265
Si	4.70895584134645	-6.25708663882666	-1.20795747098129
Si	1.19657737776348	-8.09074137542980	-1.19268074240342
Si	1.19288962675365	8.08746722640532	1.21402992669177
Si	-1.20002400005482	8.09800843896648	1.20099177568962
Si	-2.35612521141063	6.03386111088307	1.18430005426475
Si	-4.71362669163061	6.24653432723613	1.20420611268369
Si	-5.67809051452077	4.08351316790780	1.19868229571127
Si	-8.04916202922631	4.07635254498988	1.19788688501810
Si	-9.23023138374182	1.99362861693707	1.19701847865743
Si	2.35089495499200	6.02071261232015	1.21378577885853
Si	-1.15764459633682	3.99682526943474	1.18065248072164
Si	-4.47047380305362	2.04572406032258	1.23319055779435
Si	-7.96346366013357	-0.00000434413471	1.20244594415350
Si	4.70917901192968	6.24630376630552	1.21370671640770
Si	1.19373556791241	3.95033844326997	1.19606110498107
Si	-2.12716008080559	1.86556536822794	1.19133939359430
Si	-5.61173877889401	-0.00000212967785	1.20479045002510
Si	-9.23023214246634	-1.99363707594185	1.19700930477942
Si	-8.04916172510642	-4.07636017676021	1.19787516109120
Si	-4.47047142761990	-2.04572737881895	1.23319884148585
Si	-0.95880288250954	0.00000201451858	1.96083906905550
Si	2.11198239664312	1.77507095130365	1.24266451657981
Si	5.67080585318165	4.08342750107413	1.19168421327042
Si	4.45711354938036	2.05250597743984	1.17946409018248
Si	1.36652716513105	-0.00000107775146	2.58703097900257
Si	-2.12715617327443	-1.86557097427171	1.19135925626816
Si	-5.67808971307754	-4.08351608816798	1.19868039858957
Si	8.04205387882846	4.07816383882208	1.17757735991555
Si	9.22340930842694	1.99501790982383	1.17720106198744
Si	5.60305044177113	0.00000032321689	1.19216191413255
Si	2.11198071726363	-1.77507165446939	1.24266196988499
Si	-1.15764060147291	-3.99683057205054	1.18066959529289
Si	-4.71362428316829	-6.24653700452971	1.20420705513216
Si	7.95599694865940	0.00000111411710	1.18098581298840
Si	4.45711190935343	-2.05250426805531	1.17946185194234
Si	1.19373978791994	-3.95034073708726	1.19605786588518
Si	-2.35612223362758	-6.03386623770954	1.18430216980287
Si	9.22340802841900	-1.99501639397095	1.17720192687456
Si	5.67080523923777	-4.08342451999093	1.19168004924527

Si	2.35089819250454	-6.02071462599811	1.21378855622760
Si	-1.20002167146565	-8.09801398029812	1.20099218237839
Si	8.04205301818913	-4.07816232869251	1.17757557840912
Si	4.70918239783782	-6.24630234309222	1.21370410774396
Si	1.19289251008839	-8.08746910998576	1.21403022699069
H	-1.777973744469222	9.19095556891637	2.04814078293053
H	-1.75663533406349	9.20833658284003	-2.04868201297878
H	5.30965054083132	7.30783628436817	-2.09152791678353
H	8.70921080966872	5.11291058434594	-2.07223941914373
H	8.70921209296036	-5.11290637134698	-2.07224150523429
H	5.30965093873426	-7.30783297170700	-2.09153160486154
H	1.77761437715458	-9.18747724279816	-2.03284113551967
H	-1.75663081336830	-9.20833434982679	-2.04868419066580
H	-5.34302762042706	-7.27622038180057	-2.09745277249017
H	-8.71659848923273	-5.11284734556572	-2.04804842815308
H	-8.71661237065611	5.11285022223077	-2.04803098809043
H	-5.34303365519401	7.27622018500765	-2.09745240956847
H	-5.31757076460555	7.28782004902849	2.09649324941503
H	-8.72905937873761	5.11176647543388	2.04181841026776
H	-8.72906079400196	-5.11177781417410	2.04180080352037
H	-5.31757054129988	-7.28782213594097	2.09649346916937
H	-1.77796907458782	-9.19096413750254	2.04813901251533
H	1.75999401604095	-9.18639929856634	2.06102796759437
H	5.32273785490105	-7.28852606145389	2.09844553182715
H	8.72512537401696	-5.11541704207939	2.01672654175202
H	8.72512731107782	5.11541774464919	2.01672846973639
H	5.32272972848269	7.28852932845241	2.09844922857258
H	1.77760837041463	9.18747583084917	-2.03284103546369
H	1.75998985411022	9.18639777052090	2.06102798713190
H	10.45536843002275	2.03625348406697	2.03008429831284
H	10.44615814997289	2.04039411317346	-2.08977108483538
H	10.45536647576080	-2.03625209647419	2.03008609055206
H	10.44616042276601	-2.04038977436015	-2.08976900580983
H	-10.46125477659444	2.03135612949715	2.05130743640440
H	-10.44590393233577	2.02792647943014	-2.07202124076218
H	-10.44589739156681	-2.02792969777433	-2.07203305518107
H	-10.46125697613274	-2.03136541419544	2.05129608782958
H	-1.35606352280288	0.00001667932196	3.60432203455191
H	-0.36283363960774	0.00001200332095	3.64659977245726

