

Supporting information

Enhancing CO₂ reduction through the catalytic effect of a novel silicon haeckelite-inspired 2D material

Wilmer Esteban Vallejo Narváez,* Cesar Gabriel Vera de la Garza and Serguei Fomine*

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

e-mail: wilmevall@comunidad.unam.mx, fomine@unam.mx

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1. NBO analysis

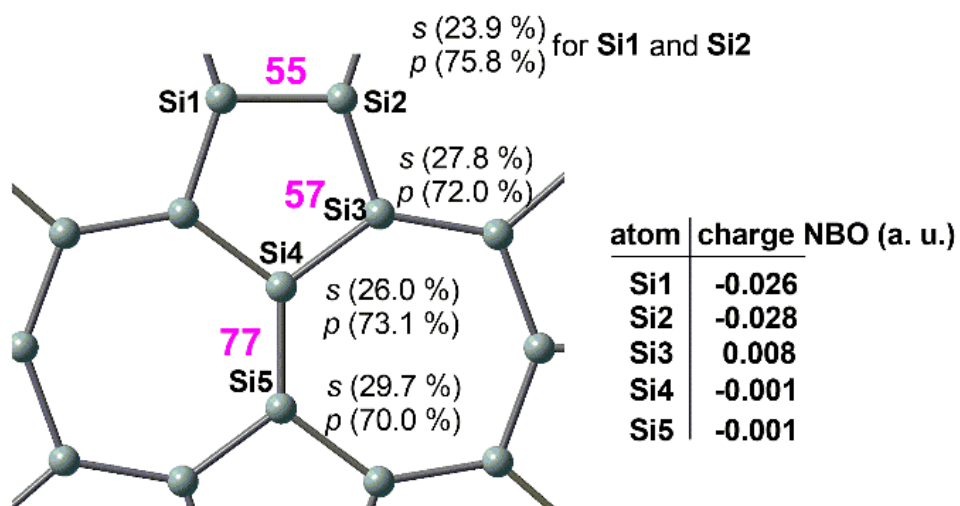


Fig. S1. Percentage of occupation of *s* and *p* orbitals and charges from NBO calculations.

2. Hydrogen absorption on Hck

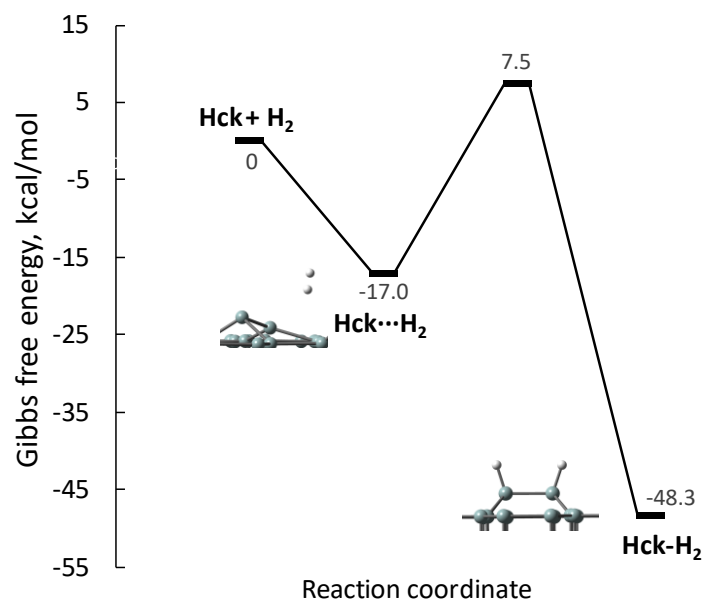


Fig. S2 Calculated energy profile of H₂ chemisorption on **Hck**. This profile corresponds to the addition of H₂ molecule on **55** position in **Hck**.

3. XYZ coordinates

3.1 Mechanism with catalyst (Hck biflake)

- **H₂**

H	0.0000000000000000	0.0000000000000000	0.37864129793633
H	0.0000000000000000	0.0000000000000000	-0.37864129793633

- **H₂O**

O	0.0000000000000000	0.00000000001365	0.12224060626212
H	0.0000000000000000	0.75884092207211	-0.48857330312557
H	0.0000000000000000	-0.75884092208576	-0.48857330313655

- **CO₂**

C	0.00000000003877	-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	-0.0000000336594
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

- **Hck**

Si	27.08323114688093	2.43721144301190	3.28018966612543
Si	26.98463681222304	-2.18965399925175	3.51018307774085
Si	29.33599504487624	3.05847096180957	3.57302441139720
Si	29.21199614360422	-2.86912415391675	3.86697839372672
Si	30.88847727515454	1.27179966701058	3.88814561166848
Si	19.16495296061406	-0.93698808099016	2.25311169833263
Si	21.13177502980807	2.80486739294699	2.35472752606264
Si	21.01842677418641	-2.38340616426839	2.61559543807146
Si	23.40238377220203	2.37739311701166	2.71933166389682
Si	23.30674359838321	-2.02559817031376	2.94083886539168
Si	25.21795557774789	3.90846658195869	2.89843621096469
Si	25.00656720709572	-5.99706455015025	3.39771675024925
Si	24.16147202240585	0.16346222321048	2.93348631376096
Si	25.28078201797687	6.29742068240895	2.78181493471139
Si	25.05528545958131	-3.60834951367248	3.27570086937244
Si	26.47611475340315	0.13141026005426	3.30483422364042
Si	18.99988711378175	-8.27914106199610	2.61189969495890
Si	17.14322829525011	-6.79346946974393	2.25460876303334
Si	14.87173915994319	-7.41846497632571	1.93902357565933
Si	13.10372036769452	-5.82153041674547	1.58544265363602
Si	13.16659499050402	-3.43310760309164	1.46379694953532
Si	11.29666355384375	-1.96035950943745	1.11558375645406
Si	9.04827778835077	-2.58426133918582	0.79565569703070
Si	7.50120924214917	-0.79800326558992	0.45635439396254
Si	7.55366083218502	1.59842845428703	0.33767409115952

Si	9.17385792263315	3.34431474357840	0.50162105451629
Si	11.39656160312041	2.66660346275383	0.88505774964336
Si	11.90460473253789	0.34577326040823	1.07947423112057
Si	14.22304048855918	0.31329909990856	1.43330409041046
Si	15.07371951481186	2.50359442242823	1.45203234305748
Si	13.32962199027637	4.08368089973527	1.08631929113007
Si	13.37788807043909	6.47266646905091	0.96909967414998
Si	15.21728312082641	8.01468477063018	1.16502107065528
Si	17.46040233323128	7.32750393436841	1.54575069617893
Si	19.38270353519372	8.75579564031750	1.75661265386560
Si	21.23969067982867	7.27263838649541	2.12420433510447
Si	20.46050283080272	5.04487387585301	2.12165906896645
Si	18.14261968125154	5.07833658275951	1.75948036450005
Si	17.36168888908528	2.86217923282711	1.77909444520807
Si	19.21511464480976	1.41411484607127	2.13408557064603
Si	23.51316409027911	7.89511873222935	2.42904769002586
Si	30.83674180034884	-1.12465891489875	4.00659372475937
Si	23.16677704153769	-7.53899729953977	3.20234935917062
Si	20.92166383598394	-6.85047817051257	2.83240805944795
Si	20.24191880944430	-4.60073858608778	2.60656583949137
Si	17.92410347905197	-4.56625038352996	2.24400245875545
Si	17.24708172177122	-2.32598160966884	2.03866380008688
Si	14.97633730225176	-1.89970759701794	1.67234762789478
H	29.64474889183680	4.26496118575864	4.40570742045531
H	29.47373178741662	-3.99928110423585	4.81488851948336
H	32.02420496449229	1.73284152697883	4.75504865762694
H	26.03633111903000	-6.57047908117717	4.32714745465410
H	26.33722277968209	6.91332278742666	3.65223977514256
H	18.84205611002008	-9.45704613737773	3.52484566791400
H	14.36539150443395	-8.59107821724568	2.72481754412450
H	11.82798599314410	-6.35941793793699	2.16533284497716
H	8.49041711019978	-3.70459366249073	1.61891808411369
H	6.15312529381352	-1.18340615504077	0.99303263587943
H	6.22457873171118	2.09309089623687	0.83058439191146
H	8.66315430063376	4.56258989006677	1.20810692560132
H	12.12987942273548	7.12514225615205	1.48852173927036
H	14.76609379230095	9.28248977331856	1.82685548136361
H	19.28099588404277	10.02563559071540	2.54594591954036
H	23.78394875703244	9.15182508259289	3.20121361953841
H	31.95614889002926	-1.54409419025944	4.91490916502153
H	23.38426155790723	-8.72354548312983	4.09590723125604
Si	27.44734343155409	2.30875489718707	0.87351410755236
Si	27.34766638537920	-2.31755562697634	1.10358786549897
Si	29.69573222044720	2.93332852479075	1.19155457872295

Si 29.57095179288539	-2.99398045042034	1.48550358947636
Si 31.24393606046259	1.14826017355886	1.53176761683887
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Si 25.41475966167561	-3.73449479622284	0.90216478731027
Si 26.83917783383074	0.00297053072572	0.90987061526332
Si 19.36144142580379	-8.40564708765271	0.23073170005449
Si 17.50377557573451	-6.92313146069318	-0.13501086103967
Si 15.23082079925089	-7.54655637050400	-0.44061579950769
Si 13.46330749684491	-5.94871811642789	-0.79288046681646
Si 13.52660490382354	-3.55976601121793	-0.90974855793119
Si 11.66129318201149	-2.08849145211027	-1.29092872762313
Si 9.40839792753136	-2.70812559638124	-1.58586665764538
Si 7.85556532378241	-0.92167804385740	-1.90013549674123
Si 7.90717925390891	1.47477024135242	-2.01879877906552
Si 9.53325256427788	3.21796942847193	-1.87981564352045
Si 11.76016825892993	2.53831613150676	-1.52118150823137
Si 12.26860815360024	0.21728491536840	-1.31540388919726
Si 14.58366445310865	0.18529724940919	-0.94635714079311
Si 15.43761952815322	2.37444823587670	-0.95245039552576
Si 13.68927305541784	3.95732286219888	-1.28722519837295
Si 13.73761583734976	6.34598136799879	-1.40915712313792
Si 15.57720997832176	7.88806056801612	-1.21438670128376
Si 17.82205435529706	7.19966208373363	-0.84312588420015
Si 19.74440380590523	8.62751321912656	-0.62452017972165
Si 21.60067598373287	7.14205180205341	-0.26492518238779
Si 20.81898646336860	4.91536098382307	-0.25507745445388
Si 18.50088430571450	4.94976715631641	-0.61709912073072
Si 17.72590776921739	2.73197605483916	-0.62697669326017
Si 19.57957509317371	1.28604379317414	-0.26531199270546
Si 23.87257804380157	7.76619660034540	0.04937942994349
Si 31.19119861011910	-1.24820626984753	1.65028072132790
Si 23.52683798725630	-7.66469247128209	0.82292139908479
Si 21.28356454472255	-6.97737147865165	0.44363021848492
Si 20.60015964557895	-4.72891816137894	0.22974497617266
Si 18.28229846067462	-4.69536938237952	-0.13243624575142
Si 17.61255280728042	-2.45523155907366	-0.36624526276991

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H	30.25198345351891	4.05413975444216	0.36789462065603
H	30.08148074097840	-4.21232316455301	0.77902590798650
H	32.59177414683449	1.53326183703471	0.99424317191693
H	26.61448394239190	-6.77576452682692	0.49949813705657
H	26.91643158771334	6.70797078587032	-0.17647273746292
H	19.46318602365771	-9.67594902351650	-0.55781341678116
H	14.96076912452921	-8.80315024931254	-1.21317759770423
H	12.40686520311772	-6.56423994425675	-1.66356920521397
H	9.10003083623929	-3.91477640653327	-2.41843523806690
H	6.72002882072609	-1.38250629576248	-2.76738761971801
H	6.78835988973206	1.89383203708176	-2.92797312811737
H	9.27303910985761	4.34820043550062	-2.82804114620211
H	12.70774672902687	6.91917428277420	-2.33860828866575
H	15.36015855019966	9.07239404008018	-2.10829869684964
H	19.90213001674566	9.80605906676024	-1.53661033957404
H	24.37828357120548	8.93901132003928	-0.73650875393744
H	32.52022931432683	-1.74244798926979	1.15683348582087
H	23.97701910588926	-8.93262134258534	0.16066777845139

- **55 (CO₂ absorbed)**

Si	27.35222470348080	2.35665506734721	2.49890646120138
Si	27.25393224235510	-2.25948939383622	2.74236929121764
Si	29.60839737372243	2.96050740025893	2.80560327742977
Si	29.47478741548984	-2.95231046755750	3.11138863589338
Si	31.16221406090076	1.17665348140867	3.12606943015698
Si	19.47810984505633	-1.08218530896277	1.46304398356395
Si	21.42831599404147	2.71578593918908	1.57320557263495
Si	21.28945774917922	-2.55985325948135	1.87471282229661
Si	23.69638383762276	2.31119114973882	1.94759015200863
Si	23.57307984893087	-2.11570721896970	2.16893959796407
Si	25.50651438835910	3.85054468824858	2.12101171073784
Si	25.30988157964161	-6.05249393952044	2.65599275471359
Si	24.40084577657650	0.09014067567802	2.20427197318927
Si	25.62114220204885	6.23727460321802	1.99980240742458
Si	25.33250372827929	-3.67770113300083	2.52579216876290
Si	26.72691585297437	0.05371566116089	2.52424169566289
Si	19.32656882338763	-8.07089589570671	1.79168521914920
Si	17.59109544428827	-6.46958830179724	1.43614915261063
Si	15.39508936545414	-7.32674853586645	1.19678614036985
Si	13.54420324571517	-5.83959500952478	0.84072814589086
Si	13.64796423929981	-3.46129244788655	0.70995581033506
Si	11.76836917034409	-2.01723556393713	0.35108440926950

Si 9.53286775084364	-2.68877661807133	0.04266033063721
Si 7.95552502884702	-0.93194365606989	-0.30983434566715
Si 7.98748718145138	1.46348148762605	-0.44435342250650
Si 9.58894992475445	3.22711242525475	-0.29185065556288
Si 11.82763191111792	2.59934003015425	0.08857816479081
Si 12.36875696726584	0.28684751566166	0.30149752208898
Si 14.68367182855549	0.27352001565503	0.70323826267838
Si 15.47058576890736	2.48214874806657	0.65496403444713
Si 13.72759607111914	4.05855134599626	0.28390075915821
Si 13.75575625626850	6.44646846564694	0.14899408485844
Si 15.60128772640082	7.97838321709001	0.34159431014640
Si 17.83636410701081	7.27196084151543	0.73143511708978
Si 19.75781537117492	8.69849711545445	0.94367879791123
Si 21.60301756386746	7.20905260819437	1.32848512706771
Si 20.82893883876082	4.97766375484175	1.34056278933876
Si 18.52097314671568	5.02386778759272	0.95289712873208
Si 17.75569013596707	2.80406818888776	0.98669840783760
Si 19.54239208321470	1.27418799385270	1.35445366749358
Si 23.86954666744338	7.84694986267431	1.63409860922815
Si 31.11009669336914	-1.21871365886872	3.24937706870199
Si 23.37821817952951	-7.45431059458137	2.43932202120796
Si 21.20313169131120	-6.61560596802486	2.01370382978100
Si 20.27743162925288	-4.54437883243815	2.40293688868579
Si 18.04713855067379	-4.49705532407060	2.59042139522399
Si 17.68086381663378	-2.62545290479183	1.25923735584877
Si 15.46834323243448	-1.94057867766156	0.89212035009438
Si 27.72802672461971	2.22722697544184	0.09581452047778
Si 27.62126474212902	-2.40370818735042	0.33732241679370
Si 29.97793209896148	2.83764094277064	0.42425099406053
Si 29.83935558125526	-3.09069705903868	0.72784992148071
Si 31.51986876838588	1.04845125063682	0.76942493590206
Si 19.86862901944246	-1.22481827800825	-0.91308426128336
Si 21.80424396373118	2.57677646225254	-0.82805496975204
Si 21.67879094736386	-2.72303254697001	-0.51753188383985
Si 24.07243319221700	2.16929916567131	-0.44935051996386
Si 23.94514043855715	-2.22882843217372	-0.22802179999771
Si 25.87186093421849	3.71310385691363	-0.25335726337730
Si 25.66627804892029	-6.19258719035637	0.27447328153771
Si 24.80262491713153	-0.04028147424744	-0.16962931237256
Si 25.98692578865381	6.09764691613950	-0.37773129587145
Si 25.68339825293166	-3.81029777981552	0.15220738353715
Si 27.13112689192276	-0.08108383780865	0.14067094964253
Si 19.69663595382478	-8.22222318204852	-0.56242725544558
Si 17.91124559121562	-6.68253691404809	-0.94700808926356

Si	15.70955581232874	-7.49813414253549	-1.18047966637837
Si	13.88405523077740	-5.98442509950001	-1.54206251323279
Si	14.00131126009152	-3.60464622748138	-1.66192330115182
Si	12.12793530792054	-2.15950079014831	-2.05729147124326
Si	9.88930650110201	-2.82894837277473	-2.34195801100774
Si	8.31023890716263	-1.06791350951064	-2.66764611003039
Si	8.34286304940050	1.32803947054245	-2.80052756756227
Si	9.94597740973281	3.09339935959152	-2.67360666754002
Si	12.18822609130932	2.46494457232369	-2.31561888939880
Si	12.70578500090684	0.14915891360770	-2.09168900665289
Si	15.01982475611793	0.14085378188327	-1.68161210241074
Si	15.83558108433601	2.33984539619419	-1.74198874739204
Si	14.09053396705073	3.91931527416812	-2.09101912296945
Si	14.12138990878800	6.30656769589197	-2.22775340849904
Si	15.96651373826043	7.84039927421522	-2.03533144450819
Si	18.20500719062301	7.13541273968977	-1.65760041547101
Si	20.12861445879215	8.55913061968322	-1.43437217989926
Si	21.97152762335251	7.06440731612390	-1.06200684938891
Si	21.18693152278398	4.83611600604713	-1.04022611736834
Si	18.87788177358917	4.88235621892404	-1.43049931647591
Si	18.12498348838724	2.65714631654033	-1.41725231092912
Si	19.92088558667970	1.13437850738552	-1.04163209459242
Si	24.23550570987525	7.70619785662269	-0.74274466704984
Si	31.46379879509369	-1.34786483872004	0.89151057404569
Si	23.76087529899748	-7.64349801755815	0.07659130056355
Si	21.59987101148776	-6.78485903335004	-0.36873894619921
Si	21.07963414699998	-4.77952179309522	-1.39768017703885
Si	18.79785690825744	-4.75602649063660	-1.84597512701143
Si	18.02261288992668	-2.70411178277003	-1.13848951829730
Si	15.81138460562120	-2.07040266637109	-1.51382970702360
C	19.79272626121432	-4.79822290607180	-3.57632662971016
O	21.12144747050113	-4.79675627851576	-3.17179044992396
O	19.46524582885539	-4.81598742094607	-4.73197321857133
H	29.91402264760904	4.16764281041912	3.63704124577197
H	29.72494133771747	-4.08361700828514	4.05973926251315
H	32.29623046739038	1.64014643304383	3.99223317890223
H	26.29332033825425	-6.65233350513285	3.61577569958801
H	26.68058972342527	6.83620307774823	2.87654348294088
H	19.15028168427718	-9.19885163790851	2.75690803024858
H	15.00561557481059	-8.49918907523361	2.04425773892800
H	12.29101480131584	-6.37575015854771	1.46606662356852
H	8.99495532267019	-3.81305976992410	0.87230796360082
H	6.61442695775781	-1.32854595207729	0.23354135541678
H	6.65359169409823	1.94886767679423	0.04215069006596

H	9.06304782215356	4.44347677493995	0.40519595696701
H	12.50792808307406	7.09779119319730	0.66708502438559
H	15.16687980542805	9.25186691811584	1.00137494037889
H	19.65575262255314	9.97147510647654	1.72588766419928
H	24.13315088332458	9.10246917176292	2.40844049481122
H	32.22540064077560	-1.64140423192347	4.15956580500307
H	23.41787163514153	-8.63348699177828	3.36143581311842
H	30.54266984283188	3.95826387549793	-0.39231965977344
H	30.35239159194388	-4.31431780996465	0.03438565335149
H	32.86961268020517	1.42726396370992	0.23502553314801
H	26.89211715937600	-6.85791374796158	-0.27582370126412
H	27.27249180660118	6.60739804308750	-0.95826103062043
H	19.79237487616892	-9.47680901212648	-1.37018489903233
H	15.55116575301762	-8.78512043272140	-1.92848210195660
H	12.84672051490602	-6.60150850703280	-2.43202335130137
H	9.59589518451926	-4.04885992893261	-3.15878382425152
H	7.18113160614024	-1.54507609478090	-3.53275346293300
H	7.21893305959812	1.73184519741818	-3.70892826682852
H	9.66206933203653	4.21591134503001	-3.62300356657109
H	13.09753331504132	6.87269650315618	-3.16631653840625
H	15.76441782055455	9.02144469340586	-2.93534986157289
H	20.29950082147341	9.73144601275263	-2.35032428870106
H	24.74003449330137	8.86912900995744	-1.54169745319773
H	32.79147686163304	-1.84383914491638	0.39921436294133
H	24.11138977702685	-8.94267779446312	-0.57920179717990

- **57 (CO₂ absorbed)**

Si	26.91681119608440	2.33650389200618	3.27170987541248
Si	27.03225662572916	-2.29619150319469	3.68155037231144
Si	29.08479432213348	3.16651999857625	3.62313434799268
Si	29.28382764565174	-2.77310705750956	4.19515872004370
Si	30.70973747942317	1.49402335834463	4.11658260637202
Si	19.40530152557026	-0.91972572269092	1.66086570131610
Si	21.07203746574858	2.62415769045198	2.09213739060224
Si	21.23751624873891	-2.33547812075230	2.07299730556797
Si	23.28998555513477	2.04351759067335	2.50322504567016
Si	23.47081753955034	-2.28618637290220	2.80462487667213
Si	25.00396503238535	3.66559828214692	2.73874704249263
Si	25.08522639285006	-6.23279879405919	3.55268955371148
Si	24.25152998432477	-0.08659296768983	2.76911382190555
Si	25.21907247665371	6.03520559228059	2.63964755211379
Si	25.20206922801718	-3.84830108847037	3.37402257889011
Si	26.51755354341371	0.00348968615247	3.35317458632392

Si	19.00787492279472	-8.07876054506472	2.58738216358873
Si	17.21494907965818	-6.56841006544835	2.13154360536010
Si	14.96215312060101	-7.24439931107800	1.86083062828014
Si	13.18556915909051	-5.67359704867635	1.52539923308978
Si	13.29300784877159	-3.29308183179578	1.39897725690611
Si	11.35366086176052	-1.89029622646353	1.17997257619849
Si	9.11954719541692	-2.60593150940783	0.98314022329172
Si	7.49320089416900	-0.87211834251261	0.74399012797464
Si	7.45287918947757	1.52526745241430	0.62950277085887
Si	9.01393020503009	3.32743655084204	0.71213898461828
Si	11.27827708346288	2.73678749997127	0.97785842186509
Si	11.83580020455174	0.43005024343887	1.10208463874968
Si	14.17924854212976	0.45475535858077	1.19816708828071
Si	14.95146658285342	2.66244336967892	1.32161460611919
Si	13.17326399324269	4.21046637514630	1.09004686528713
Si	13.33499481553495	6.59423075206213	1.04933180920451
Si	15.25200585630443	8.03793011239835	1.24913623077118
Si	17.50407996509995	7.31609847672714	1.55365846917596
Si	19.48093788533364	8.67159626951078	1.77153442499447
Si	21.29885414009924	7.13088286317863	2.02811154090287
Si	20.53014345273269	4.90229518974456	1.94811716900596
Si	18.20711572954503	5.06275486141630	1.63723090010005
Si	17.25153039974437	2.91792722788246	1.58141600174187
Si	19.07588872785491	1.39859364564316	1.85233245459413
Si	23.56927157627790	7.73945008078840	2.30632349275828
Si	30.76055917270406	-0.89608937247649	4.36015780507754
Si	23.13839081381855	-7.60225246616215	3.25716921160770
Si	20.99216780220795	-6.73684654428413	2.72539513497821
Si	20.35782673017684	-4.51693530090197	2.22534843959421
Si	18.03815828506387	-4.38280156235210	1.93413189220388
Si	17.37561359469434	-2.16023850550267	1.63647796937326
Si	15.07794044543483	-1.70443757649913	1.43488766825300
Si	27.35474850493292	2.13565348585615	0.88467739019210
Si	27.57341153851535	-2.45695790764436	1.30839290193299
Si	29.54751193304987	2.91236302217952	1.26874855943590
Si	29.81268646653877	-2.94971464739304	1.85185944189800
Si	31.20203649709433	1.27041900632943	1.79164251843641
Si	19.31182759900371	-0.86255398609532	-0.79670363902995
Si	21.42265033270263	2.52614178943655	-0.30624186710542
Si	21.91077106266641	-2.87544856288474	-0.20501430973399
Si	23.68209416042664	1.89325907512805	0.08702446628031
Si	24.07211603941436	-2.60539264661122	0.49081845700007
Si	25.43957477409076	3.50284338062715	0.38258385599163
Si	25.56811388298005	-6.43542166892110	1.19748354619411

Si	24.56505891896389	-0.30101885662360	0.39039801826379
Si	25.57859392861285	5.89362863726764	0.26284784768835
Si	25.82156489057036	-4.06519102912925	1.06258231009762
Si	26.84826112107656	-0.19512627725726	0.95195975792252
Si	19.37688416853599	-8.39685957646957	0.22086487159697
Si	17.60193116875762	-6.82222014069542	-0.24650179720274
Si	15.30616727307049	-7.39893219535602	-0.51991398653223
Si	13.50656421264628	-5.81619292873593	-0.85928341920390
Si	13.48746932557084	-3.42751904917558	-0.99084851805353
Si	11.58139677425293	-1.98777224502633	-1.24554015519674
Si	9.34343025328015	-2.70071087535266	-1.41664847070806
Si	7.70861193845214	-0.97829127001333	-1.63103802486209
Si	7.68853440774737	1.41763068327978	-1.74243526322575
Si	9.26264235934898	3.21250193089542	-1.68150168718450
Si	11.54045085996387	2.64348264109345	-1.44499641106244
Si	12.15846555261752	0.33426319831453	-1.30380735960562
Si	14.50261019369831	0.34815075119708	-1.18634147832444
Si	15.22060316213985	2.59017609796794	-1.09967434705479
Si	13.42536510006614	4.14085759861704	-1.30176834815540
Si	13.62037982823304	6.53195125145844	-1.34113079278684
Si	15.54799001149782	7.97655860072708	-1.14309361339958
Si	17.81164668946104	7.28833315130609	-0.83982090749941
Si	19.79587720364399	8.63391186283436	-0.62233869194670
Si	21.60722933859296	7.06760095253492	-0.37383183027805
Si	20.82884238733070	4.82954722967563	-0.43545258278873
Si	18.50653844112183	5.04847882971531	-0.75979476618671
Si	17.50989271637680	2.95120022744280	-0.84092694877835
Si	19.28707611404101	1.44361400309109	-0.55807153361073
Si	23.90031251413536	7.59945642729837	-0.07649522055103
Si	31.30990288042058	-1.10933902883178	2.04782531235510
Si	23.60409301152034	-7.82267802111358	0.90124914109107
Si	21.38866124627944	-7.08788280659234	0.37318338160561
Si	20.75850058895105	-4.87117959762569	-0.12122756159016
Si	18.43290180998835	-4.60418841208457	-0.41904714345761
Si	17.55538924738053	-2.41361740890259	-0.77302014234441
Si	15.28308291462425	-1.87610535122359	-0.98172295938583
H	29.25478556484786	4.44355989910466	4.38571700756229
H	29.59060295004803	-3.84003809071514	5.19967418675920
H	31.77564057826881	2.03905556239464	5.02084766859618
H	26.01886349490881	-6.84310867601317	4.55471717966916
H	26.32732349799391	6.52520871989789	3.52384283425504
H	18.80905507359488	-9.19196183516638	3.56965944025999
H	14.52700821180131	-8.42226376121970	2.67818154687642
H	11.91051903557347	-6.17856497481265	2.13232961037279

H	8.64826354896702	-3.75010284030518	1.82601079661006
H	6.19595930010955	-1.30705845253505	1.35985291746931
H	6.13297347907458	1.96726162196701	1.18956945093186
H	8.50675569995820	4.53063005733516	1.44432336680835
H	12.12941988458070	7.28246493408628	1.61734612253827
H	14.85842602114961	9.31063572797195	1.93656196108931
H	19.45530392449575	9.91109920663386	2.61268892183969
H	23.86438800242776	8.98037951331950	3.09195007955750
H	31.82928190477949	-1.20616234291806	5.36713669090871
H	23.16046484118838	-8.79667554325508	4.16171763391401
H	30.07269838641304	4.01052472765355	0.39668956792883
H	30.41509678244299	-4.16349550599705	1.21602310187475
H	32.54074060517495	1.73918566908346	1.30223859079112
H	26.76572800385794	-7.22636876288165	0.76158007545011
H	26.87131243402363	6.39303062816431	-0.31316968582678
H	19.39857201944568	-9.71907503696300	-0.48443283598821
H	14.99743077417922	-8.65440399647793	-1.27940867465712
H	12.45920215091512	-6.48459728052774	-1.70076346844021
H	9.05078857279002	-3.91583569777220	-2.24076811538378
H	6.53881750239622	-1.47202518943288	-2.43012055857578
H	6.51312257329225	1.81300384956136	-2.58713042357694
H	8.91150112608439	4.33154779950087	-2.61205586070904
H	12.60435452474283	7.21391264215537	-2.20928043442591
H	15.32656114207601	9.20733423457462	-1.97015884047724
H	19.96015171421690	9.84624424918830	-1.48674358448837
H	24.47165177595559	8.73436202065613	-0.87130303006223
H	32.70210512441719	-1.53750250691924	1.68858058421099
H	24.04597865171336	-9.13470552062040	0.32500418753459
C	21.67430395527107	-1.87474781843730	-1.84819330356921
O	20.53201441907748	-1.15273640915208	-1.99161488177534
O	22.50289682630759	-1.91941195980389	-2.73149488919349

- **77 (CO₂ absorbed)**

Si	26.84737138820347	2.41903898464903	3.18388435876663
Si	26.76372196715653	-2.17047114348667	3.41522334769544
Si	29.08958674594044	3.05334054952429	3.50676802783417
Si	28.98316154324522	-2.84864522559793	3.80039889585395
Si	30.65449308523202	1.28511641561571	3.85733570892285
Si	19.25092063873273	-0.98930943487785	1.71180422186297
Si	21.05679667709687	2.93695298008534	1.97807287078749
Si	20.94633512697731	-2.56393142554895	2.30252593532025
Si	23.26019569101158	2.36476687854135	2.45768872626568
Si	23.17820238233835	-2.05027329823960	2.69324648158105

Si	25.01540976416739	3.90983665933762	2.78718351418453
Si	24.90985551481176	-5.98491526159520	3.45185446652678
Si	23.98373587699155	0.14626518228990	2.63468428042988
Si	25.17264121707367	6.28541852817202	2.83380853652925
Si	24.87458933934982	-3.62076050015391	3.17083838668969
Si	26.27208824549395	0.12713735914733	3.16311608807071
Si	18.93205268944617	-8.44030909421551	2.96844582048771
Si	17.10057511998483	-6.96196468608737	2.45256925852654
Si	14.80157250020467	-7.50121033487981	2.14815731761832
Si	13.16050416749667	-5.81536082985073	1.66920028492965
Si	13.35639005604001	-3.45533171120130	1.42390394014152
Si	11.52421873008482	-1.94848069511920	1.10166172724312
Si	9.27154631161149	-2.56193270796136	0.81459663665667
Si	7.71858620074587	-0.77662045264525	0.50875108353639
Si	7.78780344842234	1.61975154780780	0.39399667344880
Si	9.43596963299500	3.34189017892383	0.52507247337089
Si	11.65469855767361	2.64086670507765	0.87169035073977
Si	12.13532511585368	0.33243191460045	1.01363189667980
Si	14.47678199757538	0.27882291534412	1.18884127462476
Si	15.29636336576023	2.46882599127195	1.24029759295495
Si	13.56994599852115	4.06879929605948	1.03992177472750
Si	13.44595176806819	6.44586222238058	1.04593552355846
Si	15.14320675250549	8.11301290807694	1.35629082488814
Si	17.41433640235641	7.49934632483497	1.71273840329094
Si	19.31123000684306	8.93427295476108	2.09885951459968
Si	21.20568515395767	7.45808548349442	2.29442931739762
Si	20.46431539808198	5.22707787856389	2.00441611706512
Si	18.15489642374986	5.24933370374327	1.64282827727043
Si	17.56164517928023	2.97056560867132	1.42873088723249
Si	19.32407092173520	1.36072014358410	1.51385395927898
Si	23.49966359496128	7.99567143529178	2.63292377141462
Si	30.60990869361963	-1.11157026803651	3.97505033445118
Si	23.15532688846356	-7.62386713346321	3.41615624403230
Si	20.88338613855112	-7.02756749237843	3.02696575707914
Si	20.24290092272444	-4.80313510415614	2.53676245376807
Si	17.93190538092835	-4.76333178117819	2.17289174277637
Si	17.40110961904061	-2.50126318784634	1.76327170233149
Si	15.16550157041821	-1.93941700061652	1.46938957909278
Si	27.22851335439636	2.30652540124917	0.77877137751877
Si	27.13500838112851	-2.31667256334198	1.00997214685393
Si	29.48071556559360	2.91019139473483	1.13067687830115
Si	29.36823485416356	-2.95535630865977	1.42182638659156
Si	31.05479675915615	1.15950440685751	1.50609423432977
Si	19.59166039428575	-1.59337402047728	-0.61570029876285

Si	21.52837045290577	3.14796355273968	-0.39582543386444
Si	21.37059795049568	-2.99870610582681	-0.04843702843561
Si	23.67287388722139	2.33532026943281	0.06445190960463
Si	23.56879479167556	-2.27654371336249	0.30306627780464
Si	25.44442902964198	3.88830686723813	0.42156510637151
Si	25.25583029806607	-6.25206182306944	1.08378049706439
Si	24.22830262955814	0.01798637925063	0.24196830193084
Si	25.52769784158073	6.30184522823002	0.45156581930509
Si	25.28431297948171	-3.85201867719566	0.81233513062880
Si	26.53636431488822	-0.00054162526913	0.75017632273184
Si	19.28409858089091	-8.82957640745984	0.61446911990876
Si	17.46923941887121	-7.34283935411913	0.08947249306889
Si	15.16176472350155	-7.80089566421317	-0.21390741878974
Si	13.52452349276562	-6.08357902258397	-0.69606538299473
Si	13.65661929102681	-3.68642200982427	-0.95112672512196
Si	11.87478374688945	-2.09747280115580	-1.30682928471592
Si	9.60173466438881	-2.66885243304992	-1.57237977922953
Si	8.02959369652476	-0.89730027277008	-1.85584127488511
Si	8.09056363352032	1.49518287667515	-1.97157913526959
Si	9.75585397838339	3.19774315577521	-1.86188198424633
Si	11.99299268928350	2.52595689258833	-1.53865715883776
Si	12.59255089162317	0.19924020448917	-1.36873450190843
Si	14.94721791686922	0.14428952734040	-1.16971832787739
Si	15.60585687553961	2.44107748308980	-1.16809143050837
Si	13.85284368057828	4.04791570557251	-1.34773665545991
Si	13.81357492450435	6.46166730433075	-1.33447485990201
Si	15.51125921192272	8.16085621190565	-1.02322712936007
Si	17.79853313226101	7.64047232416780	-0.67413508643815
Si	19.67674309397090	9.08966944102939	-0.27854656846152
Si	21.55443539956788	7.59911963011226	-0.09625832932959
Si	20.83491220474909	5.38024972800100	-0.36614761612075
Si	18.51083268080009	5.40193697346939	-0.72938967738770
Si	17.81783158958469	3.18091642041442	-0.97795089409342
Si	19.69119285628662	1.79309665660952	-0.87965426604812
Si	23.85829553838566	8.04600855291692	0.25195143682728
Si	31.00534797725963	-1.23278557906897	1.62343722389474
Si	23.50430752089103	-7.92398485279023	1.05231833778685
Si	21.22261430430213	-7.40754763084146	0.65944530760084
Si	20.59750556571026	-5.19412406726370	0.18397885617605
Si	18.27964969369156	-5.15525869581383	-0.18123202962737
Si	17.68060271303628	-2.93595290277715	-0.60916187347443
Si	15.49385599191427	-2.16645130443050	-0.92742332233623
H	29.37322660907362	4.27197471547515	4.32904951623641
H	29.22335003900202	-3.98955560061757	4.73967102320152

H	31.76524090400214	1.75558096140736	4.74951209572113
H	25.99964186289986	-6.42061685642680	4.38597713016837
H	26.28569542331330	6.75306915672838	3.72394188789971
H	18.75785568541474	-9.52228686000976	3.98985600598315
H	14.22532105577331	-8.58714426673266	3.00467227934587
H	11.83073867293381	-6.21052662752214	2.23958058049029
H	8.73357583703535	-3.69178638395007	1.63643621267351
H	6.38176235385108	-1.15540969562791	1.07476551905438
H	6.47809254513124	2.12786314430599	0.92109003940205
H	8.95729692872015	4.57245858943660	1.23094198057163
H	12.12912299516908	6.93477322353574	1.57194543413660
H	14.61284401489971	9.29921277578514	2.10201574804189
H	19.18109570056709	10.11032897841258	3.01686371278087
H	23.81992807976485	9.17007556868750	3.50647439305215
H	31.70884300038217	-1.53050628834244	4.90669299296599
H	23.42587453956614	-8.72141221860669	4.39971276026511
H	30.03621563153255	4.03311172617730	0.31069300963064
H	29.88576389461328	-4.17170918356008	0.71851946175735
H	32.40432164072684	1.56092931867403	0.98798242874062
H	26.52193681884257	-6.91327030375451	0.62276260947270
H	26.82279227159301	6.85400912589530	-0.06879776872458
H	19.35662077026273	-10.18069367421935	-0.02676904581565
H	14.78919977476632	-9.07431940652835	-0.91079266010857
H	12.43622171078355	-6.70977191313831	-1.51828921691588
H	9.27789914802184	-3.87207120897086	-2.40276665807432
H	6.88309182914511	-1.36420678176354	-2.70345694551969
H	6.96384712857299	1.93444062907722	-2.85954055345224
H	9.49841923424952	4.33166602910492	-2.80531341008998
H	12.74760271542090	7.04238793465230	-2.21715954795628
H	15.18507048348521	9.36857524491999	-1.84852263554538
H	19.80714078071983	10.37348408736390	-1.03813881926244
H	24.44981264285889	9.24301634274697	-0.42883546063582
H	32.33674833300154	-1.73708570385015	1.15001767758671
H	24.03387629399027	-9.20970633439365	0.49322954856904
C	19.86831420010116	-0.61403034442520	-2.25921459694891
O	20.01344489539563	-1.22505538871215	-3.29580306969801
O	19.90243121915376	0.74185181519565	-2.22928818234895

- **55 (H₂ absorbed)**

Si	26.93120699307554	2.47773298491933	3.23210786745658
Si	26.85300035450829	-2.13681017426124	3.47942092484709
Si	29.17426487263170	3.12537371796821	3.53966832294593
Si	29.08515946420564	-2.78622780589573	3.85633552674371

Si	30.74553470136918	1.35827486686688	3.87454684913190
Si	19.15394301650216	-0.85265379897704	2.20974615775802
Si	21.01200172427455	3.03471574476888	2.22394328235192
Si	20.94754491786903	-2.37833451011273	2.57026761087091
Si	23.23780460407800	2.42580232983311	2.63367835890479
Si	23.22415477704265	-2.00514474080289	2.88918692396409
Si	25.06832006675014	3.93457682221606	2.82205377376008
Si	24.97512051720979	-5.98298618992741	3.38661732181342
Si	24.00575570989416	0.20690438096661	2.85839943622943
Si	25.18067790204324	6.31174108337946	2.71977313622397
Si	24.95667844118361	-3.59476776425042	3.24442204758636
Si	26.32200301516067	0.17683921919546	3.25869642544782
Si	19.01422083594384	-8.31337261684981	2.61714625493453
Si	17.15808779222437	-6.82985185759582	2.25953596137677
Si	14.88539196431932	-7.45150293946372	1.94842795494812
Si	13.13290294811697	-5.83985387696129	1.59439157737173
Si	13.23817534575914	-3.45211638044955	1.47292990039795
Si	11.41601032518018	-1.92169508907754	1.12493444916681
Si	9.14916404200659	-2.48110218663964	0.80876056462713
Si	7.62585907794050	-0.67532902322325	0.46570084804302
Si	7.70855634829185	1.71923613144634	0.34103419095614
Si	9.36869420494423	3.42651739373912	0.50669642387554
Si	11.57131728118189	2.68804867050442	0.88782933801980
Si	12.06957373564972	0.37127587641620	1.08026573342954
Si	14.39752072146698	0.32237422486355	1.42306082323279
Si	15.26109644424498	2.51830226975005	1.47866812127318
Si	13.51238078798463	4.07636873294152	1.08403557964154
Si	13.49200575701767	6.45482230087688	0.95412047824913
Si	15.42329990818847	7.85262068513668	1.17423228058728
Si	17.55499899837367	6.91583414021804	1.55517359980959
Si	19.34415919598121	8.47598149963476	1.69821585255878
Si	21.11970666141822	6.93293341323142	2.06819095446758
Si	20.33135072939035	5.04890688467601	3.21083155521010
Si	17.97804858804709	5.08609338073079	2.94244996370925
Si	17.49597461533071	3.13109501992447	1.75735031614395
Si	19.20194041036358	1.50971541864747	2.03656528314151
Si	23.31763445562825	7.77428896994159	2.33177817287838
Si	30.70352928142814	-1.03738710385262	4.00130222907814
Si	23.16818968649257	-7.55968741427328	3.19831893703385
Si	20.92587742563716	-6.87391981198450	2.82643178343625
Si	20.24997475879600	-4.62272082069738	2.58821984003429
Si	17.93581757143354	-4.60076596069406	2.23447939334554
Si	17.30761859712693	-2.34800162922929	2.02608855145034
Si	15.04644050348128	-1.92116843411113	1.66719277241701

H	29.47248055204442	4.34227972456645	4.35964110622034
H	29.34940895485824	-3.91332592887728	4.80606506102035
H	31.86749273824524	1.83194021286062	4.75086738950961
H	26.01775507853672	-6.51839729895365	4.32274429609612
H	26.18615928357068	6.94495118838705	3.63443058205413
H	18.86639441567205	-9.48778508161088	3.53443864056348
H	14.38140844260474	-8.61847501694167	2.74217461130698
H	11.85200020165768	-6.36009289057923	2.17654187917771
H	8.56925140348964	-3.59080763963683	1.63015231076944
H	6.27423888033245	-1.04380888362925	1.00322998039219
H	6.38913009617226	2.23571818518276	0.83495408574736
H	8.88503031262370	4.65829131566379	1.20743076255197
H	12.26567258964183	7.11373567573710	1.51237664012863
H	15.13366504878888	9.13621480311890	1.88920994490880
H	19.23024897417769	9.71139334420080	2.53415929883443
H	23.44875984049212	9.05951168500258	3.08931789125238
H	31.81713422166340	-1.44877849865510	4.91887161546740
H	23.38985163975864	-8.73317006535293	4.10346959752082
Si	27.31513549490937	2.33574520108565	0.83076413597746
Si	27.22970565865397	-2.27419111806098	1.07799880292962
Si	29.55354507884596	2.98925442769205	1.15731453378066
Si	29.45998720585720	-2.91940599978293	1.47650133789031
Si	31.12111895630580	1.22603481305298	1.51932247717015
Si	19.50698217293852	-0.99728876926783	-0.18629831690343
Si	21.39549367554526	2.82587983666711	-0.17883457289340
Si	21.31205015166468	-2.51728481887743	0.16597180190531
Si	23.63540269836999	2.29278938070782	0.24755150198278
Si	23.59270586534670	-2.14780404538563	0.48834932506987
Si	25.45795135478483	3.80469140298004	0.45642744915337
Si	25.34241942715259	-6.12031567272675	1.00951263971376
Si	24.37402439144304	0.06442055190687	0.48415280323669
Si	25.57399279579890	6.17737915193307	0.34398579152211
Si	25.32739654476437	-3.73130864642696	0.87101646782781
Si	26.69307094596307	0.03772606537103	0.87059281011648
Si	19.37325811938294	-8.45175031404287	0.23833917851957
Si	17.51611117203302	-6.97124381048872	-0.13293810783183
Si	15.24057274118253	-7.58926728534754	-0.42943247374192
Si	13.49002664535917	-5.97494348213501	-0.78403610682310
Si	13.59264186297978	-3.58663454337987	-0.90348159673342
Si	11.77224765893141	-2.05920029484226	-1.27992777112724
Si	9.50276560758820	-2.61839315438745	-1.57357382843046
Si	7.97714371680551	-0.80990104398175	-1.89176810577272
Si	8.06287114421945	1.58488116000856	-2.01681789315789
Si	9.72707304951896	3.29151616895891	-1.87885944745362

Si	11.93465821863084	2.55502382527991	-1.51922049905452
Si	12.42286793037228	0.23396076317507	-1.30917303178337
Si	14.74636453955775	0.18411437047579	-0.95600141475727
Si	15.62409172484206	2.37152080798432	-0.92042655677859
Si	13.87787563803439	3.94291843487357	-1.28687727428137
Si	13.86994704963630	6.32446440691067	-1.42309296203864
Si	15.79837486886681	7.73204583947037	-1.19438585173882
Si	17.92499426563733	6.75792306548179	-0.82658704385469
Si	19.69753840464733	8.33961566198492	-0.65243902924638
Si	21.49498633144711	6.81976367734939	-0.32431524765280
Si	20.66861166679960	4.80509062272729	-1.06379085049038
Si	18.59596857001817	4.81544318622101	-1.93992374614784
Si	17.86180965351759	3.01973657019890	-0.64303000381497
Si	19.54047552021247	1.36173855969178	-0.33745834495411
Si	23.70030630224965	7.62014112525980	-0.03073492734508
Si	31.07498262384095	-1.16916007083970	1.64698753167797
Si	23.53027592644859	-7.69304354437710	0.82122041228049
Si	21.28760337423418	-7.01249743732522	0.43432985324258
Si	20.60667634578120	-4.76135441161633	0.20696932964559
Si	18.29214172043741	-4.74192820784508	-0.14859597134685
Si	17.66362725809274	-2.49136137830186	-0.37742542478480
Si	15.40279555986890	-2.05732568423462	-0.72971148126105
H	30.10506391145635	4.11454240532532	0.33782302037110
H	29.98604233996634	-4.13811790928857	0.78363256602403
H	32.46822040933012	1.61865651051718	0.98817672929649
H	26.60530628242483	-6.74708378852009	0.49725417861111
H	26.81998581375669	6.73824135349171	-0.27353891789043
H	19.47609542048815	-9.72562998458855	-0.54230978331439
H	14.96729810992735	-8.84567826687132	-1.19926204468584
H	12.42634942916382	-6.57776092208346	-1.65315654000485
H	9.16599143553791	-3.82290561553774	-2.39711080500584
H	6.83371831390186	-1.25611016313546	-2.75495926986722
H	6.95436791415214	2.02088439723820	-2.92930340128278
H	9.48320741499614	4.42894905324306	-2.82175604742760
H	12.87429472782089	6.89060555402728	-2.39137423853368
H	15.71901920105714	8.92969086404911	-2.09099584062377
H	19.83233194483341	9.46651413009637	-1.62394427588370
H	24.04361960339804	8.80586913114378	-0.87840418491879
H	32.40853534552125	-1.66155596075909	1.16675318280624
H	23.99065931868631	-8.95519677826636	0.15739167522904
H	17.24331111025533	5.15143256238963	4.24523488911386
H	20.75800005228152	5.06047480980785	4.64704128214097

- 57 (H₂ absorbed)

Si 26.99370660175667	2.42598886008292	3.27399079352754
Si 26.80823267070253	-2.24246042705125	3.48048795582200
Si 29.25895595694686	2.98319319208761	3.58324411568200
Si 29.00461141889935	-3.00080403530151	3.84433855322587
Si 30.73721930402835	1.13145615420640	3.89703904698184
Si 19.00619117378625	-0.79207896155172	3.30551798907160
Si 21.02214446700639	2.60578878662477	2.27589809398959
Si 20.80501530849775	-2.12309526472071	2.55012219372489
Si 23.32168447058112	2.34098267517576	2.64559504131494
Si 23.11806229447394	-1.93286029361262	2.87061397312124
Si 25.13182520942305	3.88476900220010	2.86767270876488
Si 24.94210028496682	-5.93995896332383	3.34556311884728
Si 24.15739161644537	0.16638922567981	2.81389696111259
Si 25.28246150549356	6.26394131345926	2.77118452286594
Si 24.83168833000316	-3.56840987640644	3.20290572186759
Si 26.44855096464175	0.10407974247665	3.28543072842750
Si 18.97862246160708	-7.99263870776615	2.56684857776381
Si 17.17989998470297	-6.45757845840045	2.23557873105116
Si 14.96627129576444	-7.21379755496509	1.92154617938416
Si 13.25012178021801	-5.58336003433592	1.57187818015189
Si 13.51003391986874	-3.22181636688752	1.47627487573797
Si 11.51749108931511	-1.95400395313374	1.09973066187919
Si 9.33399829000125	-2.78012218671936	0.81736864186699
Si 7.70136578952906	-1.06928517247676	0.47983045551038
Si 7.65386225725236	1.32897811436019	0.35511333278012
Si 9.15687376244144	3.18137446390021	0.49513352161205
Si 11.42966521383292	2.66954421046619	0.85453574450646
Si 11.99544439821610	0.36244501778220	1.04184747211047
Si 14.29779070251194	0.35634797846290	1.48006284231412
Si 15.09681896066591	2.55043202907958	1.40205724644800
Si 13.33595625349353	4.11655675380826	1.06836868928217
Si 13.39438285094620	6.50366385929124	0.95695210482442
Si 15.26813512394817	7.99604516215879	1.16895988302612
Si 17.49294164198517	7.24393812107612	1.54193280408288
Si 19.43670684289100	8.63813342577703	1.76815607012163
Si 21.27187140072853	7.13275737598416	2.11789124428091
Si 20.49643357798800	4.89665565416196	2.08650424340946
Si 18.18763218966567	4.99799663757296	1.74317977383710
Si 17.38777886563421	2.79795714421598	1.74528074765962
Si 19.11363181814280	1.18498795448391	2.04610202940074
Si 23.51230908933471	7.84940788113425	2.41657002192734
Si 30.64157026697091	-1.26706020752713	4.00138160896907