3.2 CO₂ chemisorption on silicene monoflakes

- Si...CO₂

Si	1.15450000	-7.70790000	0.00310000
Si	-1.01810000	-7.71330000	-0.39600000
Si	-2.14570000	-5.78010000	-0.00710000
Si	-4.34750000	-5.77240000	-0.41420000
Si	-5.46190000	-3.85670000	0.02850000
Si	-7.68550000	-3.83650000	-0.32070000
Si	-8.78150000	-1.92660000	0.16370000
Si	-11.01980000	-1.90470000	-0.14590000
Si	-12.08920000	0.00330000	0.31190000
Si	2.29390000	-5.79650000	-0.45190000
Si	-1.03220000	-3.86350000	-0.53870000
Si	-4.36660000	-1.93240000	-0.50710000
Si	-7.68830000	-0.00510000	-0.36890000
Si	-11.01630000	1.90270000	-0.17280000
Si	4.48010000	-5.77100000	0.02750000
Si	1.17310000	-3.85460000	-0.04720000
Si	-2.13850000	-1.92650000	-0.10800000
Si	-5.45260000	-0.00640000	0.00880000
Si	-8.77790000	1.92570000	0.13590000
Si	-7.68040000	3.82710000	-0.37880000
Si	-4.36680000	1.91280000	-0.53620000
Si	-1.02880000	-0.01510000	-0.64560000
Si	2.30070000	-1.93910000	-0.51950000
Si	5.62750000	-3.87330000	-0.40200000
Si	4.50100000	-1.93770000	0.02010000
Si	1.16980000	-0.01360000	-0.08890000
Si	-2.13650000	1.91250000	-0.16070000
Si	-5.45640000	3.84890000	-0.03190000
Si	7.82270000	-3.84900000	0.09720000
Si	8.95640000	-1.95020000	-0.34340000
Si	5.63010000	-0.02000000	-0.43320000
Si	2.30580000	1.90610000	-0.52680000
Si	-1.01870000	3.84170000	-0.58600000
Si	-4.33450000	5.75350000	-0.50120000
Si	7.83510000	-0.02110000	0.09610000
Si	4.50520000	1.90240000	0.01130000
Si	1.18070000	3.82620000	-0.06980000
Si	-2.13430000	5.76380000	-0.08530000
Si	8.96030000	1.90400000	-0.35120000
Si	5.63530000	3.83430000	-0.41830000

Si	2.30720000	5.76190000	-0.48950000
Si	-0.99870000	7.69070000	-0.48150000
Si	7.83040000	3.80720000	0.07970000
Si	4.49180000	5.73730000	-0.00160000
Si	1.17030000	7.68110000	-0.06220000
Si	11.17230000	1.87950000	0.11140000
Si	11.16850000	-1.92740000	0.11960000
Si	12.27060000	-0.02600000	-0.28650000
H	11.90520000	-3.20150000	-0.13260000
H	13.74840000	-0.02720000	-0.07510000
H	11.91090000	3.15140000	-0.14620000
H	8.57490000	5.07660000	-0.18040000
H	5.23990000	7.01030000	-0.23050000
H	1.93820000	8.94670000	-0.25600000
H	-1.75860000	8.95330000	-0.24060000
H	-5.06650000	7.02280000	-0.20740000
H	-11.73410000	3.17840000	0.12200000
H	-8.40350000	5.09670000	-0.06430000
H	-13.57800000	0.00390000	0.20170000
H	-11.74000000	-3.17450000	0.16750000
H	-8.41130000	-5.10030000	0.01050000
H	-5.08210000	-7.03510000	-0.09960000
H	-1.77900000	-8.97180000	-0.13730000
H	1.91670000	-8.97790000	-0.18480000
H	5.22470000	-7.04770000	-0.19220000
H	8.56420000	-5.12110000	-0.15850000
C	-1.73290000	0.34010000	2.98010000
O	-0.65960000	0.79780000	3.09050000
O	-2.80650000	-0.12160000	2.87890000