Si	23.09845457665507	-7.45528516635406	3.14155617287250
Si	20.91227805104326	-6.61160838627523	2.78349373917620
Si	20.18853295508881	-4.38208398697296	2.49485996448213
Si	17.86017500131119	-4.21059665933551	2.22823348293772
Si	17.09081619179764	-2.21190321993524	3.17948302425620
Si	15.35649760879705	-1.73102942580007	1.69363743380487
H	29.61195080344215	4.17136046812336	4.42324366350937
H	29.24808943205826	-4.14039923025422	4.78443105780371
H	31.88354682604941	1.55091665249670	4.77001127523381
H	25.96988626300303	-6.45686504687938	4.30708883116335
H	26.33385046494224	6.84440005460559	3.66924029664045
H	18.78777638532137	-9.16045093804089	3.48533867362087
H	14.49802809802102	-8.36487147254681	2.75927693808565
H	11.95280409489921	-6.00265753167875	2.19786053089433
H	8.85302396434865	-3.92254767792964	1.65732834061829
H	6.37272089642208	-1.50518795997955	1.02414414158500
H	6.29904704296960	1.75450664283312	0.84093544623023
H	8.56677249677375	4.36653530344757	1.19471738001785
H	12.15950267078586	7.16741195921035	1.49011482258811
H	14.85666978803315	9.26888404183894	1.84496061105895
H	19.36041140184752	9.90062000003418	2.57059298508752
H	23.73921885989533	9.10522879712109	3.20183456520635
H	31.75298207553188	-1.70062140526847	4.91167595069572
H	23.25556577511629	-8.64556657186265	4.03836338125574
Si	27.36822090012555	2.29520594656616	0.87166986201767
Si	27.17529713313985	-2.35904484445974	1.07748886703089
Si	29.63118057686593	2.85468427800748	1.20234162106600
Si	29.37239726488329	-3.10997122843555	1.46049448615730
Si	31.11347450531166	1.01368694819800	1.54424415629095
Si	19.41095243859330	-1.13680364199816	-0.87523086606535
Si	21.40140664061545	2.51033429648916	-0.11097899444567
Si	21.17313991551606	-2.26881856955559	0.11966125660283
Si	23.69522326052934	2.23771605610567	0.26023678155716
Si	23.48032710866075	-2.05441526425153	0.48015531705232
Si	25.51449415393438	3.76871387612521	0.49221825237338
Si	25.30534650535237	-6.06200499444593	0.96259829606423
Si	24.48331875391984	0.05192007561045	0.40152688511350
Si	25.65280864073225	6.14831037867964	0.39470719291757
Si	25.19784001147054	-3.69013365820191	0.83351757641603
Si	26.76470847399862	-0.01710994886623	0.89083108723637
Si	19.32873601525226	-8.11497338634248	0.18171959995384
Si	17.54533686274953	-6.56164750303139	-0.14856434701878
Si	15.33279923896765	-7.33110572922379	-0.45549400254797
Si	13.60493423413092	-5.71057251142828	-0.80399274323702

Si	13.85531463525309	-3.34706397163743	-0.89147162315881
Si	11.86868559372729	-2.08341985016291	-1.30960858425517
Si	9.68020261365427	-2.90004432015327	-1.57219076302163
Si	8.04575509183701	-1.18487729774070	-1.87911994938713
Si	7.99674390107995	1.21357346175923	-2.00302981388918
Si	9.50042004005191	3.06820403004287	-1.89014225068726
Si	11.77532871728486	2.55296385547838	-1.54972721220926
Si	12.31510943086953	0.24132804161727	-1.35073037916008
Si	14.61880402630022	0.23505707243640	-0.90974810732275
Si	15.43919611742734	2.42563035450613	-0.98150093466477
Si	13.68516907154363	3.99701373201673	-1.31669182951090
Si	13.75441484370439	6.38532059383841	-1.42278291784607
Si	15.62595992180689	7.88293384019002	-1.21194640539301
Si	17.85333653966556	7.13647875884244	-0.84567581031783
Si	19.79708925611371	8.53256509363950	-0.61589296395960
Si	21.63229592248080	7.02400757575114	-0.27787118275863
Si	20.84710741799521	4.79183350408663	-0.28998498067336
Si	18.53817320744790	4.88888431287852	-0.64451637312989
Si	17.73005156676025	2.69318988459365	-0.65634252969263
Si	19.47835759816093	1.10939318217564	-0.37055287138996
Si	23.87565321060988	7.72893620974688	0.03983346116327
Si	31.01339971340047	-1.38343568813350	1.64714475369354
Si	23.45467150025592	-7.56946625708740	0.75764171958675
Si	21.26536951453052	-6.73851162011852	0.39521803119131
Si	20.53766279513743	-4.51289292312758	0.14817891792246
Si	18.22049370819319	-4.30150693103231	-0.17368681364914
Si	17.76959922762727	-2.49799223781590	-1.58953704047512
Si	15.70885263919924	-1.85213920922092	-0.71771537501662
H	30.22686624328729	3.95906294112786	0.38554555141282
H	29.86393841264300	-4.32845314053010	0.74262769593187
H	32.47986825894341	1.36643741838287	1.03408655941509
H	26.55871706321919	-6.66714221071101	0.40507922523543
H	26.93099431314226	6.66502957406295	-0.19545262274516
H	19.38266424205309	-9.37450884018886	-0.62786746703958
H	15.13008057375122	-8.57175154710052	-1.27127947960656
H	12.54212695919586	-6.23306781053618	-1.72490587477612
H	9.43275860125539	-4.12494583932431	-2.39693844695247
H	6.92157504482687	-1.68893794250508	-2.73554661798227
H	6.84122297114970	1.56947054517060	-2.89226236753362
H	9.14154033710050	4.17364880596636	-2.83429851940073
H	12.74221264395322	6.97933835893045	-2.35690694621153
H	15.44222057899444	9.08028049153069	-2.09460104727164
H	19.96988304498679	9.71813848796538	-1.51490144677148
H	24.35339087652715	8.90292757064545	-0.75969528575781

H	32.34081662313746	-1.89425116391297	1.16873800157398
H	23.84855028408041	-8.83510276830964	0.05850923063364
H	16.54677174946757	-2.38284696543131	4.56452524836881
H	19.19558642194722	-0.42299223026977	4.74598059184282

- **77 (H₂ absorbed)**

Si	26.94251081639425	2.47044636161887	3.24402068839301
Si	26.86248597528080	-2.21047275717438	3.48650658512254
Si	29.18636239783357	3.11263963610925	3.53153692531654
Si	29.08984586276374	-2.88417093842516	3.83433608345821
Si	30.71425167955683	1.30022341090125	3.84196962345489
Si	19.00189529144497	-0.91845433213450	3.35322782127157
Si	20.96170257582637	2.48624039944694	2.31055402945015
Si	20.88032221684918	-2.13698836597320	2.60908858447245
Si	23.26491801910118	2.30565156966933	2.65878160113873
Si	23.19565386395210	-1.97175899446536	2.92776398805008
Si	25.05134792020813	3.88745747341871	2.83985828204244
Si	24.98358029112880	-5.97869574679199	3.36674404273135
Si	24.15955205830126	0.15735818145914	2.85773677584748
Si	25.24629878425252	6.25781068913653	2.74454365079159
Si	24.92052552116885	-3.59934934077794	3.24592023608459
Si	26.45586745328345	0.13366969337150	3.28519339224515
Si	19.01416034672160	-8.05953958718937	2.56189466423166
Si	17.14601685537115	-6.59773480970771	2.21848342946070
Si	14.92324095196120	-7.36482154445890	1.92244372884298
Si	13.13286829800158	-5.80147534939976	1.57676768783097
Si	13.30454976286384	-3.42617837703132	1.48393324911906
Si	11.43300407585264	-1.97671228892223	1.10148739709579
Si	9.18574827056153	-2.59757537225249	0.78277052626974
Si	7.67114964951309	-0.78346420749411	0.43583857418128
Si	7.73329904792843	1.61402337015579	0.31933726736588
Si	9.33422998639616	3.38022932330813	0.48645768707474
Si	11.55241831324533	2.69008247932044	0.86136224040270
Si	11.98262015618432	0.34989651621381	1.07068211143211
Si	14.26116079382494	0.32448523815753	1.55765035548534
Si	15.22179193322258	2.44656663720739	1.46361600980647
Si	13.49903839396542	4.06791892887781	1.08529955135751
Si	13.41571363192518	6.44255260528786	0.95569576295584
Si	15.28462528035016	7.93109802350799	1.16322800345765
Si	17.45797245458594	7.06253926860016	1.53546661209189
Si	19.38183418674512	8.47254266012773	1.75770288543855
Si	21.24480918669124	7.00554427310420	2.10303936451624
Si	20.46388564080025	4.77747950092190	2.11471007650894

Si	18.14484176968814	4.81606415830755	1.76644425875602
Si	17.52876938452500	2.54910501154421	1.80116917389624
Si	19.05511784442725	1.43088808927177	3.20180595400665
Si	23.45411352736289	7.81080395505870	2.39052261518625
Si	30.67401146881640	-1.09890621803642	3.96055799837962
Si	23.12658818125276	-7.48666386920449	3.15417776686597
Si	20.94014885755173	-6.65033021295058	2.78684893824279
Si	20.24878062538635	-4.40235687925402	2.58641386128044
Si	17.92734786364925	-4.37196134687235	2.24389855783686
Si	17.38787374388041	-2.09109547970639	2.09504778746926
Si	15.09065077375396	-1.84978658573800	1.72483789331965
H	29.51101734313924	4.31243044941208	4.36637788238057
H	29.37993774892182	-4.00759928916963	4.78069463833402
H	31.85876273184047	1.75099286884496	4.70169434737012
H	26.00411708337951	-6.52868323647544	4.31788584768550
H	26.29562092442706	6.83744228322012	3.64536379414613
H	18.86418250697599	-9.24861595657843	3.46102834701993
H	14.46978351338302	-8.54339481570804	2.72954784341934
H	11.85969701976714	-6.31803030437670	2.17763623440559
H	8.61424849325127	-3.70678953810340	1.61020600834340
H	6.31230674616721	-1.15507204577473	0.95301864333228
H	6.39681709919432	2.10251086504296	0.79630158302950
H	8.81631022450176	4.58861090060129	1.20288019833110
H	12.16652161549643	7.06340158905123	1.50579350946054
H	14.89881194504440	9.20037095846531	1.86072027374897
H	19.28358589624555	9.73382533947425	2.56072743648504
H	23.65587651355769	9.07199598898078	3.17465062597858
H	31.80913574214521	-1.49883659447768	4.85717101596112
H	23.28607034278705	-8.67780895080179	4.04952303244698
Si	27.30241056677175	2.33577252694099	0.84010527118474
Si	27.21169605255885	-2.33209537413454	1.08038632782219
Si	29.54272310317946	2.98294521141841	1.14765332153167
Si	29.43697565592911	-3.00291205900680	1.44835498013345
Si	31.06992690933732	1.17735287309052	1.48560735314599
Si	19.61105250216475	-0.86912785762042	-0.71138942124108
Si	21.30599937414677	2.36021369033579	-0.11855701220223
Si	21.24989183604917	-2.24846060138012	0.17039795967351
Si	23.60814939733918	2.19410657858324	0.26873744056520
Si	23.55004522592013	-2.08812118902596	0.54363233336089
Si	25.40846164520057	3.75707812566473	0.46873059592382
Si	25.34393116825659	-6.09431804917237	0.98553217252443
Si	24.48751330337749	0.04199738304910	0.44988212135930
Si	25.60355621596798	6.12728851238947	0.36326076277222
Si	25.26841954061511	-3.71914172017700	0.87252245950924

Si	26.77732393498866	0.00757690644450	0.88912272907059
Si	19.37302986337089	-8.16040766967578	0.17146154802039
Si	17.50137243997066	-6.70175636900308	-0.16979740504633
Si	15.28198505233223	-7.48134436169352	-0.46023005781347
Si	13.49796121919697	-5.91494785849642	-0.80385749631538
Si	13.67773851295698	-3.54366733768691	-0.88530594328363
Si	11.79981144115763	-2.11249119701993	-1.30141136197018
Si	9.55159848164598	-2.73448945302832	-1.59919317669653
Si	8.04168806798243	-0.90826918927719	-1.91840979529118
Si	8.09688309919266	1.49115010064800	-2.03548105995235
Si	9.69040566587776	3.26734980239284	-1.89795240054192
Si	11.90798214825423	2.56936105554995	-1.54354373845175
Si	12.27706813450448	0.22454349605585	-1.32990259690412
Si	14.56551384004076	0.21049497102914	-0.85454816378928
Si	15.57963022943354	2.31358167451901	-0.92441892527672
Si	13.86228053030255	3.93467642694059	-1.28420399633971
Si	13.78378651521128	6.30986462970681	-1.42413226837417
Si	15.64792257304878	7.80558240501424	-1.21919561993875
Si	17.82169902469785	6.94052088931403	-0.85227352939496
Si	19.74065765391623	8.35589966457421	-0.62851525022941
Si	21.59669617174653	6.88165170930547	-0.28731544344212
Si	20.81055916915696	4.65865324186421	-0.24131117713926
Si	18.48782091907868	4.69258400118560	-0.58978120808891
Si	17.90157469319712	2.40891626068086	-0.62327305287667
Si	19.75044060536432	1.22151515718518	-1.46425011088009
Si	23.80820867166567	7.67776014852686	0.00706793361450
Si	31.02265574672388	-1.22124019041255	1.60315363113385
Si	23.48506465990215	-7.59607105498324	0.77099086877108
Si	21.29993824792997	-6.75364373256875	0.40008320357924
Si	20.59431677310649	-4.50533452591772	0.22916689083200
Si	18.27676084541450	-4.46994345920371	-0.11333886421859
Si	17.74265750073302	-2.18891702774655	-0.34492676044329
Si	15.43883479597933	-1.94610866383197	-0.65923309307026
H	30.10371847303731	4.09678639560573	0.31932438618317
H	29.96457671752386	-4.21010340671403	0.73694238710240
H	32.42379807621984	1.55399038045208	0.95920362227122
H	26.59472541625320	-6.70790357619078	0.43140800489672
H	26.87838573500590	6.62652298189071	-0.24828686626469
H	19.47325930327608	-9.42496275985780	-0.62597674126322
H	15.07435393164453	-8.73733425710641	-1.25060579690486
H	12.44821216694517	-6.48789937230543	-1.70819802727131
H	9.21924780240307	-3.93368925089704	-2.43186740125445
H	6.89944825181631	-1.35148473143463	-2.78509749162119
H	6.96961145675484	1.89647381510038	-2.93952053735320

H	9.41138622826444	4.39426864917008	-2.84338669001937
H	12.76494011239880	6.84387184797274	-2.38595957770563
H	15.49846187736002	8.99081715349665	-2.12412810989142
H	19.89297738936340	9.54022860634689	-1.53338244730626
H	24.25474744934666	8.85043771898037	-0.81248541408129
H	32.35953120455682	-1.70074438451706	1.11820686304848
H	23.87780401234174	-8.86066498271436	0.06946307580847
H	18.85972058463315	1.94339739596501	4.59753662854192
H	18.78604869137726	-1.26611561636086	4.79726238585293

- **Hck-COOH**

Si	-7.94284272180993	2.37336154432246	-1.27587672349791
Si	-7.71541352451134	-2.25885021393511	-1.33377019867378
Si	-10.24449912904386	2.87604808927650	-1.30253663127215
Si	-9.92548848674065	-3.06708695040730	-1.36825220753772
Si	-11.73777264513438	1.01242210468825	-1.33442898345067
Si	0.30665516604223	-1.24450976368121	-1.26329855468591
Si	-1.91767716728945	2.58734851985040	-1.21608505132907
Si	-1.66273585763078	-2.61972712063746	-1.23827309229979
Si	-4.24021815312583	2.39414295564906	-1.22293007696271
Si	-3.93096471339321	-1.95765861708936	-1.25569540047895
Si	-6.08705226398354	3.89776097783879	-1.22679856231619
Si	-5.7866226216555	-5.93661049191600	-1.37548282809815
Si	-4.94441836620169	0.17039479269145	-1.30110865648516
Si	-6.12032843378506	6.28547835317601	-1.20931824970421
Si	-5.70306702059385	-3.55874072904004	-1.31571281295722
Si	-7.28715295638285	0.07883958694453	-1.28863511347428
Si	0.11524572046475	-7.90243405866848	-1.35515088743267
Si	1.91944710496089	-6.33513271102226	-1.35984866366067
Si	4.08288014093643	-7.30457679704259	-1.40468151830009
Si	5.99723141904311	-5.88139855729571	-1.37913859831464
Si	5.76233704891564	-3.52542059819609	-1.30172264678912
Si	7.76917078286918	-2.22534034208248	-1.35803397610278
Si	9.99444278859557	-2.98771814794845	-1.40540139880105
Si	11.62608383825585	-1.24245281554866	-1.40337586333742
Si	11.64493731550265	1.15872414389112	-1.37000393379358
Si	10.08204884277517	2.96386407698670	-1.32442890518380
Si	7.80126116583004	2.37797112736622	-1.28773353898392
Si	7.23661524257467	0.07242226944359	-1.28826895098047
Si	4.89181123087763	-0.01778780510936	-1.16281343228925
Si	4.10320730882620	2.19482748479735	-1.21070791046740
Si	5.86645171595467	3.79588326213327	-1.22103006287057
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Si	1.83235062660589	7.08875983816733	-1.19147726259996
Si	-0.08856392143965	8.53005379572922	-1.18139968241430
Si	-1.98666607242752	7.05881455227830	-1.18867787034654
Si	-1.21558633707925	4.82507820727464	-1.19117889410128
Si	1.12290487752007	4.83682068997780	-1.18739525714114
Si	1.80818543579368	2.58941315397848	-1.20625852799269
Si	-0.04866064516364	1.10406975385889	-1.20656448324967
Si	-4.24667128009261	7.79268631023903	-1.18805299732353
Si	-11.62137095734733	-1.38538996513329	-1.36089124471105
Si	-3.87480604295617	-7.38412692335207	-1.37373966400085
Si	-1.72220566612666	-6.39683139365829	-1.28887061942118
Si	-1.17696988780431	-4.50367131583967	-2.51422890703634
Si	1.03964130146960	-4.28059114261430	-2.02349085480250
Si	1.94702159250484	-2.26380180144777	-2.64623297804315
Si	3.81667252224562	-2.13750909687574	-1.25622782202767
Si	-7.98377952829970	2.35476252069583	1.15848841542527
Si	-7.75839427974418	-2.29132484327742	1.10178175315076
Si	-10.28615959553646	2.85425372505789	1.10842415558380
Si	-9.96773999357914	-3.09705145684551	1.04753813659457
Si	-11.77463473069820	0.98638023560834	1.05067804675535
Si	0.24387295357896	-1.19823141922435	1.16173709148687
Si	-1.94278674149704	2.58285068990873	1.22233850260790
Si	-1.75518220442238	-2.50221647133095	1.18208503261976
Si	-4.26920833437580	2.38166775527690	1.20360998182708
Si	-4.03276172238187	-1.97449769102805	1.16351725048944
Si	-6.12178796362171	3.87841054782696	1.18063379938550
Si	-5.84685804029816	-5.99578217787567	1.03482768903730
Si	-5.00625185854105	0.16764672218854	1.11448202217736
Si	-6.13457323350220	6.26700599942103	1.19842007574814
Si	-5.76015041133008	-3.61565109993729	1.08291349097896
Si	-7.34906541987113	0.05415530704218	1.12874909042607
Si	0.11601736042176	-8.02227524288303	1.02826172238003
Si	1.96506745911249	-6.51953993223896	1.05697256689328
Si	4.13880963162980	-7.43041480490063	0.98749883729620
Si	6.02695390162863	-5.96284312213798	1.02469559859915
Si	5.84510100717541	-3.59861426183283	1.09596524311171
Si	7.82826520574173	-2.25837478965436	1.07614678046460
Si	10.05399757047454	-3.01959776906294	1.01143854261326
Si	11.68319667677201	-1.27415107763976	0.98240318019277
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Si	10.13371518354253	2.93497249748466	1.08706128427533
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Si	7.27446167932539	0.04720159968303	1.12725770925482

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Si	4.13070912715940	2.20567814754088	1.21094338178871
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Si	5.93018783912687	6.18162676394145	1.19697964205194
Si	4.11266626437077	7.76070231797704	1.21962347606649
Si	1.83513388902236	7.08265728079182	1.23136916446063
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Si	-1.98949800584231	7.05284223324389	1.22980406067962
Si	-1.22178633373672	4.81697589032023	1.22141760530342
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Si	-0.04309516586605	1.13634646806827	1.21831961220098
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Si	-11.65928416210757	-1.41160185046082	1.02680070462405
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- **Hck-HCOOH**

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Si	-11.76445657519957	0.87049305628403	-1.21334630729343
Si	0.30340254847879	-1.14535564516639	-1.35577426638207
Si	-1.98048475133163	2.61200211658524	-1.28123256783637
Si	-1.64156986226305	-2.51658949455591	-1.27155039146560
Si	-4.30405615411495	2.42527459479520	-1.26227441340780
Si	-3.92091126955645	-1.91439085614924	-1.29188583727541
Si	-6.18064502820459	3.89388153225240	-1.21960057344728
Si	-5.70205364446152	-5.95680228131473	-1.31657849156069
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Si	4.11386840610269	2.22308759496801	1.08410676702415
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- **Hck-HOCHOH**

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Si	-7.67294946414374	-2.37215756408862	-1.42481233991528
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Si -1.18800151575597 4.91966746759705 -1.12915551960043
Si 1.15330590361508 4.95774676942758 -1.11766878908031
Si 1.89699306103376 2.74339247531320 -1.27025665215005
Si 0.05284712606477 1.25104774414930 -1.35220148475991

Si	-4.21041062662209	7.82449125702794	-0.99868971105628
Si	-11.59973593222419	-1.33003839452578	-1.39788902965888
Si	-3.88564538168368	-7.20045941449627	-1.33690402418229
Si	-1.84010394793154	-6.10135153066633	-0.92790304107553
Si	-1.04809114833542	-3.99824571707395	-1.44093750677255
Si	1.27232355488384	-3.87937807980591	-1.04645690701683
Si	1.79361363223922	-2.29202140229049	-2.71241352259760
Si	3.81933624200518	-1.89797635218895	-1.53283580522552
Si	-7.85281766784358	2.28426829562734	1.15309525601102
Si	-7.73407501526180	-2.31067067857983	0.98471163507422
Si	-10.14997026275450	2.81175309107770	1.16532627812682
Si	-9.94129388843160	-3.12574232495526	0.94411735542226
Si	-11.67764683212490	0.97756463936601	1.07840019151485
Si	-0.05674859984082	-1.30035218577201	0.82774353366881
Si	-1.82180949736076	2.51942009148340	1.13782202208361
Si	-1.79636737630420	-2.43904968815660	1.98592179712427
Si	-4.13185354885340	2.19753228725903	1.14861316152067
Si	-3.86367792930351	-2.12976969353578	0.98793322668792
Si	-5.94702185101459	3.74214065137556	1.21635817105778
Si	-5.90563631214138	-5.95143255249728	0.97524399308518
Si	-4.88031156863413	-0.01462856783088	1.13245071309876
Si	-6.03101306051315	6.12828148591141	1.31613953504003
Si	-5.71625822353766	-3.59367364192937	0.95193795432708
Si	-7.22213220755827	-0.00540564504402	1.05794377785499
Si	-0.01366436239973	-8.11230832959288	1.12908714576727
Si	1.92750718073497	-6.76013308156411	1.42735433619855
Si	4.12641881365179	-7.52703377676936	1.01021476870217
Si	5.88955791620958	-5.90506313299439	0.92295185817283
Si	5.65863601262173	-3.55519010113456	0.89511986990147
Si	7.65787791472924	-2.26371418004401	0.97244549559699
Si	9.84729684928609	-3.11846489600796	0.96675413535545
Si	11.55040626151484	-1.44824241696614	1.06157657515697
Si	11.65128433478937	0.94647790896323	1.18152272538714
Si	10.15053789201425	2.80150756714974	1.26544670251671
Si	7.84188686368349	2.32961684323007	1.20062877875007
Si	7.17308628294856	0.04793512924340	1.05960139601491
Si	4.82230297962558	0.11153990905873	1.03375745257736
Si	4.17455878769501	2.35208272053690	1.16169731768087
Si	5.99917351868251	3.86693685945341	1.24901373090443
Si	6.01331112947523	6.25368483387560	1.36561680784108
Si	4.15543923878320	7.78122174942024	1.44365492862780
Si	1.88269004189935	7.07722331501148	1.41790405883117
Si	-0.05408272205995	8.50266007350286	1.48536512173025
Si	-1.95132695518323	7.02625439209224	1.39957780806653

Si	-1.19247289047341	4.78851826922006	1.27253879887290
Si	1.14318604646942	4.83929879428611	1.29437192142631
Si	1.87278312745526	2.61910370738503	1.16694830496472
Si	0.07264403787331	1.06053034397383	1.06909178942189
Si	-4.22639301577663	7.71301695933581	1.40707787817056
Si	-11.61236279818355	-1.42060958711041	0.98733241190049
Si	-4.07294838849130	-7.49187933104709	1.03167058316753
Si	-1.89558625981742	-6.66612471393472	1.43807873117694
Si	-1.12500779150201	-4.67266143197832	2.30113392530982
Si	1.22866761045712	-4.73133766210675	2.32839765955799
Si	1.71063696358216	-2.82115092798516	1.10604948246556
Si	3.86277123222979	-2.03512634046945	0.88682387348354
C	0.61781994426699	-4.63581838401367	4.13671140744140
O	-0.67616091966262	-4.66367987839483	4.15895608300612
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H	-10.29659985628430	-4.19403205169813	-2.35243668500128
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H	-6.94002463119707	-6.54409439971480	-2.26896714136090
H	-7.17681641978143	6.83059533179216	-1.81718091684116
H	-0.01661029956484	-8.54173847391385	-2.34594159827634
H	3.74631028347721	-8.33684082393915	-2.32599325397391
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H	10.25310356744973	-4.16137439598869	-2.32879595087908
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H	12.96934500376150	1.47264725349918	-1.86128464066090
H	10.71887516377609	4.11783462927813	-1.89666035678816
H	7.16607264270126	7.02220942717986	-1.74641123926663
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H	-3.73203133824632	-8.32899566789374	-2.30734710936002
H	-10.62325730885346	3.92817220219613	2.04396055159419
H	-10.29379888209210	-4.34357722283118	1.74146354638671
H	-12.94478140004559	1.34868081864612	1.79172661814952
H	-7.06741614894858	-6.46645751086760	1.77048879188592
H	-7.21485326713375	6.65406328036281	2.07242723117758
H	-0.08474154949556	-9.46499436928647	1.76249979396584
H	4.57674388442054	-8.79493182993222	1.66905153042773
H	7.08383728270993	-6.37987693674650	1.69589716685181
H	10.15818407083634	-4.34988059855742	1.76088136894986
H	12.76361972018664	-1.98401886117324	1.76363657929313
H	12.91216794632629	1.29323040666944	1.91813320851787
H	10.62131735675357	3.89736053034220	2.17109633049094

H	7.16786670883664	6.82048506334712	2.13741258423641
H	4.49076600276059	8.97260383048370	2.28936714692449
H	-0.07474827094820	9.68104207846384	2.41038877877195
H	-4.59301518918899	8.89099286787646	2.25820477563357
H	-12.84736356274604	-1.92633130053344	1.67306581522736
H	-4.42794364888582	-8.78365690634482	1.69967618033340
H	1.09933912231990	-4.53219021245047	5.12816195158621
H	-1.79755472277473	-1.94562603181926	3.40268363255625

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Si	27.34228015831011	2.22954578418788	2.37618164922349
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Si	29.61528288584083	2.77963609448051	2.65873176070442
Si	29.34588914437753	-3.12661234393841	3.07708151172816
Si	31.12494638289079	0.96372798780757	3.00887743775944
Si	19.50474558796106	-1.17445763017656	1.48579025908747
Si	21.42598062450868	2.64189966839373	1.47683038722633
Si	21.21248932985317	-2.79183237352889	1.83580910895297
Si	23.69478236360109	2.24404860680268	1.83770076211404
Si	23.45571812256662	-2.16873904838054	2.12311144111951
Si	25.52658317518020	3.75548363297615	1.97577084043691
Si	25.15263371735736	-6.13480370623185	2.68964940192258
Si	24.35204755955354	0.01112315918489	2.12507101493527
Si	25.63423665443990	6.13946128525124	1.80385058447768
Si	25.18579760497654	-3.75609952752421	2.50793348288751
Si	26.67740471829200	-0.06037880630851	2.45305927602611
Si	19.28687061221015	-8.14987324249288	1.91302109285124
Si	17.49147782375533	-6.62463688365922	1.55857230166486
Si	15.26197413321887	-7.39161050472553	1.34822528941931
Si	13.40908494675280	-5.92120702556790	0.97088588383732
Si	13.52773438160579	-3.55111563056646	0.80876601018635
Si	11.67619852019587	-2.07666437432167	0.42830458355810
Si	9.42796951278365	-2.71395019162351	0.14050933910746
Si	7.87602157056879	-0.93933042341698	-0.23396223290021
Si	7.94298233257345	1.45282512527877	-0.40443410369921
Si	9.57370908218512	3.19233224684552	-0.28393210605508
Si	11.80327868632178	2.53233049121302	0.09461935520255
Si	12.31590308725695	0.21644163277871	0.34017541880785
Si	14.63322074992114	0.18212670397013	0.72592108689162
Si	15.45581551496702	2.37699635549780	0.64925039281956
Si	13.72549526351673	3.96685894429752	0.25645317077985
Si	13.74659535302356	6.35209583238339	0.07379063315269
Si	15.59135306058398	7.89052086953488	0.21882206979316

Si 17.82365702308779	7.17642265015439	0.60225135111547
Si 19.75365066605002	8.59813841857241	0.75892222475428
Si 21.59942259522634	7.10927400391207	1.14704359961084
Si 20.80156186296816	4.88866658871065	1.20304319823276
Si 18.48560371961110	4.92338955079812	0.86332618263174
Si 17.74880182034935	2.69120806688597	0.95115080286244
Si 19.55472349439971	1.17891596605491	1.32232508196903
Si 23.87469498656271	7.73669542514413	1.42125694576104
Si 31.02036667482011	-1.42761219394689	3.17901326070640
Si 23.22713637960723	-7.55533791005615	2.49923184379219
Si 21.10260349720148	-6.60855401181553	2.05710039990442
Si 20.41792341163458	-4.61236176909435	3.04643432763980
Si 18.33684055991595	-4.58736315023128	2.21550130619888
Si 17.60771184682119	-2.59170299548429	1.36582458324208
Si 15.36408546762900	-2.04759065411379	0.96153878939946
Si 27.69807013555936	2.04523537784887	-0.02613592912598
Si 27.49962095800070	-2.56903269856706	0.30185153514122
Si 29.96765862983109	2.59785314895276	0.27942939195221
Si 29.69891452656437	-3.31152374843816	0.69504529628130
Si 31.47217599488953	0.78216466371165	0.65434300699503
Si 19.82295308613031	-1.36997769187606	-0.89569038858576
Si 21.77250915271366	2.44960448135353	-0.92490900306042
Si 21.58712290779759	-2.92948794497626	-0.55628321424926
Si 24.04418641392716	2.05832350583495	-0.55688302391089
Si 23.82536751735852	-2.34569913872057	-0.27449588048451
Si 25.87462446608399	3.56932896143415	-0.39796841498396
Si 25.52475772491298	-6.32290986210588	0.31579785874881
Si 24.71623252972569	-0.16782359383807	-0.25178627007063
Si 25.98009612518454	5.95227728518608	-0.57217185969347
Si 25.53922221917065	-3.94162666908428	0.13938183774683
Si 27.04362191793847	-0.24515786817647	0.06823266205526
Si 19.61524246730102	-8.34237778037135	-0.44248707488673
Si 17.80227660284607	-6.82996237614342	-0.83673789813808
Si 15.58190688584491	-7.62987422874181	-1.01851421379216
Si 13.76289903216146	-6.10855978652178	-1.40723900851648
Si 13.88669777133579	-3.72990387617217	-1.55991575153260
Si 12.02743973892913	-2.26752928530466	-1.97563604480488
Si 9.77520952455221	-2.89821226990558	-2.24258365248380
Si 8.22321076375408	-1.11652314365677	-2.59017623151637
Si 8.28611582921134	1.27672789640765	-2.75973106329426
Si 9.91561874163053	3.01932716270672	-2.66589180892636
Si 12.14589576042681	2.35288796348601	-2.30947009936337
Si 12.63388231105824	0.03446287290343	-2.05304809034865
Si 14.94856041046173	0.00344768394889	-1.65743985215360

Si	15.79816595496171	2.18686768304379	-1.75076557040401
Si	14.06988369467603	3.78122727925572	-2.11708306793563
Si	14.09177535588321	6.16458869047044	-2.30270964354819
Si	15.93432300278335	7.70508138579183	-2.15804886103319
Si	18.16794344372804	6.98778880925990	-1.78808600684729
Si	20.09639832248730	8.41073173297713	-1.61973127225020
Si	21.94361029406916	6.92020481986942	-1.24315296591420
Si	21.14477071603103	4.69865380728672	-1.17829004256233
Si	18.82770728874191	4.73461722750324	-1.51631415706334
Si	18.09189307646776	2.50186495526147	-1.45232442940350
Si	19.89398041414807	0.98776133685332	-1.07543610999953
Si	24.21851958098226	7.54787207883600	-0.95536581858506
Si	31.36844331947952	-1.60953958098129	0.82361686998136
Si	23.62135907005628	-7.77446718745045	0.13901329369801
Si	21.49076957059046	-6.86526653885658	-0.31577092805348
Si	21.00909352273672	-4.95022793682648	-1.50528807268616
Si	18.69329489711045	-4.89449404078982	-1.76238983603481
Si	17.93614158004334	-2.81831911938168	-1.03618650328311
Si	15.71484043789522	-2.20916748365741	-1.43511637016537
C	20.59023899504342	-4.98846953531317	-3.42863705162011
O	19.13408062792223	-4.94067284924623	-3.42965348485091
H	29.95986448851392	3.99546354320172	3.46207182891906
H	29.58076308200173	-4.24654793884756	4.04283730499652
H	32.27387966960912	1.41660973122582	3.86119486631469
H	26.14959325326820	-6.69673813004248	3.65910143170094
H	26.69823029935884	6.76191004060783	2.65848941776940
H	19.13431849003373	-9.25610665896357	2.90681827634996
H	14.91353218277929	-8.54154963741628	2.24201759785092
H	12.16464335681581	-6.46196422945683	1.60921400163158
H	8.87684270072968	-3.81684113475227	0.99012323878816
H	6.53086184437252	-1.30947269761593	0.31789814083560
H	6.61916095442415	1.96626068959450	0.08072727276563
H	9.06982218697604	4.42602500672786	0.39880527109051
H	12.50076927988382	7.00953802877779	0.58916421965692
H	15.16185688316749	9.17450038279722	0.86122473237492
H	19.66821944487819	9.88722741165623	1.51652634968666
H	24.14630807924935	9.01143376914624	2.16105124550177
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H	19.70926173753807	-9.61406234277293	-1.22483226099071
H	15.38629574741508	-8.93202511483227	-1.73106322396093
H	12.72340085733053	-6.73804037537905	-2.28597971582982
H	9.45380200167552	-4.12567808104459	-3.03750664330647
H	7.08473444323283	-1.59146984603629	-3.44426227118937
H	7.16340539491062	1.67960299798200	-3.67003200966916
H	9.64595340422022	4.13255579260151	-3.63024795707666
H	13.05532091476069	6.70458833755370	-3.24296142606356
H	15.72745051182764	8.86550656324579	-3.08344751590400
H	20.24960422577205	9.56547808780489	-2.56103198993809
H	24.71871836782725	8.69789785494061	-1.77596735551857
H	32.68351875518541	-2.14487340182987	0.33820683110382
H	23.95581303651338	-9.08054271855480	-0.51297009968810
H	20.93423982491711	-5.90998151836035	-3.93483489578248
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Si	27.31433193108118	2.24512579026790	2.39103955513298
Si	27.05063064427516	-2.37033480748014	2.63880506349166
Si	29.58666856710128	2.76113054383668	2.73335817171314
Si	29.22867927287008	-3.16146670678350	3.04625092044027
Si	31.05678640916322	0.91368796409441	3.08731049823598
Si	19.42078040623026	-1.25803053103299	1.08184509179214
Si	21.41973944631746	2.60284156028659	1.37621836725658
Si	21.15210700654913	-2.78795279162502	1.60464592317005
Si	23.69394271887813	2.27942154675884	1.74978756723982
Si	23.36515962035192	-2.09768203410938	1.91789334793183
Si	25.51850679568818	3.78540948852292	1.97789893931605
Si	25.09053108365260	-6.05634067987918	2.59561008235364
Si	24.34176694999570	0.04593979356093	1.97945955950611
Si	25.63820418361511	6.16918865556651	1.87438210931083
Si	25.07082792275561	-3.68850584618495	2.36389547147225
Si	26.64958497898195	-0.04192097452469	2.40863742658146
Si	19.24024098682105	-8.13117689840821	2.06648032914202
Si	17.37337502709611	-6.67099633140070	2.01860573831396
Si	15.17414008041982	-7.34505280539903	1.43072556698337
Si	13.45599445973006	-5.76377749599478	0.89910098139293
Si	13.74088812865378	-3.45169227902387	0.57407022785660
Si	11.82242737567219	-2.07352626813255	0.31024457697034
Si	9.59162312743068	-2.79640620970071	0.11906658428060
Si	7.99096622100130	-1.04348427949700	-0.14332433288992
Si	8.02190274522195	1.35259361403894	-0.25348734747884
Si	9.62973818723859	3.11246830431215	-0.15596274704956

Si 11.89226421681403	2.49938090090157	0.08269429331060
Si 12.46739439833848	0.19655150339517	0.25512477814744
Si 14.80558214122946	0.12711696208157	0.53884815085730
Si 15.52914434161777	2.35175265122100	0.49466923121492
Si 13.79346567792005	3.94684152146815	0.21797215872766
Si 13.78636481402316	6.33544143742367	0.11596734024935
Si 15.60708427288944	7.89238959921343	0.29128738673689
Si 17.83909946029881	7.17334343650452	0.65095418017058
Si 19.76026154423179	8.59417209118500	0.87263677048504
Si 21.60822360520881	7.10029379242663	1.22266367934752
Si 20.82295915622914	4.87039356364952	1.18828639780517
Si 18.51597660281352	4.92002353910568	0.82137192984417
Si 17.79684768135035	2.68909833853462	0.80626446636607
Si 19.55328700111291	1.12209637750975	1.13029838357822
Si 23.87052237769669	7.75948623701840	1.52169841130636
Si 30.91678237892518	-1.47941515322076	3.21554777078024
Si 23.19102754059922	-7.51496374665688	2.45545084531036
Si 21.03546653578692	-6.54451824904220	2.23812024905508
Si 20.51266497652879	-4.45598794465711	3.16537434627576
Si 18.33365153039538	-4.63995972748168	2.59711824867857
Si 17.75040457282968	-2.89380848832558	1.22185999791298
Si 15.66254177199147	-2.09017133978200	0.60375788838997
Si 27.71602801686602	2.10340949672755	-0.00649757748105
Si 27.45948911337794	-2.51980444222777	0.23940908999236
Si 29.98801550219412	2.61210995250887	0.35994169935104
Si 29.63665981903717	-3.30690895520378	0.66929750622596
Si 31.45550302239160	0.76591952058815	0.73846451517719
Si 19.76089330578275	-1.26383128567976	-1.30470871607892
Si 21.81554290101411	2.52470261140059	-1.02634312682554
Si 21.55291077333476	-2.76758640493413	-0.83184508083853
Si 24.08638335997786	2.15559774643136	-0.63988264988915
Si 23.80296104607563	-2.25776876297145	-0.46634809171509
Si 25.91844172629868	3.65744109906466	-0.39198483833387
Si 25.46341132705032	-6.25183302136240	0.22036295739429
Si 24.72380033944150	-0.08720926098430	-0.39753793788339
Si 26.00842753946165	6.04633926309341	-0.50172050361388
Si 25.49309826228497	-3.87696881931920	0.00865994149739
Si 27.03251506749025	-0.18594456969416	0.02508335564586
Si 19.49425546626204	-8.03632753000805	-0.30840518499018
Si 17.73617397518566	-6.43871381752267	-0.38964674520349
Si 15.66489923251560	-7.41031928040836	-0.92052131521220
Si 13.79168237680536	-6.03883231547010	-1.47313379981260
Si 13.97939487197227	-3.67184489552190	-1.80181849245376
Si 12.06941793081029	-2.23403768328451	-2.10920781019996

Si	9.82639411776906	-2.92434139827770	-2.28368585924104
Si	8.23963493792415	-1.15485493893866	-2.51586264007707
Si	8.27288484416084	1.24420920461508	-2.62418454050520
Si	9.86287599243044	3.02804736648177	-2.55531244015028
Si	12.12791790622591	2.41193015037459	-2.33765520890013
Si	12.61401288517269	0.08792303375722	-2.15762744394783
Si	14.93764093455440	0.04921983018762	-1.85743623169986
Si	15.81497926010143	2.23117116526826	-1.90809278033606
Si	14.06995644421380	3.83635516413809	-2.17346285499129
Si	14.10382897527307	6.22855594087290	-2.27057772552645
Si	15.94449139442811	7.77337704379157	-2.09042754467638
Si	18.18913259728899	7.06927514099360	-1.74582752477630
Si	20.11330974947326	8.49317211346248	-1.51063400501719
Si	21.96137580343727	6.99540187593094	-1.17089721141038
Si	21.16842812576512	4.77147150044722	-1.19732814044867
Si	18.85282594636699	4.80791749687280	-1.56217461281865
Si	18.11672134642653	2.57161006687786	-1.60082034025601
Si	19.94773871464561	1.07747578326168	-1.26012977280830
Si	24.22962636999978	7.63316436197484	-0.85618628439152
Si	31.32155000710351	-1.62702485467210	0.86667816773748
Si	23.48365011063229	-7.58359233895394	0.06820124702870
Si	21.35529001018690	-6.59424623418744	-0.12125708768783
Si	20.64359719884419	-4.78729825814551	-1.35799981177294
Si	18.42420469659862	-4.23621736320663	-0.69341508258577
Si	18.06002418444763	-2.59076793284311	-2.32455486564649
Si	15.83175986515324	-2.13133999103354	-1.79979933619188
C	20.34954395959162	-5.40728544272248	-3.16051440174474
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H	29.43226197987154	-4.29923681072992	3.99829292037480
H	32.19395398049114	1.33344113382748	3.97194125773304
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H	19.24198171258016	-9.33731180021528	2.95102144203799
H	14.59597268219104	-8.51007091193381	2.17540585931840
H	12.15452489291151	-6.10866818103178	1.55814228745389
H	9.11613261075508	-3.92670227018552	0.97856445814438
H	6.67809203697823	-1.45215781404384	0.45698537158074
H	6.71163586541032	1.83667997125857	0.29477846627573
H	9.14929009860253	4.31560844621575	0.59493501286586
H	12.53275603002686	6.94602474286596	0.66869511916318
H	15.17037623607131	9.15430168432884	0.97129092899361
H	19.65928071949309	9.85572973352912	1.67357693426771
H	24.11922727592119	9.01862592812505	2.29532587836492

H	31.99842909450448	-1.93346538318339	4.15134187308825
H	23.38665118553127	-8.72094146536574	3.32319088627809
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H	32.82774683223469	1.10216298776512	0.23260930035929
H	26.65419087978266	-6.98086155654665	-0.32839017003628
H	27.27985427520735	6.59029067384482	-1.08311835642638
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H	9.50120815693205	4.16174076157029	-3.46426152322599
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H	15.72316478952362	8.95636657824268	-2.98365432471718
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H	24.72544087227794	8.80683470733271	-1.64566030678506
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H	23.66988288703699	-8.85644559019034	-0.69944065936867
H	21.28978368232466	-5.83987679963606	-3.56237508149847
H	20.04548010564357	-4.57067345634141	-3.82130555096744
H	18.34565770565992	-2.95254953189306	-3.74757759220525
H	19.13371736344242	-6.77304499053469	-3.92865054360483

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C	19.77868394220170	-5.95228048908543	-3.45639921669099
H	19.79473843791153	-4.85062479906351	-3.42219463546038
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Si	27.05763978946286	-2.38155239839583	2.45223491035437
Si	29.57507171964156	2.65543787675932	2.75398425373692
Si	29.20288992325385	-3.25334534355059	2.86838524438211
Si	31.04110648404659	0.79665331483048	3.05144425852669
Si	19.55069487846764	-1.25191732116398	1.06662470369625
Si	21.39652496933588	2.53312165542140	1.34438885169180
Si	21.05279138466594	-2.90620327098039	1.84607232972332
Si	23.66345740158186	2.21302248736502	1.72926610787210
Si	23.23681300753966	-2.09965136970103	1.75167968861952
Si	25.49063822224829	3.71928698949330	1.98515401446607
Si	25.09478546954753	-5.90956931680096	2.51018563843822
Si	24.26752429861954	-0.01598389936841	2.05806896037159
Si	25.61716701358867	6.10553016796616	1.93340194054362
Si	25.02321361650290	-3.57708818024689	2.16534663774690

Si	26.60372967582314	-0.07453799891049	2.29777047095881
Si	19.26402573408187	-7.95365443751975	2.14100726505427
Si	17.42762808945360	-6.46465320717582	2.01172655909717
Si	15.28672028459005	-7.22554104263521	1.35261221498412
Si	13.53271097223281	-5.68250210966686	0.83438265564174
Si	13.81287493453391	-3.35723096941839	0.59827613551940
Si	11.85443591060747	-2.04743560976469	0.27901848996364
Si	9.65938423118104	-2.85103188375321	0.03117472577855
Si	8.01719486526406	-1.14452442987581	-0.26683790144636
Si	7.98480668688380	1.25291793501624	-0.37096790451091
Si	9.52551674277576	3.07243449032862	-0.23848288892401
Si	11.80078404427918	2.53758689808112	0.06886683097684
Si	12.40843907949827	0.24278312641579	0.23778337457075
Si	14.73784193418978	0.23036858434602	0.54252820402686
Si	15.44275352979551	2.45219716889086	0.52796350417274
Si	13.68059489956802	4.01713075801421	0.24605622387069
Si	13.72338266467490	6.40287610037058	0.16553710408333
Si	15.58613902733151	7.90492950292311	0.38906640320416
Si	17.81191561102380	7.14656860570741	0.74521975028716
Si	19.75582990944130	8.53554506329397	1.00600885432470
Si	21.60083132863824	7.02837202258268	1.30710418478767
Si	20.80544268543082	4.80526791529250	1.20886045550256
Si	18.50049473927441	4.88878979025831	0.85623359694385
Si	17.73532084453673	2.67132716451022	0.81172374595881
Si	19.50893365455652	1.10280238721807	1.13462008816699
Si	23.85404249689474	7.70462278657812	1.62189867294883
Si	30.90794020497248	-1.59763161565737	3.09788984249079
Si	23.22324978981110	-7.40766219456197	2.51566158117153
Si	21.06062841490343	-6.42493239092749	2.50324002166999
Si	20.45119780946736	-4.39109319566390	3.57698198285211
Si	18.32020670158579	-4.46101185157391	2.75403801261134
Si	17.73691973021138	-2.70325643261276	1.37081616224038
Si	15.67816425787248	-1.93104332971570	0.69510026887569
Si	27.75309971492252	2.15152213572672	-0.05259776534495
Si	27.47894616784004	-2.50308114419831	0.06227330522892
Si	30.01997031632495	2.61988874651632	0.38216104676464
Si	29.63168077404000	-3.34742071035590	0.48919325717550
Si	31.45060466508586	0.73240714664358	0.70096076498305
Si	19.68023599935189	-1.18331736994270	-1.39509091731113
Si	21.79076892627774	2.48141764442392	-1.05045646571555
Si	21.68297567985742	-2.40304402556794	-1.64925438216457
Si	24.07553814291333	2.12355616296338	-0.64744538871641
Si	23.77009678226915	-2.13112111263759	-0.66889502696593
Si	25.89708008986014	3.64279229465294	-0.38855513644250