- **TS Si...CO₂ → Si-CO₂**

Si	1.09363600	-7.67732600	-0.12362300
Si	-1.07522300	-7.72704300	-0.53118200
Si	-2.19277200	-5.76606400	-0.26244800
Si	-4.40793200	-5.80825100	-0.60125900
Si	-5.48020500	-3.87603500	-0.11896500
Si	-7.72797400	-3.85315100	-0.25796100
Si	-8.74983300	-1.93511400	0.34011000
Si	-11.00874400	-1.91299200	0.32205300
Si	-12.01189400	-0.00519500	0.90958900
Si	2.22391800	-5.78717500	-0.67779000
Si	-1.09336500	-3.90710300	-0.99640800
Si	-4.44482400	-1.95549900	-0.78509400
Si	-7.73300000	-0.01248300	-0.32317600

Si	-11.00669500	1.89667800	0.30647600
Si	4.38563800	-5.73041200	-0.10954500
Si	1.10354900	-3.81454900	-0.46003900
Si	-2.19312500	-1.96245700	-0.59032100
Si	-5.47012700	-0.01320000	-0.20018000
Si	-8.74776200	1.91658600	0.32434500
Si	-7.72390400	3.82862300	-0.28939400
Si	-4.44267000	1.92327400	-0.80053500
Si	-1.10914000	-0.01892000	-1.06077200
Si	2.25588900	-1.93702700	-1.02991900
Si	5.56938300	-3.85263100	-0.50788600
Si	4.38889900	-1.91770900	-0.25635400
Si	1.12242900	-0.01807600	-0.45570300
Si	-2.19103500	1.92928900	-0.60506600
Si	-5.47614200	3.85018300	-0.15007000
Si	7.69362400	-3.82874300	0.23776100
Si	8.88607500	-1.94392600	-0.08118200
Si	5.58627400	-0.02083800	-0.62238100
Si	2.25774500	1.89563900	-1.04350600
Si	-1.08912100	3.86956400	-1.02573500
Si	-4.40172200	5.77739300	-0.64735400
Si	7.70286200	-0.01867600	0.18959300
Si	4.39102300	1.88007800	-0.27071800
Si	1.10755500	3.77880700	-0.48825700
Si	-2.18673500	5.73565800	-0.30739800
Si	8.88810500	1.90300000	-0.09722200
Si	5.57328100	3.81177400	-0.53827900
Si	2.23003800	5.74836500	-0.72219200
Si	-1.06684700	7.69304500	-0.59204400
Si	7.69777500	3.79162000	0.20674700
Si	4.39183500	5.69390200	-0.15401700
Si	1.10187800	7.64426600	-0.18362300
Si	11.01270200	1.88002000	0.67577200
Si	11.01066200	-1.91675000	0.69173700
Si	12.16347000	-0.02007800	0.42553700
H	11.76929300	-3.19544700	0.55176000
H	13.59360700	-0.01904600	0.85440800
H	11.77270000	3.15669100	0.52514300
H	8.44898800	5.07621600	0.06913200
H	5.14211500	6.98455700	-0.20612400
H	1.89107700	8.90891100	-0.26651900
H	-1.81985600	8.93311300	-0.23864400
H	-5.09760900	7.01164000	-0.16881300
H	-11.68095200	3.17018400	0.69709200

H	-8.40783500	5.08340700	0.14959900
H	-13.50192900	-0.00401900	1.00042000
H	-11.68433100	-3.18258200	0.72297600
H	-8.41321600	-5.10361700	0.19117800
H	-5.10485700	-7.03790500	-0.11250300
H	-1.82950100	-8.96326900	-0.16718700
H	1.88140600	-8.94350900	-0.19596200
H	5.13451200	-7.02227100	-0.15076700
H	8.44347100	-5.11522400	0.11072800
C	-0.60128000	-0.00995700	1.62363000
O	0.63794400	-0.01139700	1.48704100
O	-1.51838000	-0.00652600	2.35966100