Si	25.45480783675316	-6.14420457515631	0.14028220374291
Si	24.84209744133528	-0.07081432560721	-0.34363806548778
Si	25.98047385163107	6.03419691690444	-0.44643164377024
Si	25.45257476334242	-3.77436385029549	-0.18558656455302
Si	27.16210921856691	-0.15211016113124	-0.05456904400457
Si	19.59115199304961	-7.70097283091202	-0.20915085467010
Si	17.84995937305003	-6.13377684103747	-0.40034800386522
Si	15.83301749918730	-7.18296759614446	-0.97906425834198
Si	13.93095033842419	-5.86874283348537	-1.53739297556119
Si	14.16150548633113	-3.50567920466885	-1.77896517635557
Si	12.18276723518985	-2.18773647528933	-2.13660498910069
Si	9.96942061516880	-2.95868497626643	-2.36390402816791
Si	8.32843382896120	-1.24355195003158	-2.63223737380362
Si	8.28790834558797	1.15495255067105	-2.73521077476694
Si	9.82397703717509	2.98158839220485	-2.62976408664932
Si	12.10136690457935	2.44166240722287	-2.34096255475366
Si	12.68525967977617	0.13344927901840	-2.16384421979073
Si	15.00978506065434	0.09751158950443	-1.84662503881343
Si	15.74724932101893	2.32832795550924	-1.86716398159909
Si	13.99594475284496	3.91734288735681	-2.14516456145905
Si	14.07106514461769	6.31170416977398	-2.21571559374142
Si	15.93348340558245	7.82666044887770	-1.99332455126311
Si	18.17028577892097	7.09858155655380	-1.64545969206455
Si	20.11001476892401	8.49265006093669	-1.38253628268998
Si	21.95240966877350	6.97985002159986	-1.08685543109154
Si	21.16578012901567	4.75200362516781	-1.16599967610730
Si	18.85019919613332	4.84354863726858	-1.52852132779518
Si	18.04438473111688	2.65047231382577	-1.60122792401152
Si	19.84479936015800	1.14594982488679	-1.31313804222428
Si	24.21134180108745	7.63551483049154	-0.76041891313721
Si	31.31007750405615	-1.66561137969407	0.74585439511389
Si	23.43223514229540	-7.38708244879031	0.11814699893375
Si	21.39773935556607	-6.22977023342724	0.12911262273672
Si	20.82554388496735	-4.03332322976732	-0.24895354696945
Si	18.47025770950687	-3.89741919230682	-0.60444428092311
Si	18.16850533674494	-2.62944772360463	-2.58602554955302
Si	16.06341843478156	-2.02086829874928	-1.69832240428097
O	18.47286456315554	-6.35054950804167	-3.02687141366512
H	29.89830499333063	3.81431499364425	3.64522906869239
H	29.35204927760810	-4.41603388125362	3.79954860624556
H	32.17303471304312	1.19528960362106	3.95200560736813
H	26.14353938114256	-6.27495511180379	3.51728790474829
H	26.67635335318704	6.66040297767044	2.83859683526286
H	19.17404470499856	-9.25031437683010	2.88030174828072

H	14.74840884217340	-8.43612157218186	2.05303094973490
H	12.23216784597404	-6.06455755386177	1.47508274778240
H	9.19947808150870	-4.00034697938414	0.87400968331203
H	6.69911988831135	-1.58390538403307	0.29978827211439
H	6.64798039556117	1.69558136666581	0.14794602856540
H	8.97305023246675	4.25979151846863	0.48774792712574
H	12.48124784924010	7.04729240315220	0.70541246930920
H	15.17751143842731	9.16735540049139	1.08562102627751
H	19.68042965959029	9.77616786423010	1.84222137890920
H	24.10247919377634	8.94081647666784	2.43144938489089
H	31.98564082912403	-2.09030734169038	4.01789434010512
H	23.57551386731283	-8.59894310103177	3.35692222696736
H	30.68893603990155	3.73993567717415	-0.35225351428992
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H	32.83233298483295	1.06580943103556	0.22009532084040
H	26.61340245626510	-6.88721696115314	-0.45481975173185
H	27.25667362275192	6.57335241631937	-1.02137392638772
H	19.71218627579650	-8.78946155141632	-1.23752223891628
H	16.04911843903931	-8.42198501013731	-1.79743520759224
H	12.98896994569068	-6.59652495899842	-2.44980892236032
H	9.68586825589709	-4.17943757375303	-3.18388689487403
H	7.19398869198242	-1.73909538877515	-3.48026912512683
H	7.12473593968944	1.52920096677456	-3.60664961689158
H	9.46316968502505	4.10332692680675	-3.55385045529380
H	13.04990933822996	6.92703954370950	-3.12653627158157
H	15.73139598180866	9.03330332756721	-2.85927758456870
H	20.27764481777547	9.70201665636699	-2.25018009566921
H	24.71267259513532	8.82243898512945	-1.52587613250513
H	32.63389370233413	-2.18456176976281	0.26696351379283
H	23.40034965796890	-8.60478801628891	-0.75305579184413
H	20.57268211648296	-6.34099379852821	-2.78632145281383
H	19.97835726801395	-6.28026199813169	-4.49393945437984
H	18.41775026476223	-7.32259114801673	-3.08267536650999

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C	21.10857391270108	-6.03702210286885	-3.60884582137207
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H	20.84624322956619	-6.45476832706125	-4.60048038301348
H	21.93187746196680	-5.30592451611442	-3.72736293741530
H	21.46789293707706	-6.85806962212039	-2.96646904970841
H	19.64773334899188	-4.71466272289422	-3.47660692833881
Si	27.31680249070262	2.31896779184303	2.44208418400067
Si	27.09659126607885	-2.26644821362236	2.50839973673249

Si 29.58168606468289	2.80894663913786	2.87194646165574
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H	24.73935975897792	8.96354596403360	-1.33714905219672
H	32.69995317939384	-2.03080262493520	0.47965036943658
H	23.64017840929657	-8.56895465297687	-0.73798806610502
H	19.06949143519862	-3.52600362453642	-4.18978421536333
H	20.03575998948989	-2.31398673161262	-3.94298805913681

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Si	26.91121030842263	2.11094197603312	3.42007220310427
Si	26.77523812906104	-2.50981359944307	3.40481242103833
Si	29.17224502486099	2.66317093864188	3.78626737442548
Si	28.97964719943683	-3.25616817481550	3.76175316312215
Si	30.70276914537448	0.84721669852104	4.03023729183373
Si	19.17701650728748	-1.28897825616362	2.14046707587919
Si	21.02192003736840	2.54521675949523	2.43795496106560
Si	20.87764957411518	-2.91370371623153	2.35413924557085
Si	23.28419807387751	2.11797714035140	2.79748193230054
Si	23.09515056771739	-2.31690978301137	2.76616316864031
Si	25.08467581566705	3.64090370524077	3.09233249260801
Si	24.82361017133840	-6.27442007192283	3.08008068822370
Si	23.96820599045119	-0.12683968842035	2.88471738176896
Si	25.14510730689627	6.03303647041163	3.10260977590668
Si	24.84923592048441	-3.89302771580725	3.05685495333514
Si	26.28017690367771	-0.18474503701230	3.31259468319546
Si	18.96306145596058	-8.26113997806640	2.11896184396964
Si	17.10184807495617	-6.79068055704570	1.82380918333944
Si	14.86609715779682	-7.49928334837525	1.44778746344250
Si	12.99878420646404	-6.02737210694476	1.13228880793589
Si	13.09674405705391	-3.65411419411336	1.12367995297656
Si	11.23287243709593	-2.17580774749590	0.82615840326818
Si	8.98362381460548	-2.76693601161456	0.45515642496654
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Si	7.53943683207937	1.44747658803227	0.19875169227385
Si	9.17811034943409	3.16222776380266	0.47325333865581
Si	11.39011199747630	2.44542948591105	0.84153246759475
Si	11.87373672522529	0.11426344895683	0.91464894236216
Si	14.18855296734032	0.03712656065623	1.30317072741188
Si	15.05615102607403	2.21147016963954	1.44426710038198
Si	13.32870551847396	3.82709524846505	1.14598878162928

Si	13.30690285530284	6.21642363965108	1.14373394648996
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Si	17.34453928485031	7.04687557597172	1.81448863730302
Si	19.23646595098819	8.49300742381370	2.12476657301340
Si	21.10420650738848	7.01448135071194	2.44067215334504
Si	20.33878527035919	4.78541637047852	2.31480785522496
Si	18.03038094361901	4.78581226542115	1.91715479307767
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Si	19.19192018405938	1.06009536899975	2.11273397759741
Si	23.37061163817884	7.63328287655470	2.80749363659511
Si	30.63084129249808	-1.55097040789987	4.02163056470246
Si	22.88885323838777	-7.65831147597941	2.77232111054526
Si	20.75016967106847	-6.70814206980547	2.43654583681943
Si	19.97089874680370	-4.75961313024486	3.42119472726494
Si	17.99277024774879	-4.70793178379120	2.32641120969142
Si	17.23239692387993	-2.59580024658081	1.77164804323095
Si	14.94862507848751	-2.18698025366308	1.43790384976657
Si	27.31296225154172	2.10771834550922	1.01895685503748
Si	27.17693760572596	-2.51462695325042	1.00040694622949
Si	29.56965483275422	2.66173648070363	1.40742771548026
Si	29.37767628182006	-3.25927364037696	1.37993985178652
Si	31.09450607619765	0.84474442256358	1.67548681680192
Si	19.57045705055204	-1.28202923676818	-0.27684368827030
Si	21.42039194588161	2.54651524347088	0.03394785859296
Si	21.28160235974202	-2.89971210430991	-0.05664086108930
Si	23.68253829747550	2.11975267203607	0.40009409588811
Si	23.50359936063784	-2.31901312635186	0.36190816349670
Si	25.48265632633373	3.63947857614426	0.71925578703981
Si	25.21534206237152	-6.28862200361015	0.70095816474884
Si	24.36112208167777	-0.12511434300401	0.51137056615278
Si	25.54049161095773	6.03177891666406	0.72657080613309
Si	25.24751801196969	-3.90400054777229	0.68926321499831
Si	26.67564751154696	-0.18866464566759	0.92438544828158
Si	19.35532081893190	-8.26516219849238	-0.23398555808570
Si	17.49603000183177	-6.79360976314434	-0.55721855299429
Si	15.25998955568871	-7.51082834600892	-0.92254521582865
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Si	13.48132677563132	-3.66690167992165	-1.25030458296020
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Si	9.36873896713334	-2.77184651520813	-1.92833657688538
Si	7.83647658752793	-0.95560694636648	-2.16540050317634
Si	7.92027785318626	1.44272763142919	-2.15724270187560
Si	9.56412451141568	3.15757385995663	-1.90870096179905
Si	11.78041367691953	2.44123007648250	-1.56047308596220

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Si	15.44985342844914	2.20849178176221	-0.95678571015914
Si	13.71636476331630	3.82456265312644	-1.22878460488718
Si	13.69811637983600	6.21504057044727	-1.23398923030997
Si	15.50688860493249	7.77194479889089	-0.93599755014092
Si	17.73873908349384	7.05022390767962	-0.57517511354997
Si	19.63127412833841	8.49397846931230	-0.25361588323945
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Si	20.72839856552193	4.78529118935993	-0.06816449384626
Si	18.41906220748661	4.78800593387516	-0.46160105376439
Si	17.73440814523240	2.53583809257466	-0.57621109465778
Si	19.58749400937208	1.06428813142844	-0.28427486841485
Si	23.76315954093329	7.62949987763383	0.43071004595769
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Si	23.27266971482387	-7.66444481058573	0.39761476771660
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Si	15.33507636212766	-2.19113078959550	-0.96865018033471
H	29.48532116618970	3.82061234753288	4.68341202416737
H	29.20970304230283	-4.44117761188911	4.64784554854991
H	31.82909723493471	1.25203979564761	4.93539629586971
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H	15.30304352733589	8.99407791387669	-1.77888875404668
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H	24.26637860561882	8.84598050453452	-0.28577342346412
H	32.35396145028218	-2.03408127842898	1.16705749350734
H	23.59186030422696	-8.92523645290803	-0.34624872450232
O	18.84975071285740	-1.59112352082389	4.73244551313238
H	19.78235143426268	-1.48211646026102	5.00266066893647
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C	18.22872435923765	-7.35986728308411	5.65349917043874
H	18.22107658113882	-6.60141991035340	6.45222796412439
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H	19.26409659456972	-7.51694356440846	5.31053892610367
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Si	27.44982717930822	2.36745002750328	2.49707110210793
Si	27.35122373132117	-2.26254874317823	2.76720611071727
Si	29.70198725824681	2.99049151314717	2.79174739139494
Si	29.57833075603494	-2.93522428450063	3.13716760472856
Si	31.25355476294205	1.20720663258752	3.12773263266175
Si	19.54105039151732	-1.02312409817011	1.47528301744962
Si	21.50579791876033	2.72620009821964	1.55158977546598
Si	21.39283341568542	-2.46761878061344	1.85335308948528
Si	23.77470069939559	2.29813125850018	1.92675693555089
Si	23.67786188230295	-2.09939751862198	2.18880985329775
Si	25.58623346568362	3.83487746294787	2.09617614271716
Si	25.38263808042233	-6.06973742639938	2.68288657585402
Si	24.53787802616456	0.08730727981768	2.15726171910042
Si	25.65819346219719	6.22218776759178	1.95835480004259
Si	25.42294563189250	-3.68218521302569	2.53868001379064
Si	26.85192465814649	0.05900155237350	2.54068168394326
Si	19.37986335211584	-8.35969299385280	1.88749319277070
Si	17.5269022224899	-6.87300818790626	1.51060926874074
Si	15.25868089870411	-7.50762285512655	1.18430549808180
Si	13.48560936854759	-5.92132460178832	0.81175089976349

Si	13.54905643929621	-3.53368385083380	0.67749803636294
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Si	14.61180996250347	0.21730372904474	0.65114210509758
Si	15.45994630380748	2.40817188076688	0.63160856800473
Si	13.72032643140462	3.98790678488992	0.24026133747491
Si	13.76088118530997	6.37585363247227	0.09940617500459
Si	15.59671622735969	7.92285802736601	0.28994011391777
Si	17.83967520467318	7.24228502975093	0.68556348353840
Si	19.76355698258182	8.67031943132769	0.88898025867965
Si	21.62141489747924	7.19326136971596	1.27733089538245
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Si	18.52349024711523	4.99595667075707	0.92513537214678
Si	17.74531502282493	2.77890768946706	0.96439861633899
Si	19.59237211223154	1.32819987563168	1.34498462110994
Si	23.89381332319877	7.81846671999147	1.58473005306561
Si	31.20088240683642	-1.18838879030840	3.26706301627236
Si	23.54887896517537	-7.62013940856495	2.49297740059540
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Si	13.85996115030679	-6.06219149507551	-1.56384931030484
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Si	12.06354955340290	-2.20895488551780	-2.10289956776653
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Si	8.26431960746774	-1.04314981196706	-2.74563020389094
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H	30.45658331689993	-4.30557505370031	0.06452673664202
H	32.96571759016477	1.44380336784034	0.23843986537956
H	27.00629270945356	-6.86823121838017	-0.20157932464083
H	27.30534036712795	6.60118776186684	-0.99768982993864
H	19.85914021704128	-9.76864865017140	-1.27131116999616
H	15.37981387269717	-8.90888985606582	-1.95627255968921
H	12.81141556671356	-6.68404904512929	-2.43802668127534
H	9.50607289743710	-4.04347113268767	-3.22604859213981
H	7.13418044320805	-1.50868592159851	-3.61596728528669
H	7.20661795136569	1.76528079808302	-3.80097554205651
H	9.68728781013617	4.22254240071574	-3.70015674068477
H	13.10592654689440	6.78576464011387	-3.21541612713404
H	15.75352435819818	8.95142523103518	-2.99114897965382
H	20.29433680770694	9.68727020528518	-2.41144715649536
H	24.76805729100019	8.83300074073341	-1.58681339506679
H	32.89544071264348	-1.83061958413100	0.43204569242624
H	24.36281754989790	-9.03153303333354	-0.53834317970471
C	19.70277270742762	-4.37504501651835	-3.44922712679801
O	20.35438597333147	-3.50327603373475	-3.80469851371127

- **Hck-HCO-H**

Si	23.07199759659025	-3.30893814561805	4.31938917209486
Si	22.76423022895795	-7.92774187474243	4.61446867876508
Si	25.36790347135155	-2.86513636561390	4.61284671851807
Si	24.91047398295813	-8.81121952937008	4.98495526761825
Si	26.78520739865971	-4.75945569357508	4.94973625075484
Si	15.28478619710188	-6.67463469603961	4.04920979160746
Si	17.13269378335585	-2.97178007115758	3.41007762874670
Si	16.85178192519668	-8.02964552747368	4.92839927596340
Si	19.40860153047550	-3.32371201972803	3.76107288170647
Si	18.93113927165671	-7.59169035073847	3.97764169217884
Si	21.23432683021985	-1.80876778265328	3.91226236545959
Si	20.85923655059885	-11.49499628581475	4.55193033487416
Si	20.11447301026320	-5.54867393310795	3.94057984407617
Si	21.26646916813250	0.57786058327614	3.73020900587360
Si	20.71736201463213	-9.13232849408404	4.34397788914095

Si	22.41911325437880	-5.59806330463818	4.38252023618431
Si	15.02660836357817	-13.72575000490173	3.83907285190786
Si	13.15769660664591	-12.29543503278101	3.44563530411565
Si	10.93226138736165	-13.06239105260399	3.17635244518388
Si	9.15782056048219	-11.50294413107706	2.77713009210172
Si	9.37586349776298	-9.14008830567312	2.62255590405697
Si	7.45108782385243	-7.77163059545879	2.21239926868971
Si	5.23086582558668	-8.47933289666412	1.89201539239352
Si	3.66968257667236	-6.71760527522936	1.47767647504787
Si	3.67461952252604	-4.32300264370602	1.28064090798825
Si	5.22428526237957	-2.50915120792865	1.40693770046205
Si	7.45715026965042	-3.11334818794523	1.84235031610580
Si	7.93205063443538	-5.43795740917208	2.10013888777610
Si	10.24291856898851	-5.41280565127273	2.46349290747586
Si	11.13726908851973	-3.25916065605590	2.47211186052301
Si	9.38453906548642	-1.69782917541669	2.03487793574106
Si	9.36885271669275	0.67852477870645	1.83092280675711
Si	11.22320868002453	2.19988608062869	2.00613011174214
Si	13.42797152044840	1.43697635843372	2.43980763056953
Si	15.32789661976022	2.89430648787255	2.60068121327950
Si	17.20711123807625	1.45670090499710	3.03136004994951
Si	16.42025223910292	-0.76306346075291	3.11738206096441
Si	14.11079860756904	-0.80738262770586	2.74975330784698
Si	13.44020252442858	-3.06224611083666	2.83629373769086
Si	15.30328938117455	-4.48659936717523	3.32988356923925
Si	19.46897310153872	2.12886341500454	3.32500684525052
Si	26.62395790844878	-7.15113341021502	5.10379960921235
Si	19.05128831046869	-13.05507347391738	4.39685003193080
Si	16.87885944856254	-12.22566567754892	3.97430874399878
Si	16.30296049023436	-9.95123317980302	3.71924757496869
Si	13.97751638145782	-10.08710063952661	3.41515383509775
Si	13.45082382772910	-7.82271160228680	3.20509498975587
Si	11.15816954988556	-7.54366694294674	2.77141970356051
Si	23.42475830572107	-3.48908247857550	1.91872321974514
Si	23.12420557529065	-8.09971881894098	2.20842052818802
Si	25.71892438628779	-3.04372947906729	2.23253214230418
Si	25.26738989322107	-8.98543035923105	2.60026390199821
Si	27.13631776990639	-4.93335018981807	2.59648438255636
Si	15.71264776134410	-6.84376637296341	-0.07150698681551
Si	17.48246839424094	-3.19369337704608	1.01676935942937
Si	17.53834113477835	-8.35548680982297	0.14547183820242
Si	19.75939920740340	-3.50200299380287	1.38243237629150
Si	19.29797689537085	-7.77558660532324	1.56921096412697
Si	21.58753394007815	-1.98686634502735	1.53139940758137

Si	21.22031401817372	-11.67829289485841	2.18012808552841
Si	20.44883332665306	-5.72567385598855	1.55904737377764
Si	21.63989168318070	0.39671879268517	1.35657063475668
Si	21.07255915949739	-9.31209905296948	1.98279139304181
Si	22.75090253240197	-5.77379834114848	1.99523495497371
Si	15.38090609303759	-13.92016017938314	1.45934253820613
Si	13.51474410764866	-12.48714564927560	1.06224194929314
Si	11.29070893959048	-13.26197680082726	0.79846391490966
Si	9.52708330242561	-11.69196127520833	0.40027353587444
Si	9.75833006681245	-9.32898920681956	0.25951084725683
Si	7.84436116610534	-7.95721110974693	-0.18171761974788
Si	5.62276444452041	-8.66943372939720	-0.48313325691710
Si	4.05482228319047	-6.90944734919708	-0.86985615065008
Si	4.06815280283153	-4.51534010321232	-1.06393949939169
Si	5.62666652064954	-2.70636086945692	-0.96430260496693
Si	7.86491550319236	-3.30876282849201	-0.55005757311146
Si	8.35018017085538	-5.62952777584720	-0.27310308603515
Si	10.66030875892393	-5.61900717811606	0.07407764111550
Si	11.54682225611079	-3.46617596965951	0.09395079576221
Si	9.79247143029821	-1.89592820059356	-0.33215899603097
Si	9.75687908673986	0.47986404623869	-0.53713247793316
Si	11.60885823370124	1.99923724341732	-0.36159355214854
Si	13.80836856045984	1.21627029237345	0.05506652218787
Si	15.70454150701366	2.67586399996583	0.22675853358142
Si	17.58381468559420	1.24044666943590	0.65293789435799
Si	16.78804147297313	-0.97833546953730	0.73919730641714
Si	14.48182365869284	-1.02925666218370	0.38207079502194
Si	13.85119341379493	-3.29768189717390	0.45760582300907
Si	15.68219726508542	-4.73845755552864	0.93661475046706
Si	19.83842608324624	1.93550077115763	0.95070769327691
Si	26.97881462387502	-7.32544852764829	2.74988203067329
Si	19.43054935921407	-13.26037713210370	2.02827788805324
Si	17.25667250110363	-12.44920048860043	1.60151368102614
Si	16.68407922833232	-10.18969128046701	1.32822772900862
Si	14.35401960315536	-10.28221585571765	1.07391828792299
Si	13.84987966897341	-8.01695388580867	0.78563173663248
Si	11.55678826393760	-7.75353394303887	0.39410204717549
H	25.77663745731796	-1.67541030867497	5.42508346586964
H	25.09966099376170	-9.94175294668163	5.94836440106689
H	27.95454789698888	-4.35671884439300	5.80004873375247
H	21.89360979651224	-11.94905241713628	5.53895587315609
H	22.30168481586981	1.23553366180974	4.59395463807797
H	14.91628828397958	-14.86904840306577	4.80112302364262
H	10.47949168577903	-14.21132513021298	4.02525167277978

H	7.87616969349067	-11.97516793730796	3.39534732944664
H	4.67650788505049	-9.58077828012024	2.74126183510711
H	2.31934030415478	-7.10532594442493	2.00482882022027
H	2.31965834781138	-3.85694992540536	1.72654018918833
H	4.65946301682250	-1.28725267013997	2.06240264355811
H	8.11645311059971	1.32862255119234	2.33859988083415
H	10.79989354449553	3.48827984689243	2.64391222355748
H	15.20244326454911	4.19266738807306	3.33719604667703
H	19.71425716676949	3.41214452069277	4.05969855063280
H	27.72088489776442	-7.60430415649845	6.02177309331530
H	19.18577670197296	-14.19161556427952	5.36432676529914
H	26.36443346405967	-1.97594507495110	1.40463204917547
H	25.69554414433797	-10.23936218786962	1.90285699291085
H	28.50955476830140	-4.62796858797160	2.07357054311810
H	22.49508360064955	-12.23323619750648	1.61640837565350
H	22.90840696885217	0.93206169310224	0.76160742516315
H	15.50828157836517	-15.20243283807413	0.69551918817817
H	11.07826241853950	-14.54430077201969	0.05278022653332
H	8.47446444417290	-12.26832372869318	-0.49846782363189
H	5.35137144657154	-9.90574700702364	-1.28281390616054
H	2.93206654052948	-7.40802986530825	-1.73145889573098
H	2.94581693549904	-4.15472570064298	-1.99256468547699
H	5.34088878131974	-1.62045394627361	-1.95469057811100
H	8.74299696374100	0.99493021357429	-1.51451953928205
H	11.45283771129908	3.15727856041121	-1.29959040845698
H	15.84219215410994	3.81955178349241	-0.73060409493079
H	20.30718374063157	3.09743685866105	0.12826526337823
H	28.28586025225507	-7.88360729788307	2.26867586241665
H	19.84616726521990	-14.52993889559499	1.34911666096056
C	15.30236242698895	-6.41559304327709	-1.93565117759744
O	14.85532429593459	-5.32654974304378	-2.25421303096348
H	15.45304059602144	-7.21475737022242	-2.71651741935166
H	18.03965577920881	-8.68880702681470	-1.22780001890624

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Si	-7.81139390804850	2.31551623351424	-1.30287254149573
Si	-7.78093037247713	-2.28764360255961	-1.34813940377868
Si	-10.09426078985440	2.89481882056853	-1.32174535404508
Si	-10.00385818689707	-3.05730343488772	-1.37619110303717
Si	-11.65545402263234	1.08754634930249	-1.34877337458437
Si	-0.35477370217432	-1.22785438991670	-1.39715587387291
Si	-1.83266850166944	2.58682491461287	-1.26475389315936
Si	-2.01259685159859	-2.22117508991331	-2.77108591113824

Si	-4.11847671510372	2.13197548808709	-1.25107028658069
Si	-3.81468862897704	-2.20067128998584	-1.27882367171404
Si	-5.87772119629270	3.73844979737679	-1.24788331463772
Si	-5.98432986754175	-5.93765108621282	-1.31569415843875
Si	-4.90106082817296	-0.08510588672077	-1.16819977048066
Si	-5.92355589798865	6.13359823746610	-1.23489029159887
Si	-5.76713178934080	-3.57928474660219	-1.29213944024557
Si	-7.24695155406229	0.00967959589114	-1.29440000547295
Si	-0.12800378930748	-7.79260872275689	-1.39207593833112
Si	1.70706019821769	-6.28292435064238	-1.41291050776400
Si	3.83299491209934	-7.32792436187203	-1.44498495897502
Si	5.76918723750679	-5.91418852172174	-1.43714384030405
Si	5.65581692768699	-3.53866403849727	-1.37407519149705
Si	7.67125341066066	-2.24499793175916	-1.33434402835375
Si	9.87228659528340	-3.07784836443299	-1.32628867063365
Si	11.58034880031781	-1.41068931478597	-1.26118565463562
Si	11.70324185098555	0.98622628233003	-1.21034225822700
Si	10.22112491232772	2.85998120269268	-1.19446746140544
Si	7.91264362013205	2.38174205379562	-1.22871176846780
Si	7.24466047016836	0.09273136998606	-1.27840428935126
Si	4.90263320899185	0.18760377016747	-1.34091749249638
Si	4.21106347484019	2.41412302401609	-1.24562831968351
Si	6.05902347245642	3.91391973259220	-1.20111723504021
Si	6.08423933348164	6.30262649764671	-1.16170037748408
Si	4.20902216118400	7.80964723596552	-1.14692092740623
Si	1.94707359035205	7.07905271269523	-1.17393675447154
Si	0.04404992625365	8.54485787044766	-1.16057800212549
Si	-1.86949145246196	7.09355716976858	-1.19859098003052
Si	-1.16095265567287	4.84096637254718	-1.21685858682491
Si	1.17903166294498	4.84512722069544	-1.21460915039971
Si	1.88958010788985	2.61314318529770	-1.26422487114637
Si	0.03349222084321	1.11452648791901	-1.28197696878175
Si	-4.14723631814546	7.75637954793010	-1.19962648682358
Si	-11.63726549908743	-1.31378899076973	-1.37170247551961
Si	-4.01037821053821	-7.26815970188448	-1.33512942137656
Si	-1.89803453729220	-6.20652761783876	-1.39705095190352
Si	-1.02957664025606	-4.21794672832076	-2.22817316614079
Si	1.18183760133737	-4.48256008977581	-2.79881150170068
Si	1.62061769631203	-2.62122994623727	-1.46512332796451
Si	3.88258944596498	-1.93821792457515	-1.35389852828853
Si	-7.83992260963421	2.29882423791476	1.13023058763205
Si	-7.82476903059119	-2.30192179295644	1.08597710517716
Si	-10.12623556802941	2.87176055661295	1.09033645189256
Si	-10.04630656647303	-3.07637608969973	1.04209005152302

Si	-11.68956341851625	1.06545899867968	1.03677892229913
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Si	-1.84829137274958	2.56646291485249	1.16475949114837
Si	-1.92878236454688	-2.35298707649816	2.36627953397907
Si	-4.13573675595821	2.13995336270246	1.17135920287328
Si	-3.91815419484761	-2.20821252838813	1.16056398779960
Si	-5.90961114243289	3.73026399003466	1.16264589208420
Si	-5.97241075621464	-5.97088534708340	1.09067204387434
Si	-4.91152804140385	-0.06875869746743	1.23453097828128
Si	-5.95450125436261	6.12241285435631	1.17551462570752
Si	-5.82661445914407	-3.61335908158759	1.10851487213336
Si	-7.25366715196640	-0.00695345306303	1.12063244178182
Si	-0.15045025515505	-7.87762945303710	0.98549254504013
Si	1.77350490762735	-6.50770447036404	0.99507256154889
Si	3.93042482514332	-7.43717070833149	0.95217103018077
Si	5.81685251208590	-5.97742027294690	0.97349553076382
Si	5.65415200025226	-3.60745237153181	1.02338281819987
Si	7.65687471657844	-2.29842484385838	1.09999557590649
Si	9.85610399557747	-3.13192391077116	1.09058658356061
Si	11.56054913438696	-1.45932950648604	1.12680952291346
Si	11.68733534217247	0.93784336675922	1.17469482561106
Si	10.20932258975976	2.81358734340990	1.21668198391248
Si	7.90195063783328	2.33570205948885	1.20553352348306
Si	7.25106517261775	0.04185322695227	1.13703903355261
Si	4.90697346588601	0.15284483957021	1.07158625985870
Si	4.20664429382357	2.37666774841924	1.18067983904991
Si	6.05343576555434	3.87345614740429	1.20675361108510
Si	6.07226281376933	6.26294198458668	1.24634616691428
Si	4.19754415555599	7.77230364714379	1.26157095227030
Si	1.93494815835115	7.04513747053141	1.24535716573117
Si	0.03007556106464	8.51098665982028	1.25219026602463
Si	-1.88657342694204	7.06185736744029	1.22572574612815
Si	-1.16688490849778	4.81332784526466	1.18587923871745
Si	1.17188232435079	4.80924017259500	1.19815671124413
Si	1.88811950914259	2.57533630555871	1.17558493405774
Si	0.01402871446547	1.09573447015545	1.13959526024902
Si	-4.16555343942679	7.72975117494039	1.20897545491491
Si	-11.67995669321996	-1.33525874776357	1.01421764328889
Si	-3.98245987884083	-7.28525225455680	1.05738021114615
Si	-1.86437539036656	-6.22844837240483	1.02750769930191
Si	-1.24829748493511	-4.58981810379065	2.59984259443071
Si	1.08586023572640	-4.53735114444576	2.02607033876803
Si	1.62789526092059	-2.54375208887707	0.92492253441832
Si	3.90533178613480	-1.98788868858069	1.06744933850413

C	2.08349919557468	-4.37790698440823	3.56966410408828
O	-1.57621290443539	-5.14743052206895	4.16331571849974
O	2.74472191976734	-4.26647371293282	4.51038590197648
H	-10.53283367024508	4.06368728466915	-2.14857222012267
H	-10.38044316095075	-4.23025215794250	-2.22784677197392
H	-12.90490492166973	1.51396623442209	-2.06241945085788
H	-7.09333010976432	-6.50758840080139	-2.14678499839145
H	-7.09527680464054	6.70355505602188	-1.97869700651502
H	-0.18967162705432	-8.96764641918041	-2.31368036217742
H	4.00784313523492	-8.54325892967263	-2.30217311195920
H	6.89228698657175	-6.48949447077851	-2.24702065435569
H	10.21655319096526	-4.25586835991356	-2.18400575272394
H	12.80759313467974	-1.90111267358114	-1.97140790345002
H	12.98378005444835	1.36831291113833	-1.89294926228547
H	10.72592181406626	4.01514680944842	-2.00216351964142
H	7.23896381377357	6.92194191189329	-1.89101068180900
H	4.53195770912408	9.05579310000098	-1.91448181694447
H	0.05918365570330	9.78287877808352	-2.00360255829797
H	-4.51982790693503	8.97518436307417	-1.98786384234929
H	-12.86707302940115	-1.75870619037220	-2.10717009508250
H	-4.07063689654357	-8.51510256950392	-2.16049801477527
H	-10.59448368136645	4.02140665996250	1.92806991980549
H	-10.43900804984311	-4.26285665971209	1.86747794295211
H	-12.95685117206714	1.48482536291522	1.72273599592257
H	-7.04717087284347	-6.58617852953430	1.93493660865394
H	-7.14019383078464	6.69105602194465	1.89779959678972
H	-0.23526366683690	-9.06652559687217	1.89015630564447
H	4.08756872066633	-8.69827881183228	1.74289149425954
H	6.95966649591553	-6.56126916621276	1.74901102460626
H	10.19046464043440	-4.34480916390896	1.90286354117510
H	12.77497182399812	-1.97996771624492	1.83771900490844
H	12.95918704933489	1.28631783565946	1.89078401500547
H	10.70600542256399	3.93517580204961	2.07508829127740
H	7.21763940118906	6.85929903510616	2.00892074554814
H	4.51716961669536	8.99194205135145	2.07194277141338
H	0.03753208987739	9.72455725155191	2.13038402211845
H	-4.53934907198159	8.93380304296810	2.01916446506642
H	-12.93471387413756	-1.79118615781047	1.69892509655353
H	-4.03357133972520	-8.53053389710298	1.88873995778197
H	-2.00937070509597	-1.76610131967233	3.74097323360286
H	-1.66311107812341	-6.11524052065966	4.23658512993894

- **Hck-CO+H₂O**

Si	-7.88647170586605	2.46105062879534	-1.22884852396292
Si	-7.82758321051376	-2.15787507041118	-1.32225928323793
Si	-10.17771987548844	3.01075425763173	-1.18691255399582
Si	-10.03656296632143	-2.95936372200751	-1.31592601730946
Si	-11.70953263707611	1.17692782246550	-1.20119165453886
Si	-0.20351612393922	-1.19849175997782	-1.34971359729377
Si	-1.82747004974221	2.59283272467903	-1.23820587853164
Si	-1.89127260394117	-2.42233835609132	-2.36645518668449
Si	-4.13798030667696	2.28072182462420	-1.22600231884589
Si	-3.95763413760237	-1.97258679327176	-1.55972947073121
Si	-5.92775679709871	3.85256822042270	-1.19245559212320
Si	-5.97864254500430	-5.79693174055029	-1.39427397314652
Si	-4.99302741198712	0.09987399815220	-1.22375749380569
Si	-5.92559072141488	6.24424200548292	-1.15898773139178
Si	-5.80129194908116	-3.43179494383374	-1.35253075935518
Si	-7.34055256881515	0.15477677233128	-1.26014738069623
Si	-0.02076266011712	-7.98684769274941	-1.35808882583985
Si	1.68743393741619	-6.30906824080071	-1.23699058209308
Si	3.81979614080005	-7.34920134157276	-1.27305940253479
Si	5.79304607298308	-5.98735199389049	-1.29854714665327
Si	5.73241824664318	-3.61003982071888	-1.28733353464637
Si	7.74092811249866	-2.30569991159029	-1.28972800680962
Si	9.95638429986722	-3.10182073614555	-1.29307278949831
Si	11.64983981752925	-1.41889809177336	-1.27171514806988
Si	11.75305424513722	0.97890175713001	-1.25935617963822
Si	10.24689150234006	2.83248771386248	-1.25835133383143
Si	7.94583061921671	2.32235323292380	-1.25847879327704
Si	7.28118884272690	0.02796116462484	-1.27009013916760
Si	4.93717738625652	0.10158517101125	-1.33173278113384
Si	4.25718707357921	2.33551245470817	-1.25547820692885
Si	6.09376306387467	3.85423401802658	-1.23566702081322
Si	6.11712451016161	6.24469536756290	-1.21428046370333
Si	4.25904463156105	7.77538380951610	-1.18805268788053
Si	1.99531076887762	7.05694836500814	-1.18823006032003
Si	0.09537229557523	8.52285421470047	-1.15815314545989
Si	-1.82518155926615	7.07703947162169	-1.17001352027480
Si	-1.10429787031940	4.82849554911520	-1.18647695594378
Si	1.23507058048650	4.82070676869557	-1.20475281347182
Si	1.94206175298287	2.58545827423937	-1.24559853864446
Si	0.05542394473109	1.13208716896394	-1.26530588801240
Si	-4.08991373642841	7.79430995490926	-1.14543579616041
Si	-11.67598710260223	-1.22382561820732	-1.24953621508112

Si	-4.17949954071659	-7.37587521246041	-1.44148534351571
Si	-1.94889897545692	-6.60002275759818	-1.47320265911026
Si	-1.07907469416317	-4.41239804149691	-1.50199436906920
Si	1.01198509132868	-4.54563244790760	-2.62307070580067
Si	1.66430854263846	-2.69526532250247	-1.34352175220022
Si	3.93134657519038	-2.03406400469938	-1.29404338972791
Si	-7.86800964834402	2.40843812636448	1.20659709242623
Si	-7.80261041856864	-2.20674741851979	1.10731180850873
Si	-10.15978773348465	2.95785599481261	1.22627437930527
Si	-10.01331896120570	-3.00782948314209	1.10361135529404
Si	-11.69396194210978	1.12810760617939	1.18481259294978
Si	-0.29370291612447	-1.21941747240895	1.14983168778926
Si	-1.82226165335194	2.57158622541731	1.19439546819532
Si	-1.86543334330916	-2.51749128705415	2.30578613566746
Si	-4.12792591372224	2.24366336672561	1.19228090622362
Si	-3.88842630985637	-2.03823718941014	1.33318623885395
Si	-5.91966945220674	3.81494072658518	1.21986597107739
Si	-5.97729952178928	-5.83654119778853	1.00563503784653
Si	-4.94670884227845	0.04777485197864	1.21226006544544
Si	-5.91631919135799	6.20890406156403	1.25173861314288
Si	-5.76746452263821	-3.46816947196048	1.06107076955017
Si	-7.29427240589786	0.10417114978621	1.14516145958511
Si	-0.11070191030733	-8.06805581789870	1.03222052019584
Si	1.73299832681905	-6.58784915081234	1.18236874752742
Si	3.92544077880136	-7.43384226487062	1.12483184637408
Si	5.83661424219721	-5.99991221765528	1.11360722996140
Si	5.74840573611081	-3.62889849776842	1.11292921905790
Si	7.75471532203976	-2.32213590413078	1.14626136541931
Si	9.96727795243667	-3.12162295563670	1.12385407276403
Si	11.65417050671021	-1.43066110919547	1.11626411933425
Si	11.76038682179908	0.96806122913010	1.12622241602367
Si	10.26130416620799	2.82754369500146	1.15278650466759
Si	7.96245024106207	2.31433652273266	1.17576057354103
Si	7.33692046518507	0.01484062483490	1.14650905744964
Si	4.99283936008515	0.10695423469764	1.08410650359935
Si	4.26711623482063	2.32334792077829	1.17294636893483
Si	6.10330818473399	3.83661430327127	1.17230447800729
Si	6.13017167886679	6.22413941633262	1.19344856718963
Si	4.27153029935314	7.75224699645810	1.22048901430115
Si	2.00796803676243	7.02908503223532	1.23483479807517
Si	0.10677207197380	8.49438073697997	1.25650612614873
Si	-1.81489606841627	7.04932096264711	1.25018532145463
Si	-1.09641676323397	4.80296222164850	1.22058096360904
Si	1.24259441241511	4.79230748665084	1.20264845428691

Si	1.94817319290826	2.55272586659044	1.18734892551882
Si	0.04988933785372	1.10550489157576	1.17293667078610
Si	-4.08068690122960	7.76097384474123	1.26569893865902
Si	-11.65503123984660	-1.27226227186398	1.13661185871174
Si	-4.18260030975769	-7.41206964987416	0.96454314591765
Si	-1.97639842648790	-6.58774257537442	0.93943951350016
Si	-1.29513287051657	-4.33963854655975	0.94109392917638
Si	0.88728975899635	-4.54046002519686	1.80279797297038
Si	1.70366265661266	-2.50320409237300	1.05911864484525
Si	3.98931653181797	-2.02159632187444	1.13259495250132
C	0.85317910396492	-4.27059471348347	3.67644438395164
O	-1.08797544313532	-5.77426840644694	4.10041538247950
O	1.07874568463430	-3.96178292864188	4.76136402848782
H	-10.65650843222171	4.18209414964902	-1.98721871268980
H	-10.41458647037362	-4.12234044181143	-2.17955312729753
H	-12.97917720590162	1.59856257993000	-1.88085018304062
H	-7.16227613881369	-6.25796778014864	-2.19062338030333
H	-7.09062839232894	6.84448608309442	-1.88857094707711
H	0.14823516586001	-9.17281601453234	-2.25516669601126
H	3.98337910051531	-8.58160214028304	-2.10944858393587
H	6.90477673589917	-6.60119859217010	-2.09577822962666
H	10.30586041759868	-4.28871170783257	-2.13645424889799
H	12.87485081764368	-1.90966290596678	-1.98573184732717
H	13.02105411131199	1.36562461786277	-1.96254098096300
H	10.72324663210466	3.98019803086341	-2.09374475044406
H	7.26477316764425	6.85809533087323	-1.96004178940090
H	4.58235023515931	9.01315741481595	-1.96871930913771
H	0.09992736508380	9.75809126042081	-2.00552715854157
H	-4.43494881105294	9.02845644001390	-1.92246686166061
H	-12.92359746061823	-1.66531813212386	-1.95600257985905
H	-4.52363785529440	-8.56610875045221	-2.28402189507369
H	-10.62037384925426	4.09439655026144	2.08526891424884
H	-10.38010716100444	-4.20344087080538	1.92691325913554
H	-12.95489057160141	1.51970803098549	1.89781027577103
H	-7.15650137730014	-6.32048680285176	1.79509498934852
H	-7.07347215103261	6.79088697999621	2.00832178312995
H	-0.17934557982536	-9.25386144883427	1.94424522741995
H	4.13241478826079	-8.69128145179956	1.91174019396128
H	6.96677958809222	-6.59561970466242	1.89875759867918
H	10.32783463128077	-4.31882634621658	1.94798144063872
H	12.88172016700100	-1.92726614297438	1.82196017189652
H	13.03404454923914	1.34185757368987	1.82628168603901
H	10.75112973295943	3.96957486997595	1.98813650680707
H	7.28804356410845	6.81946155947907	1.93790773165428

H	4.60218360191754	8.97454772735675	2.02221928959952
H	0.11512693264774	9.70926684748440	2.13287089615108
H	-4.42233936348512	8.97206643988822	2.07975774696743
H	-12.88899571036248	-1.74683063991411	1.84576678628210
H	-4.44958151249926	-8.63466839093505	1.78829381764249
H	-1.74676175423466	-5.13121013672402	3.76215634145621
H	-1.11645720787819	-6.48237130232815	3.42299403813178

Transition states

- **TS1'' (Hck...H₂ → Hck-H₂) in 55**

Si	26.9292914	2.4708135	3.2061685
Si	26.8708473	-2.1395963	3.4623246
Si	29.1684722	3.1328589	3.5068453
Si	29.1067200	-2.7757924	3.8384520
Si	30.7475850	1.3743490	3.8432123
Si	19.1965430	-0.8484490	2.2404306
Si	21.0250364	3.1407784	2.2474510
Si	20.9750910	-2.3906255	2.5841365
Si	23.2260053	2.4113780	2.6101519
Si	23.2521865	-2.0238835	2.8889279
Si	25.0581751	3.9152501	2.8049182
Si	24.9846740	-5.9999848	3.3833926
Si	24.0082286	0.1966204	2.8563495
Si	25.1779012	6.2909968	2.7060312
Si	24.9839212	-3.6113301	3.2401489
Si	26.3287738	0.1707277	3.2365521
Si	19.0055823	-8.3022561	2.6263224
Si	17.1546414	-6.8098927	2.2775980
Si	14.8856678	-7.4421172	1.9634675
Si	13.1216741	-5.8444102	1.6071040
Si	13.2274831	-3.4582141	1.4963786
Si	11.4005564	-1.9354444	1.1362755
Si	9.1357213	-2.4842021	0.7856792
Si	7.6296092	-0.6662278	0.4276334
Si	7.7222901	1.7279501	0.3124639
Si	9.3821995	3.4319462	0.5087203
Si	11.5756928	2.6805179	0.9174439
Si	12.0520817	0.3572557	1.1065211
Si	14.3750542	0.2912485	1.4600978

Si	15.2431748	2.4832916	1.5535418
Si	13.5209580	4.0635914	1.1365755
Si	13.5003998	6.4414553	1.0094439
Si	15.3974985	7.8809786	1.2365069
Si	17.5679507	7.0424547	1.6054287
Si	19.4542268	8.4748497	1.7295322
Si	21.1328641	6.8185703	2.0716095
Si	20.4681257	5.0572112	3.4685896
Si	18.2135013	5.0660503	2.6010740
Si	17.4978659	3.0175836	1.8206969
Si	19.3016383	1.5124073	2.0779626
Si	23.3048548	7.7401003	2.3162280
Si	30.7170694	-1.0204629	3.9762947
Si	23.1681962	-7.5675705	3.1996926
Si	20.9267154	-6.8755337	2.8326071
Si	20.2547804	-4.6249524	2.5945852
Si	17.9379413	-4.5819991	2.2705405
Si	17.3235227	-2.3225708	2.0648448
Si	15.0492893	-1.9407033	1.7070432
H	29.4638623	4.3527119	4.3235038
H	29.3768297	-3.8992904	4.7906215
H	31.8701688	1.8530221	4.7159082
H	26.0251416	-6.5438446	4.3170784
H	26.1875856	6.9181348	3.6206408
H	18.8541597	-9.4784963	3.5406520
H	14.3848700	-8.6108700	2.7563771
H	11.8437452	-6.3729292	2.1875163
H	8.5347264	-3.5919048	1.5941824
H	6.2682746	-1.0304276	0.9427913
H	6.3976278	2.2475662	0.7879364
H	8.8923124	4.6606825	1.2099640
H	12.2678770	7.0970111	1.5571540
H	15.0887624	9.1614664	1.9487293
H	19.3959471	9.7118764	2.5674133
H	23.4299156	9.0245846	3.0767516
H	31.8338496	-1.4253555	4.8927381
H	23.3836935	-8.7430319	4.1038975
Si	27.3122746	2.3241038	0.8043388
Si	27.2440659	-2.2830338	1.0607853
Si	29.5460208	2.9930871	1.1247585
Si	29.4782018	-2.9140139	1.4587738
Si	31.1214075	1.2381324	1.4884362
Si	19.5368713	-0.9864855	-0.1586228
Si	21.4233345	2.8552366	-0.2014150

Si	21.3309193	-2.5203897	0.1800300
Si	23.6376560	2.2708653	0.2246925
Si	23.6140728	-2.1693960	0.4900210
Si	25.4510960	3.7884896	0.4382002
Si	25.3460127	-6.1408963	1.0062865
Si	24.3788285	0.0467706	0.4850389
Si	25.5814807	6.1602437	0.3307511
Si	25.3480966	-3.7524571	0.8660475
Si	26.6998531	0.0268157	0.8486665
Si	19.3581203	-8.4364557	0.2460212
Si	17.5127151	-6.9417807	-0.1144467
Si	15.2437121	-7.5751370	-0.4137974
Si	13.4864658	-5.9720811	-0.7701453
Si	13.5971037	-3.5855462	-0.8794011
Si	11.7808287	-2.0609305	-1.2651193
Si	9.5169957	-2.6146607	-1.5923383
Si	8.0114290	-0.7938377	-1.9249175
Si	8.1098836	1.6011196	-2.0407572
Si	9.7717715	3.3066407	-1.8723029
Si	11.9687331	2.5574958	-1.4858355
Si	12.4295212	0.2320057	-1.2792293
Si	14.7486677	0.1700851	-0.9168720
Si	15.6484981	2.3459702	-0.8408684
Si	13.9187893	3.9310762	-1.2286277
Si	13.9072914	6.3133832	-1.3631857
Si	15.8117539	7.7562104	-1.1282993
Si	17.9504327	6.7959895	-0.7807090
Si	19.7662364	8.3330270	-0.6272648
Si	21.5346187	6.7803230	-0.3527409
Si	20.7163061	4.7989912	-1.1503292
Si	18.5728593	4.8235099	-1.8548501
Si	17.8862649	2.9986691	-0.5910702
Si	19.5954930	1.3706819	-0.3074140
Si	23.7160092	7.6075289	-0.0421847
Si	31.0855178	-1.1566131	1.6215350
Si	23.5247599	-7.7036875	0.8221731
Si	21.2842870	-7.0132327	0.4395778
Si	20.6169486	-4.7585650	0.2131946
Si	18.3003075	-4.7169819	-0.1117531
Si	17.6799779	-2.4641898	-0.3401065
Si	15.4134551	-2.0655179	-0.6882810
H	30.0900567	4.1179719	0.2998617
H	30.0087013	-4.1316889	0.7678096
H	32.4671538	1.6344059	0.9565040

H	26.6022692	-6.7782712	0.4914035
H	26.8332767	6.7125249	-0.2827107
H	19.4429818	-9.7077372	-0.5403714
H	14.9813399	-8.8321696	-1.1863728
H	12.4260501	-6.5668723	-1.6484077
H	9.1888770	-3.8149748	-2.4249762
H	6.8753882	-1.2269823	-2.8039362
H	7.0151322	2.0422948	-2.9668032
H	9.5469434	4.4485265	-2.8141218
H	12.9100436	6.8726980	-2.3337476
H	15.7034387	8.9523031	-2.0235066
H	19.8903935	9.4688682	-1.5899211
H	24.0486587	8.7983292	-0.8867779
H	32.4195567	-1.6467907	1.1407100
H	23.9758896	-8.9690094	0.1582131
H	17.5700918	5.1541817	4.1464769
H	18.5789946	5.1450802	4.2741515

- **TS1 (Hck-CO₂ → Hck-COOH)**

Si	-7.94076868513584	2.36613408475388	-1.25784292322211
Si	-7.70983707984750	-2.26578918986941	-1.35891476535498
Si	-10.24106979513447	2.87182077613816	-1.29856226312289
Si	-9.91859442434716	-3.07568407590743	-1.42020460094498
Si	-11.73087490125494	1.00652617246134	-1.36154263047439
Si	0.32809795566991	-1.27519338217143	-1.18560108441383
Si	-1.91930575499582	2.54799070892493	-1.14856283236394
Si	-1.65916085033960	-2.61307053556254	-1.17951859542350
Si	-4.24262350288944	2.38459149622118	-1.16638797755677
Si	-3.92705669050692	-1.95184991822357	-1.23348365585596
Si	-6.08633237749806	3.88911601303008	-1.18301112301561
Si	-5.78951993572172	-5.93410312594874	-1.42795133247137
Si	-4.95386672601289	0.16598685414479	-1.25591210951237
Si	-6.11371522025146	6.27461415715602	-1.15703117188562
Si	-5.69281544469290	-3.55856435144347	-1.33469630763123
Si	-7.29546216112470	0.07056760337207	-1.28129679036318
Si	0.11506638038252	-7.93206060346144	-1.34419963420153
Si	1.91074944070736	-6.35985958898939	-1.28337803931274
Si	4.06806066631732	-7.33021734464617	-1.33482610987449
Si	5.98276890466163	-5.90841786980387	-1.34221785737329
Si	5.78655411054996	-3.54128525776981	-1.30253103813423
Si	7.79335692830726	-2.23809266113067	-1.37914980555501
Si	10.02109417923702	-2.99191585388186	-1.44366115142306
Si	11.64294760144464	-1.23698554339873	-1.46017594301675

Si	11.65943271599074	1.16456267576588	-1.42961819028900
Si	10.10091981088029	2.97373646168304	-1.36926265186743
Si	7.82249291078189	2.38122676437126	-1.31132335431323
Si	7.27791283465428	0.06810427130910	-1.31025180254587
Si	4.93530092761290	-0.01385270700055	-1.17449152845275
Si	4.11500473261255	2.18699050316801	-1.18737333437038
Si	5.87931347346938	3.78788248759157	-1.21909531299512
Si	5.91655859806156	6.17934170719383	-1.20698193053170
Si	4.10044325849781	7.75123164999550	-1.16518154024400
Si	1.83945054830816	7.03639984664625	-1.15173874311519
Si	-0.07686709640579	8.48210816573610	-1.14125594590800
Si	-1.97875916608447	7.01886240000109	-1.14243820791309
Si	-1.20996831616527	4.78341946552329	-1.13096479381634
Si	1.12830770274767	4.78703060761030	-1.13652301881805
Si	1.81465962716956	2.54296233612011	-1.14891966521265
Si	-0.04635993587498	1.06625642522940	-1.12369900884203
Si	-4.23275780452451	7.77040326596227	-1.13383548737237
Si	-11.61235562253294	-1.39127520667314	-1.41147222084779
Si	-3.89587568555044	-7.40316927155668	-1.43457610026662
Si	-1.73510705193662	-6.44617783846291	-1.28510287531513
Si	-1.13824608797192	-4.51021990569923	-2.41081675844172
Si	1.07006755897116	-4.29287476718388	-1.94382068179320
Si	1.94780217145071	-2.25812784884064	-2.60395536631057
Si	3.85423396849096	-2.12849075734857	-1.27275394591995
Si	-7.99662944029094	2.32827377525766	1.17621713221231
Si	-7.77298943459540	-2.32317539134536	1.07757458288791
Si	-10.29966683661890	2.82554555707954	1.11162677072679
Si	-9.98178748493182	-3.12818275478887	0.99451391980690
Si	-11.78526195909253	0.95621615050975	1.02280208137342
Si	0.16613639322669	-1.22012351278589	1.30222147103295
Si	-1.95582792526654	2.55593233009634	1.28675313181424
Si	-1.78849292786147	-2.59487669788013	1.23152413204250
Si	-4.28367569408795	2.35633441727958	1.25895458890276
Si	-4.04942740747774	-2.00124956486901	1.18551801879724
Si	-6.13582128294062	3.85599500683866	1.22504503222866
Si	-5.86636937832674	-6.02638831605544	0.98132780793198
Si	-5.01963167283919	0.14039799234475	1.15960901463652
Si	-6.12731965600853	6.24588412600863	1.25022416492522
Si	-5.77227325473997	-3.64397717283565	1.06244384087340
Si	-7.36241997937182	0.02462248529325	1.13595119736055
Si	0.09550747400299	-8.08769731163724	1.04073221442370
Si	1.92596553380807	-6.55807020151650	1.13847969468375
Si	4.11950972193269	-7.43007374858912	1.06168235303125
Si	6.01664057548705	-5.97129516356955	1.06187196849684

Si	5.90193471171856	-3.60658316104282	1.09881433964193
Si	7.87835674812021	-2.26304640217092	1.05541464707172
Si	10.10432634186092	-3.01853900836136	0.97259515879826
Si	11.72556380330095	-1.26563912540842	0.92524753316800
Si	11.73622344672107	1.13510396838832	0.95473149833219
Si	10.17790840569255	2.94457552645563	1.04213644300607
Si	7.89550751724038	2.36183357556576	1.12176025035551
Si	7.33952050760344	0.04667977753469	1.10377875067768
Si	5.00024680962027	0.02137353899304	1.23257517590215
Si	4.15792430192371	2.20579251921994	1.23419675215830
Si	5.95061384437091	3.77686899154403	1.19121615726004
Si	5.95734488843772	6.16767554029046	1.20334165097076
Si	4.12428816922903	7.72837293555694	1.24448752556341
Si	1.85042416475922	7.03600014573443	1.27224265661809
Si	-0.06963489987172	8.48357959886230	1.27299911667664
Si	-1.97467459418539	7.01805678140206	1.27841786906153
Si	-1.21560125158727	4.78126718752578	1.28110935762020
Si	1.12630656411418	4.78702501186656	1.26864669672437
Si	1.84819180010096	2.54989735763997	1.28215912728380
Si	-0.05422101227596	1.11637417371434	1.29879066781893
Si	-4.23866141021004	7.74356137562612	1.27475305294125
Si	-11.67145332800023	-1.44149968862461	0.97523062202982
Si	-4.02006263085748	-7.55605911093541	0.95890974332947
Si	-1.83364128821486	-6.69854301305513	1.11222583109911
Si	-1.21630490676656	-4.68534099559364	2.00823795648811
Si	1.12164355144477	-4.58694602087022	2.05378723545687
Si	1.99166359638974	-2.43332530952312	2.10852183246099
Si	4.06402981504670	-2.12338260561405	1.16975860555613
C	0.37591047334402	-4.47104415620518	3.89383842386449
O	-0.92052457222799	-4.74892515464860	3.81591279542890
O	0.87455675689552	-4.01094369440091	4.94123636834382
H	-10.70327431288161	4.03201829276669	-2.12438209297450
H	-10.24655677235470	-4.24970248376339	-2.28971156861108
H	-12.98875602469598	1.39306452149337	-2.08271713288418
H	-6.92002220206048	-6.48382251209390	-2.24550949066018
H	-7.25983723118269	6.88605406329889	-1.90603175499683
H	0.18987550043782	-9.07132618582249	-2.31029849281700
H	4.18328501013024	-8.54998939351037	-2.19451073199224
H	7.10619891326726	-6.45170484240180	-2.17226231450670
H	10.39040400310262	-4.15947662293566	-2.30534891958214
H	12.86289629294600	-1.67467360302601	-2.21607600943555
H	12.89653937982429	1.59283591564707	-2.16311187910034
H	10.52109822259031	4.14450823759864	-2.20277152045876
H	7.07402157988768	6.75942762422596	-1.96442933687787

H	4.43210412543377	8.98145902315740	-1.95387631305216
H	-0.08370396868889	9.70775637220326	-2.00234629296504
H	-4.53330219678681	9.01695092884828	-1.90961471395776
H	-12.81936738132868	-1.87500517937281	-2.16021642605866
H	-4.08433350398462	-8.58227393467759	-2.33812506162957
H	-10.81919804220050	3.94761006417238	1.95595241695865
H	-10.35225367013768	-4.33764858149755	1.79582750952562
H	-13.07498094383391	1.31366454246448	1.70164230720453
H	-7.03367630801308	-6.62847982688012	1.70563198684102
H	-7.26820307759632	6.86750823801398	1.99952431978856
H	0.15712549241891	-9.32380832842435	1.87997973082656
H	4.34626595921658	-8.68563872715094	1.84488160397768
H	7.14372137059727	-6.55539467130842	1.85918456388140
H	10.51682679125764	-4.20467161579356	1.78823265676761
H	12.99314057983173	-1.72097174772498	1.58630111428222
H	13.01662334636458	1.54965458812352	1.61867535505913
H	10.65986185527853	4.09179516120061	1.87508164339835
H	7.12669212816686	6.76582298170483	1.92813850998052
H	4.48692073610007	8.93989708104195	2.04893599068674
H	-0.07978849007287	9.70860508760244	2.13519285104218
H	-4.56137783127291	8.96847991191913	2.07613301430608
H	-12.91423408663845	-1.95181848605244	1.64343865661502
H	-4.28289614938758	-8.82443344195669	1.70887662419335
H	2.31719961857347	-2.51148103167232	3.94706005691265
H	1.84051790977061	-3.15200727885409	4.44062438842125

- **TS2 (Hck-COOH → Hck-HCOOH)**

Si	-7.99625711240153	2.30040669089382	-1.24842142093195
Si	-7.71846676283445	-2.33401971224977	-1.31176425308617
Si	-10.30455122030220	2.77624226322544	-1.24850898901086
Si	-9.92023110560212	-3.16593214060964	-1.32784764621834
Si	-11.77526124947038	0.89445143802100	-1.26969958743487
Si	0.29953410456549	-1.22475599032570	-1.33712602514637
Si	-1.97186515054368	2.56792438253405	-1.23001571385394
Si	-1.66455618426572	-2.59320900194666	-1.29278884777901
Si	-4.29541796459572	2.36024649910148	-1.23553493248916
Si	-3.94460646029893	-1.98389906728753	-1.28609493981499
Si	-6.15623449631616	3.84862067305677	-1.21334237315104
Si	-5.73586502369029	-5.99954298964258	-1.33706639466141
Si	-4.98012254333924	0.13040035100161	-1.31260999534439
Si	-6.17959089339351	6.23796087215197	-1.18069635690832
Si	-5.69261361625539	-3.61730659276009	-1.30844375224058
Si	-7.32032977372164	0.01029970406981	-1.27112747300556

Si	0.12878877324070	-7.93101214360107	-1.39636823012017
Si	1.97885541242450	-6.41445303469948	-1.48162545858927
Si	4.18323385138411	-7.29257723257524	-1.52121503869000
Si	6.01599300842383	-5.77012730553393	-1.41862496488569
Si	5.75209905531830	-3.42412787867424	-1.26653866760127
Si	7.77854114202860	-2.16233037102953	-1.31436917448132
Si	9.99480825742778	-2.94901925613557	-1.38981466205232
Si	11.62513758887738	-1.20164531928138	-1.40303069765607
Si	11.64294884879141	1.19894080240008	-1.37481278292240
Si	10.08427538746749	3.00563610119412	-1.32285813525377
Si	7.80071643064806	2.43288672394218	-1.23947984236681
Si	7.23775900982490	0.12812344537875	-1.22051493945600
Si	4.88984784098624	0.02836170465592	-1.17609984011146
Si	4.08747112925273	2.23372389128038	-1.17038244712119
Si	5.85677664301575	3.82858660463685	-1.18096038296543
Si	5.86439222233421	6.22181578086484	-1.16998497833422
Si	4.04098656693508	7.78654470540982	-1.14114748995520
Si	1.77903461410407	7.07002043032035	-1.15215238243197
Si	-0.14692682269942	8.50595131426481	-1.13213386337367
Si	-2.04239202655510	7.03284041594363	-1.16155303189638
Si	-1.26154434574691	4.80317894460076	-1.18299887928394
Si	1.07627550822189	4.81849874231466	-1.18226191280045
Si	1.79044101364154	2.58390128492458	-1.20602964088496
Si	-0.07548253628172	1.11087729950063	-1.24843680363923
Si	-4.30793619316435	7.75146687544804	-1.15266915540424
Si	-11.63312898602036	-1.50206840393774	-1.30192503168374
Si	-3.79407723239037	-7.40097589078318	-1.31395957953854
Si	-1.66041692477536	-6.38440117647773	-1.20591694142077
Si	-1.10891099356401	-4.52163844455483	-2.45949052317471
Si	1.10507693701090	-4.32494225373398	-2.03821674372631
Si	1.96758827011001	-2.26571540687937	-2.64440194314423
Si	3.79904833976960	-2.06594942043748	-1.25045203530403
Si	-8.01387540254304	2.27303836604928	1.18650817382721
Si	-7.74001418630778	-2.36865781338747	1.12551248548993
Si	-10.32176108927987	2.74825196385805	1.16197382895161
Si	-9.93940833795287	-3.20165089819514	1.08785694018700
Si	-11.78879849647035	0.86334157592718	1.11552454370337
Si	0.19379685876387	-1.20966327656715	1.12952634774075
Si	-1.99471156126613	2.54160543389772	1.20477726317691
Si	-1.73174415192423	-2.60015336679412	1.10622173680929
Si	-4.31539252241695	2.33213896938147	1.19023693907613
Si	-3.99769362490133	-2.01546507684679	1.13789168100185
Si	-6.17227028587942	3.81903726893009	1.19485663776585
Si	-5.77551273840566	-6.03569703662644	1.07469152266293

Si	-5.01782807585450	0.10808816292200	1.10269484606927
Si	-6.18861691606873	6.20667323946975	1.22660565483048
Si	-5.72054670253461	-3.65679961843515	1.09216202824227
Si	-7.36080169845750	-0.02192992183926	1.14707817390827
Si	0.16353558894921	-8.08248196869437	0.98515834381956
Si	2.01862043186435	-6.59245826742084	0.92828130618589
Si	4.20951172172112	-7.45157104384333	0.87127205470374
Si	6.03919964588996	-5.90979587727428	0.97910766185064
Si	5.87092914590284	-3.53883414000305	1.13591127836766
Si	7.86780600261115	-2.21468944034817	1.11758600256588
Si	10.08505304256445	-2.98913553461624	1.02661046007987
Si	11.69770998768621	-1.22828674419510	0.98230545678169
Si	11.70510638726278	1.17437024591532	1.01001797858347
Si	10.16944169521106	3.00646827219297	1.08829314803536
Si	7.88385445773516	2.43957183088699	1.19385359267033
Si	7.38716050791872	0.11283738948399	1.18545089609918
Si	5.04560915815932	0.08029597138534	1.24177849543392
Si	4.12559382068948	2.23474731750686	1.24841105669064
Si	5.90858988392438	3.82031982644781	1.23048094093928
Si	5.89215211005200	6.21178611644989	1.24075070375482
Si	4.04666235363895	7.75394617742225	1.26918964699913
Si	1.78069706148614	7.03510533590163	1.26873592344260
Si	-0.14863912870933	8.47169042433888	1.28251635686636
Si	-2.04751540017047	7.00071015741585	1.25908485441481
Si	-1.26877559544627	4.77001474181285	1.22703434549981
Si	1.07186652040496	4.78204587201576	1.22272170698871
Si	1.80697116262282	2.54664997137005	1.22753598426478
Si	-0.09197334534121	1.11216297968228	1.18583031815213
Si	-4.31469969666656	7.71825757851631	1.25579643611027
Si	-11.64822431250862	-1.53354077394327	1.08575635167725
Si	-3.88767505746796	-7.51091172586551	1.08011855324168
Si	-1.70571888123377	-6.62585539592711	1.21820864034567
Si	-0.98522634763096	-4.58384818224810	2.02071663429728
Si	1.34737518458287	-4.61886038781943	1.86649550163833
Si	1.93078951595417	-2.36225022473471	2.16468936616431
Si	4.04878282972746	-2.03156014627024	1.30286470136833
C	0.77988527957084	-4.46038314508911	3.76391429023198
O	-0.57740863821523	-4.42525315980906	3.76566497719155
O	1.25609453490465	-4.97846825981959	4.92343511138045
H	-10.79845745761013	3.92341371852601	-2.07428294465734
H	-10.25054940302568	-4.34979746807891	-2.18317351918329
H	-13.04915940734584	1.26299051701543	-1.97212428067369
H	-6.85254818947095	-6.60831173332856	-2.13183890020140
H	-7.32496821080168	6.85849202052182	-1.92385668807407

H	0.05232201741461	-9.06416199537687	-2.36977703559127
H	4.41327358848307	-8.46481473427102	-2.42325263367641
H	7.18370330030155	-6.19153028586856	-2.25823230339038
H	10.34289731548698	-4.11336327349640	-2.26442430823924
H	12.84569426505517	-1.64710322385845	-2.15328104743117
H	12.88434055010246	1.62933307499024	-2.09967782266502
H	10.48840040764196	4.17073233408070	-2.17198847292524
H	7.02272900268227	6.80510474399904	-1.92382590726744
H	4.38833506007475	9.01757312703569	-1.92212872281699
H	-0.15436363890354	9.74394409302604	-1.97562018495933
H	-4.62754860138425	8.99693558633822	-1.92283890672398
H	-12.84859043817875	-2.00415602342630	-2.02456266849236
H	-3.93481384325728	-8.60679942706718	-2.19086080880255
H	-10.83363169411003	3.87300126320270	2.00746534968829
H	-10.28279735993285	-4.40881345961124	1.90467821057807
H	-13.07067372740225	1.21248253648761	1.81340967799026
H	-6.92303057145678	-6.63527814620778	1.83174149903431
H	-7.33820658908295	6.80910197981580	1.97811563910090
H	0.30105877034104	-9.31550181395009	1.82087715732371
H	4.44496963424370	-8.72011471386493	1.63123254545894
H	7.18123107411215	-6.48148513759547	1.76508733047607
H	10.50450996540845	-4.17740098053902	1.83554114417612
H	12.96685735194271	-1.67283451629683	1.64764257426170
H	12.98750272650576	1.57991943880495	1.67594874864655
H	10.68278673187239	4.15413492692384	1.90162100409180
H	7.05470832404455	6.81613661237434	1.97127154031717
H	4.38573057424570	8.96710301721272	2.08135066194605
H	-0.16625175090816	9.68490260162603	2.16132423268816
H	-4.64139938020029	8.94024401256076	2.05997216107129
H	-12.87301188293332	-2.05243791781675	1.78023414664750
H	-4.13470979946768	-8.77351956448265	1.84566511466944
H	1.23171967672730	-3.10426218808133	3.73780339131009
H	2.22182157506428	-5.09053067187082	4.83296604736096

- **TS3 (Hck-HCOOH → Hck-HOCHOH)**

Si	-7.92826302563646	2.30021034186433	-1.26953591589101
Si	-7.70042579375145	-2.34199947898505	-1.43549933795541
Si	-10.23020401695538	2.79291188730913	-1.18206230677256
Si	-9.90451978366560	-3.16548173772011	-1.41107956311703
Si	-11.71039818743112	0.91725134639302	-1.21141848514771
Si	0.27419147722624	-1.11595713912629	-1.64033050668676
Si	-1.88929414853582	2.60855211541477	-1.34737270612522
Si	-1.69849634637547	-2.32747747052144	-2.19156319625643

Si	-4.20587583046373	2.29246227493491	-1.31665185929213
Si	-3.91968038167039	-2.03299368532201	-1.51560737692006
Si	-6.04974335011084	3.80146787801754	-1.22217497473154
Si	-5.73005349978738	-6.03169403245784	-1.44089623320034
Si	-4.96743122445864	0.07652766114412	-1.30664078976417
Si	-6.13839017767369	6.18934041736529	-1.12943979330919
Si	-5.68795107248844	-3.65053304505006	-1.47984125683397
Si	-7.31059816542915	0.00095422955758	-1.34886623875931
Si	0.24334928631464	-7.72233230342934	-1.14567428602832
Si	1.99928135267862	-6.16421835349505	-0.80017905411279
Si	4.05227262192456	-7.22936422348679	-1.25772886826297
Si	5.98234867061585	-5.85055174478257	-1.44560081309591
Si	5.75933841555471	-3.46992973759818	-1.53408633551831
Si	7.75296915643816	-2.12192584695656	-1.52495124191060
Si	9.97850820345872	-2.88875497220509	-1.50954181907797
Si	11.63129221165191	-1.16750434643580	-1.42437466959300
Si	11.67223694982985	1.23218751790476	-1.34249644103088
Si	10.13075080591364	3.05758758770817	-1.30226762301201
Si	7.83830842617358	2.51088838471820	-1.36754968002267
Si	7.25139975946918	0.20147102904228	-1.45127965020784
Si	4.90398043582643	0.16467564056156	-1.45397024820416
Si	4.16223529699941	2.39485604804557	-1.37444031656346
Si	5.93232156885743	3.98688519980785	-1.30575591199736
Si	5.90107825466231	6.38090794180930	-1.21312426742455
Si	4.04056833184984	7.90895689696625	-1.13249869572882
Si	1.77386324282720	7.19472276354091	-1.13584371931434
Si	-0.17421363205307	8.60047012488520	-1.06045701420962
Si	-2.04259426517325	7.09401437129714	-1.12109789285165
Si	-1.25503257095577	4.86842022305092	-1.21787564919431
Si	1.08555457821416	4.94088549978246	-1.22627831732764
Si	1.85266711031893	2.73291872429089	-1.35650173204476
Si	0.03564184435022	1.20873819589122	-1.41791287365768
Si	-4.32025241084332	7.76487982660557	-1.07761063895822
Si	-11.59406889315846	-1.48000993414984	-1.30281501374306
Si	-3.75022597509341	-7.35066160048627	-1.33963104346238
Si	-1.66323828466954	-6.33909057609273	-0.92259764828610
Si	-0.95720577601372	-4.17535074266258	-1.20562255670505
Si	1.38374159844635	-3.92496526140408	-1.00884538073063
Si	1.87822803852808	-2.46609913788663	-2.81451743243553
Si	3.86863876658287	-1.96424731393110	-1.61259209238003
Si	-7.87215324499695	2.20171523912476	1.16249495021124
Si	-7.65814375318453	-2.40910746057008	0.99835381766295
Si	-10.17571349693760	2.69204541142547	1.22705510292396
Si	-9.85643866254645	-3.24728688914569	1.00399261670998

Si	-11.66714557442041	0.82822819898955	1.17229937328347
Si	0.14078106967267	-1.31049439964868	0.78129976412496
Si	-1.85131398504904	2.49854744284628	1.07982713895363
Si	-1.67776497730747	-2.67225865694815	1.44580802592776
Si	-4.16239872887803	2.21808377653686	1.10119138394521
Si	-3.86545336861333	-2.12796121055717	0.87584884825421
Si	-6.01228635900674	3.71605865970699	1.18782078207918
Si	-5.75134929226901	-6.05244624957216	0.96776287698120
Si	-4.86308375772308	-0.00825681914879	1.10810368406558
Si	-6.12144502576262	6.10055694102257	1.27801301716151
Si	-5.64124582751629	-3.68605761150403	0.92088979864013
Si	-7.20765826373732	-0.08403310533652	1.06352526866077
Si	0.21643821943882	-8.21541903276832	1.19165176778066
Si	2.07654025811902	-6.74940841071481	1.54517153129230
Si	4.28572765108158	-7.48988850860164	1.11185866906763
Si	6.02934268854055	-5.84666516998462	0.96579416389708
Si	5.77539544510232	-3.50394012328068	0.86584003417087
Si	7.74457691532194	-2.16858317137152	0.91179635048123
Si	9.95837234716486	-2.95952273151219	0.90690439471127
Si	11.62041891102068	-1.24689688267372	0.96217066636355
Si	11.66075158341281	1.15104568428787	1.04216320992151
Si	10.10491701410597	2.96026344562259	1.10691124775380
Si	7.81172080189836	2.41646277261578	1.06384700722953
Si	7.18416166552759	0.12422716964525	0.96515357943250
Si	4.83287674364806	0.11435685057391	0.95066535275556
Si	4.14497474664722	2.34423229209392	1.04801321096287
Si	5.93034434325924	3.90605886882461	1.10331017747571
Si	5.92071130536764	6.29410117089490	1.19395572860603
Si	4.06422627502901	7.82172873062098	1.27404546046630
Si	1.79763196884191	7.10007183357270	1.28255999396756
Si	-0.15770198419771	8.49852721661762	1.34948124854143
Si	-2.03100728680427	6.99290613355577	1.29837561299836
Si	-1.23672483806372	4.76861385596908	1.18949465481068
Si	1.09698361871010	4.84737065690345	1.18685805128030
Si	1.84481851142391	2.62917498929493	1.07356817168362
Si	0.05485191923577	1.05252728099592	1.00580807918941
Si	-4.30637017956308	7.67502625787321	1.32867517391208
Si	-11.55255158651287	-1.56782548708396	1.08299229866391
Si	-3.94376911299112	-7.62968071890998	1.03200472656434
Si	-1.74549935623565	-6.86395174774976	1.45109382527977
Si	-1.00586527143428	-4.80828793616404	2.18119721813685
Si	1.30303667676898	-4.74386656281901	2.45309680786117
Si	1.81602944956178	-2.90272058275583	1.14621717209605
Si	3.92716377487715	-2.05591884618692	0.81275386969513

C	0.59647245116973	-4.45974735695143	4.28595815039706
O	-0.88934773769736	-4.31657479759133	3.94322038003625
O	0.76516695826024	-5.45441872786463	5.21848742802769
H	-10.75227848846378	3.96410471746213	-1.95481994289534
H	-10.27113110940787	-4.32870639655848	-2.27964109525980
H	-12.99930235912167	1.30659692171713	-1.87383841182484
H	-6.79855977778192	-6.71043423406684	-2.24386152614346
H	-7.31254454616261	6.78759844124304	-1.84556044446611
H	0.32621562704796	-8.69504385614665	-2.27889131930888
H	3.90195959472094	-8.37351185503042	-2.21149360684077
H	7.05993957207430	-6.50925618943432	-2.25446918223593
H	10.37515129010715	-4.04727104804003	-2.37194441545228
H	12.87393041166755	-1.60185707491029	-2.14485360338168
H	12.93972603373159	1.66368546367763	-2.02065936341879
H	10.61447323949673	4.24276347611136	-2.07955578581181
H	7.04096973711065	7.03811461813135	-1.93397916121773
H	4.35687099809824	9.17028014968784	-1.87791709093045
H	-0.21482311072074	9.86138460405694	-1.86791317443433
H	-4.68561349699456	9.01169889231385	-1.82474611094059
H	-12.83142684451140	-1.95212114708505	-2.00791252411370
H	-3.65057830113588	-8.48812018211367	-2.30685221547649
H	-10.64418604853785	3.79881571737360	2.11994032381085
H	-10.17328422465842	-4.46845258282390	1.81057909513672
H	-12.92755650691222	1.17290979684984	1.91003860952277
H	-6.92802677474448	-6.56409569127534	1.74329490639545
H	-7.29113510973765	6.62535114674031	2.05604127905295
H	0.20295863841607	-9.56630436145936	1.83489443078073
H	4.78051577783938	-8.72990264506540	1.79271475334585
H	7.23384511379410	-6.27851576518339	1.74794393255818
H	10.30684986184448	-4.16904924345993	1.71883901399683
H	12.85092025997194	-1.74085771923307	1.66478338185335
H	12.91577804335012	1.54562882243502	1.76451732136627
H	10.54462340105936	4.08558921399742	1.99191102155053
H	7.08141949357406	6.87397338663472	1.94671472323069
H	4.40039697262566	9.02314645749797	2.10482490606135
H	-0.19634728382761	9.68676352545871	2.26102664989505
H	-4.65943836334730	8.86251243677886	2.17212944317298
H	-12.76261502891759	-2.09763570741131	1.79439196884103
H	-4.36198556156009	-8.90431944962655	1.69694132923206
H	0.86848419857972	-3.50400525209937	4.76233569233501
H	0.73670336167783	-6.31908775891695	4.76466405685580
H	-1.68210297668088	-2.29046462285501	3.25682243006179
H	-1.31793436764111	-3.11935243129523	3.72819943785642

- **TS4 (Hck-HOCHOH → Hck-OCH-H₂O)**

Si	-7.83876681328449	2.35949952306765	-1.26916417589279
Si	-7.70187480820841	-2.25512869817115	-1.46570813302843
Si	-10.13411104169261	2.88835731345686	-1.24245873903452
Si	-9.91207655453228	-3.06155865511135	-1.50496488951850
Si	-11.65218611889939	1.04559387342176	-1.32121022672417
Si	0.06214924021254	-1.09407353933426	-1.56059237397068
Si	-1.84230883576468	2.66154331747432	-1.25472207843412
Si	-1.77826754335163	-2.20326709525812	-2.63036446416978
Si	-4.13738553625104	2.25677626806563	-1.24251568808774
Si	-3.79010976684404	-2.08781615574332	-1.40450651270323
Si	-5.93276806511593	3.81985442902964	-1.16861530318830
Si	-5.88297436860058	-5.91609480903363	-1.48560175554012
Si	-4.88496864806907	0.02874664888375	-1.24623671142848
Si	-6.00047947397147	6.21116243431589	-1.05978454030856
Si	-5.68665778504013	-3.55172251019901	-1.46413188882124
Si	-7.23234730837551	0.06117979120002	-1.35718666923981
Si	0.00274183188874	-7.57237175951838	-1.25485202833363
Si	1.83042127586166	-6.11032936124853	-0.86451933662188
Si	3.86825380029831	-7.20083343242329	-1.35409596894802
Si	5.81970517758561	-5.84695442127681	-1.50065042650699
Si	5.63948841394511	-3.46410647078270	-1.51625737059763
Si	7.67594218127445	-2.18623293318120	-1.48033547796152
Si	9.87443300150349	-3.02600054708155	-1.47758175236954
Si	11.57374678585058	-1.35150832199697	-1.35974684350118
Si	11.68294379964396	1.04471401233730	-1.23556766841896
Si	10.19967835666006	2.91738045264908	-1.16588678628430
Si	7.89082605597417	2.44450998136802	-1.24381413687840
Si	7.25366283716199	0.15014944305052	-1.37232941966489
Si	4.90764658976941	0.18039794301158	-1.38133845662502
Si	4.20975538183479	2.41847347875728	-1.25100142686565
Si	6.02026844151868	3.96297732122217	-1.16028895043512
Si	6.01971292490797	6.35409295965742	-1.03486455415379
Si	4.15941537904813	7.88093787517747	-0.94527718130652
Si	1.88707516160250	7.18234447743146	-0.97344008086725
Si	-0.03615280511240	8.62179898079908	-0.89463288557926
Si	-1.92939052133188	7.14869454415341	-0.98621027052455
Si	-1.18800909202081	4.91046586088454	-1.09625128367823
Si	1.15333553299694	4.94369221884083	-1.09205279024533
Si	1.89779885630755	2.73047077564824	-1.24740553500078
Si	0.05396179471693	1.24002169187766	-1.32917050554838
Si	-4.20722550350435	7.81288329647510	-0.96319158895525
Si	-11.58025977944055	-1.35286427975722	-1.42786710086389

Si	-3.89774513015380	-7.21670677871806	-1.42463404081257
Si	-1.85104312819424	-6.10752892712715	-1.04272983168440
Si	-1.03863408728898	-3.99246566998462	-1.48387188575600
Si	1.26652905363591	-3.85211201775692	-0.97871955780412
Si	1.77155645813874	-2.32850310047293	-2.72188361247983
Si	3.79144175152676	-1.90732073887214	-1.54290036251055
Si	-7.84243370187895	2.25088493586123	1.16191553778160
Si	-7.72733339777256	-2.34371759817447	0.96587937534384
Si	-10.14102899750941	2.77438155177887	1.16693343289596
Si	-9.93300416039969	-3.16218624292372	0.91096482067803
Si	-11.66748894999566	0.93978006939600	1.06220072983971
Si	-0.06196464005736	-1.30797085247581	0.85748381592711
Si	-1.82439690736862	2.51418960463577	1.16901949037588
Si	-1.79453707376655	-2.46212545686505	2.01872879630452
Si	-4.12935428612122	2.16803818898571	1.17670961087516
Si	-3.85852559517020	-2.17033713992857	1.00472534213693
Si	-5.94110653648849	3.71619021597100	1.24146357538409
Si	-5.91058534912169	-5.99116572740538	0.92095654947896
Si	-4.86671094349800	-0.05018779340120	1.15975318277726
Si	-6.02184592100078	6.10346268876029	1.34756634484765
Si	-5.71290750319648	-3.63318611756331	0.93416718656421
Si	-7.20838183850062	-0.03885832171826	1.05718428549639
Si	-0.02798331333016	-8.10945898072635	1.06493286404428
Si	1.91501980379159	-6.77004934954636	1.46281431370535
Si	4.11258180107186	-7.52925492860949	1.00103432228638
Si	5.87601372361236	-5.90738843090417	0.90979600343043
Si	5.65414425352685	-3.55788296874003	0.88083281897568
Si	7.66156921895289	-2.27786484145038	0.95386468809186
Si	9.84871568537564	-3.13868123695191	0.93705500850281
Si	11.55587980626966	-1.47196069576878	1.02507453078820
Si	11.66258624942552	0.92244785509960	1.14704352998730
Si	10.16526844920136	2.77975268067249	1.24075986329560
Si	7.85561795316444	2.31174847577150	1.18580385948929
Si	7.17990213890250	0.03345022734466	1.04156734455780
Si	4.82931486973862	0.09734065848365	1.02082582318063
Si	4.18283765531592	2.33718615754336	1.16656649826604
Si	6.01245233467110	3.84734888001084	1.24799510162317
Si	6.02523223095805	6.23356914397093	1.37113023364775
Si	4.16614401468929	7.75968443849636	1.46006529450436
Si	1.89123352458828	7.05971510958296	1.44197910133887
Si	-0.04162427718366	8.49150360485811	1.51412916344003
Si	-1.94282092025768	7.01922999221287	1.43189357929564
Si	-1.19018378341939	4.78026850850920	1.30542165010972
Si	1.14607591980252	4.82284091434382	1.32095941377861

Si	1.87941570694053	2.60284921368410	1.18753240506321
Si	0.06696671409242	1.05406269989504	1.08925433088037
Si	-4.22159852600391	7.69479529033864	1.44210199697457
Si	-11.60453236715061	-1.45789933930882	0.95662224851104
Si	-4.05876939265770	-7.50831550420996	0.94613607016217
Si	-1.89377664966844	-6.63651518144418	1.32002454284771
Si	-1.12780669091533	-4.69956109495468	2.32145408674319
Si	1.22087414637706	-4.72502722911719	2.34836015881179
Si	1.71021158063855	-2.80597576940338	1.17549830989255
Si	3.85590019464623	-2.04278812158098	0.87753937129559
C	0.65510899534059	-4.88358426266500	4.23862557635696
O	-0.80173520444808	-4.89915365164090	4.16267860775778
O	0.71014875432939	-6.32539519208582	4.72316480411615
H	-10.61319133131198	4.07491256175463	-2.02019751902559
H	-10.27381415398393	-4.21223042299428	-2.39287235201371
H	-12.91748712702748	1.46536110229055	-2.01049354139354
H	-6.95763827667320	-6.53142186114280	-2.32919333676499
H	-7.17066289557914	6.81130427875041	-1.78169156739136
H	0.06642029318835	-8.52556433879125	-2.40556940454697
H	3.69178382963589	-8.31494032342461	-2.33798012573447
H	6.88530804995560	-6.50280494595107	-2.32739776158307
H	10.23771317694838	-4.17969198630842	-2.36099349457714
H	12.80567833931276	-1.80876295513531	-2.08448544220821
H	12.96581963369509	1.44866683505129	-1.90170441843855
H	10.72320824890662	4.09953230317977	-1.92156221392106
H	7.16811761456116	7.01061931642244	-1.74249463405263
H	4.48821058551319	9.15300993817733	-1.66700736189654
H	-0.04542294061377	9.89316709774297	-1.68676059559380
H	-4.57397515878705	9.06443911628109	-1.70180091428059
H	-12.80614255651203	-1.79864564269628	-2.16950368016994
H	-3.76180949789545	-8.34540732105205	-2.39736476540768
H	-10.62096972017997	3.88399816704766	2.05076980896368
H	-10.28835757714848	-4.38480504295156	1.70007757877195
H	-12.93805826597595	1.30722351856151	1.77160979675043
H	-7.06092037312487	-6.53196507538176	1.71615600523992
H	-7.20621846739016	6.63101115840292	2.10218238349612
H	-0.13446865563447	-9.45915850842075	1.70413494548102
H	4.56145200576677	-8.80068620984426	1.65518907151099
H	7.06925195757118	-6.38725704477580	1.68164720032570
H	10.16141202578588	-4.37124570854555	1.72900604279259
H	12.77139720834712	-2.01162296870598	1.72034709531088
H	12.92822916680358	1.26565769496978	1.87727800242460
H	10.64224971158117	3.87343140405616	2.14589770139262
H	7.18131736494344	6.79998788153520	2.14107418890414

H	4.50712240053289	8.94892628880819	2.30675876431809
H	-0.05682906441307	9.67012314732791	2.43911433870300
H	-4.59420553957566	8.86892968430342	2.29612112060622
H	-12.84334409473895	-1.96684996493997	1.63328576310798
H	-4.37238743118686	-8.80824677040317	1.62009382846110
H	0.99861001687242	-4.26770980766601	5.08264447012783
H	1.04520381863595	-6.87645876825726	3.96062890064826
H	-1.79652106415903	-1.97181731356795	3.43660965760243
H	-0.46057242400467	-6.11093827955736	4.56632713947401

• **TS5 (Hck-OCH → Hck-CH₂O)**

Si	-7.81490568798427	2.33218138667111	-1.22105485519780
Si	-7.55807485756795	-2.25230908390253	-1.34746119178457
Si	-10.11948354568678	2.81667574842289	-1.21081869300125
Si	-9.73913260789445	-3.12894708350509	-1.39379976282738
Si	-11.58928499297193	0.93674617567227	-1.27683578385504
Si	0.05637923655057	-1.18161934054132	-1.71359931315765
Si	-1.81380332821036	2.64263501519681	-1.31059934390298
Si	-1.79619586298319	-2.31104338729223	-2.74310207206261
Si	-4.10765225333399	2.28693652820624	-1.24088766299847
Si	-3.61320962686601	-2.05394021903958	-1.27439901184646
Si	-5.92118310128117	3.81291732115291	-1.16574791113415
Si	-5.85958253726143	-5.80918756935969	-1.47834421333452
Si	-4.79235421608864	0.04992248390304	-1.10996273692426
Si	-5.96460889852247	6.20524461052286	-1.08589985847112
Si	-5.51735724723795	-3.47583898756508	-1.36765397948817
Si	-7.14439202377408	0.05770756308047	-1.27022986805937
Si	0.00468239190372	-7.63788023592282	-1.19076379327790
Si	1.77427657416856	-6.14141150737539	-0.73884349679666
Si	3.79885133906474	-7.28665027539961	-1.08555878171027
Si	5.77468040909467	-5.96691816030449	-1.25306295744817
Si	5.61605335271907	-3.57930933482387	-1.39657170923120
Si	7.65145388924640	-2.29986049257988	-1.35655354489680
Si	9.85505807088978	-3.12657169359293	-1.29697230460100
Si	11.55169829300477	-1.44866839294192	-1.19889012083975
Si	11.66682569062305	0.94874003958209	-1.13062249375342
Si	10.18608412883874	2.82505756502981	-1.12472331929835
Si	7.88073409189200	2.33720707674880	-1.22349761197120
Si	7.24119969874585	0.04164872164353	-1.31282368318027
Si	4.89918756104501	0.07235195438103	-1.39869462192941
Si	4.18940316368874	2.30553881342783	-1.32061144396079
Si	5.99915893505590	3.84922545425669	-1.19733246396059
Si	6.02588773607702	6.24435592457063	-1.10211801754750

Si 4.19834669690171	7.81220786977192	-1.02769644425064
Si 1.92865892483604	7.12349232436512	-1.05049818814668
Si 0.02064944038172	8.57868388264254	-0.96867958968711
Si -1.87831827745448	7.11262870450162	-1.05448642411237
Si -1.13229664249786	4.87776994476684	-1.15802236669889
Si 1.20853518128792	4.87976703872663	-1.16106127089845
Si 1.88642232497607	2.64445893426136	-1.34273650551275
Si 0.03892804599505	1.15430128477407	-1.42559579574844
Si -4.15418277210007	7.78795744520049	-1.02463127273805
Si -11.45032420500291	-1.45917563163613	-1.36259978051630
Si -3.95589679279901	-7.22042478662894	-1.48746980800496
Si -1.88090422637998	-6.19596067818589	-0.99567611057766
Si -1.10227614004383	-4.03521824209960	-1.41260878598240
Si 1.24251736674804	-3.90395225365809	-1.03344509976817
Si 1.80950076761567	-2.42781303316840	-2.79082443416635
Si 3.77257591677725	-2.01047527553622	-1.52347468404119
Si -7.81317662228637	2.25747425897435	1.20258157092699
Si -7.62169922562473	-2.33482886367642	1.09845075085959
Si -10.12608604300599	2.72541912449150	1.20039102589432
Si -9.80174697462597	-3.20649260598600	1.02060683183917
Si -11.61045000420564	0.85349745693814	1.10725467851792
Si -0.06350999966933	-1.40507513362729	0.70394665177807
Si -1.79106691472581	2.48746373092933	1.10755044567009
Si -1.64330461972680	-2.62987534427643	1.95152286934999
Si -4.10100360655397	2.20649469292302	1.20080667255160
Si -3.75607847788785	-2.11788169862411	1.20185046450703
Si -5.91589646745768	3.74394374896469	1.25764446923417
Si -5.90550424773083	-5.96262058258237	0.92138474606783
Si -4.80572783403005	-0.011111705775255	1.28448438728424
Si -5.97497747588988	6.13479989632205	1.32126276336134
Si -5.59492917542902	-3.60538471980371	1.04258755527753
Si -7.14023271519621	-0.02609635925715	1.15147597681781
Si -0.05011715052591	-8.21197880588104	1.13007616045085
Si 1.73712129680802	-6.69675321282379	1.61858061183071
Si 3.94737758819260	-7.49133355307838	1.30021976621466
Si 5.76216882225632	-5.92413198474654	1.15623585588152
Si 5.59717320221884	-3.58054918745795	1.00945669564251
Si 7.60978532796464	-2.32616731544027	1.08691359456639
Si 9.79826021543122	-3.18051073034738	1.11770120930092
Si 11.50424781208007	-1.51193187691988	1.18847625105668
Si 11.61876436699159	0.88391842783431	1.25415178453440
Si 10.12224819612450	2.74395381843686	1.28451743170043
Si 7.81869661327545	2.25506690839941	1.20608744069074
Si 7.15061741013696	-0.01895148702240	1.10570249843033

Si	4.80222002993750	0.04344851145494	1.00608777860335
Si	4.14072036045905	2.27459937939375	1.12775235557303
Si	5.96672374959549	3.77665063924247	1.21418766581362
Si	6.03095350739717	6.15867143333407	1.30321176504561
Si	4.20298231792101	7.71541241682186	1.37881864672613
Si	1.93495982840491	7.00707780569773	1.36517796399549
Si	0.01905626608042	8.45234202386914	1.44043174486583
Si	-1.89087188090742	6.99036112511197	1.36506934603721
Si	-1.15049197233657	4.74902750648148	1.24180745900185
Si	1.18348200765249	4.76873708505422	1.25057377473175
Si	1.84670903674979	2.52532408958833	1.12261792471281
Si	0.04653564783181	0.95872260237186	0.98656197533953
Si	-4.15761628052158	7.70212634704590	1.38381404666604
Si	-11.51042036222130	-1.54305346091861	1.02345734552041
Si	-4.19225523903018	-7.63717677384674	0.85811507527808
Si	-2.01418108345622	-6.89166350387529	1.31327479591883
Si	-1.35750687765860	-4.94254588375251	2.28095109352388
Si	0.97160936577890	-4.63242861849939	2.48880261456962
Si	1.65913723545345	-2.90987053551836	1.11954232052287
Si	3.78913853880835	-2.08677103511133	0.90405917385064
C	-0.01456467827940	-4.16396674359901	4.09974746818451
O	-1.12483594490947	-4.92413769824227	4.07771586812194
H	-10.61466711115190	3.98735542893510	-2.00181701613218
H	-10.05153563678859	-4.29351590263718	-2.28228171432621
H	-12.86405687294374	1.31193522039745	-1.97386204496529
H	-6.98842943758767	-6.28572100253442	-2.34026525652710
H	-7.13365819512598	6.80382191365566	-1.80966397608362
H	0.10906085276238	-8.57159499480677	-2.35525777849872
H	3.64680963641366	-8.45199609622615	-2.01337218376364
H	6.85774448407764	-6.66053813466826	-2.02493518678533
H	10.23116004499082	-4.30051964327564	-2.14734267657652
H	12.79281479472354	-1.92334337623054	-1.89602862574734
H	12.95721183959608	1.33446928089703	-1.79271240802483
H	10.71912941046615	3.98772198563664	-1.90337371426249
H	7.18403651462108	6.86606859158950	-1.82495990793984
H	4.54449787073027	9.06711445906173	-1.77041730300422
H	0.02004234929786	9.84613716227165	-1.76641684485998
H	-4.52098558354067	9.03154240195878	-1.77628782987793
H	-12.64830513968903	-1.94798914967423	-2.12214797043467
H	-3.87545441808231	-8.28074456533350	-2.53916318694634
H	-10.64112921517079	3.82893829699100	2.07171850189720
H	-10.12523782495779	-4.43238540771866	1.81727735091348
H	-12.89031430785586	1.20873769870678	1.80569679339138
H	-7.10220529356289	-6.44506950824970	1.68532124170472

H	-7.15489069022885	6.67921927839860	2.06955485010023
H	-0.08190580280254	-9.58090341673115	1.73047278231795
H	4.39711989398116	-8.72621930590346	2.02099103389031
H	6.93562404823994	-6.38190452606982	1.97019323192931
H	10.09542780942955	-4.39316648053688	1.94469220865411
H	12.71043772729528	-2.03720760416199	1.91012262886991
H	12.87540386343945	1.24262047746787	1.99199986371489
H	10.57883428602562	3.86003695047699	2.17232540972969
H	7.20298733082812	6.69353968635789	2.07076188970668
H	4.54481418542428	8.90487936710426	2.22401995962669
H	0.01391481556786	9.63025443962616	2.36585094240943
H	-4.50319158813632	8.89472182377727	2.22286812114980
H	-12.75008050456766	-2.06335405746767	1.68895563284376
H	-4.62811031240955	-8.93193127197312	1.46972610654299
H	0.26395986689885	-3.75146314384892	5.08438217826263
H	-0.68428294405044	-2.80323127869645	3.40319971755965

• **TS6 (Hck-CH₂O → Hck-H-CH₂OH)**

Si	27.33061457339752	2.22443687400618	2.38409538024454
Si	27.10267368769633	-2.38277575629206	2.70625514351052
Si	29.60694763582233	2.75679405496552	2.67691359794586
Si	29.29721566051667	-3.14582770042463	3.08545385941345
Si	31.10376067088423	0.93132447079865	3.03282487609882
Si	19.48867225394439	-1.19490537899276	1.47018515750014
Si	21.42860431155968	2.65505654412122	1.45393325250815
Si	21.17548469270604	-2.86469761998096	1.83519066543715
Si	23.69475361787161	2.25362938256814	1.81915643182937
Si	23.40174496599128	-2.15863027275259	2.09639989097539
Si	25.52608108051011	3.76153622374049	1.97505956291728
Si	25.13377964881635	-6.11679989822160	2.68523585571275
Si	24.32654681028172	0.01240842180388	2.10080254978909
Si	25.63626540090992	6.14568514300607	1.81273813550408
Si	25.13727660778913	-3.73934891749681	2.49621746511296
Si	26.64903022291102	-0.05943308525140	2.45348992305286
Si	19.32302560855845	-8.10224845424952	1.92693980120913
Si	17.51137805210451	-6.59356824701200	1.57119102033789
Si	15.28208182655454	-7.37449954321660	1.36716097292021
Si	13.43830218167006	-5.89833872718640	0.96830696821532
Si	13.58709536030940	-3.53892775358273	0.75734545462126
Si	11.71515271821351	-2.08668824922428	0.41736242690981
Si	9.46691143685092	-2.73569191569816	0.15666366656491
Si	7.90772299969944	-0.96140391367417	-0.19282140472723
Si	7.96880373045869	1.43149593008289	-0.35825009525766

Si 9.59728109808712	3.17344949564038	-0.25288507963062
Si 11.83180600680911	2.51447129992306	0.09182244504467
Si 12.34983743936940	0.20046212564030	0.32125932001463
Si 14.68064408039743	0.15187934381491	0.63033530758706
Si 15.48943560483637	2.35424351055094	0.60714523592754
Si 13.75467039617827	3.94355370243754	0.23867881161730
Si 13.75277444757564	6.32877319117349	0.06792730178151
Si 15.58426170460663	7.88186477779050	0.21464937955078
Si 17.82041217748624	7.18018854026646	0.59304177706874
Si 19.74649479293118	8.60511285810912	0.76268735301634
Si 21.59901451342048	7.12193758332931	1.14616807723667
Si 20.80148393297638	4.90114927307618	1.19091976495595
Si 18.48827898489247	4.92733555762493	0.84163979731917
Si 17.77423183438804	2.68683247698213	0.91635220358601
Si 19.57491347025269	1.17010173742973	1.28089886115526
Si 23.87586260417840	7.74203165654808	1.43082447357856
Si 30.98409083944232	-1.45963599297863	3.19939818466323
Si 23.20223681806193	-7.52431092178154	2.47956859735220
Si 21.10590016601539	-6.51407336831366	2.02879941928850
Si 20.44902821550338	-4.60446147699338	3.21698573580714
Si 18.36168590914376	-4.54962926608344	2.25859046525953
Si 17.62168514223987	-2.59560141672512	1.48298855590952
Si 15.44895522229206	-2.06815206142012	0.91839818260625
Si 27.69488221116876	2.04244012228126	-0.01687115861982
Si 27.47167538579128	-2.56470404674264	0.30334736681595
Si 29.96872764697150	2.57374089603725	0.29925136540976
Si 29.66227125673135	-3.32747163911226	0.70433541536364
Si 31.46268391418979	0.75067671751410	0.68005591429904
Si 19.82799393451742	-1.34828229444618	-0.88598672761591
Si 21.78750011261451	2.48471508928244	-0.94401617614676
Si 21.56583183461554	-2.94412491117252	-0.55686613268621
Si 24.05408495771544	2.08102196089883	-0.57465397454783
Si 23.79960087992793	-2.33985513144532	-0.29459616919586
Si 25.88832056019680	3.58397008237013	-0.39778730960747
Si 25.52638740334327	-6.31027273611633	0.31398113979508
Si 24.68844357445205	-0.15778833212821	-0.27409367508452
Si 25.99030536218224	5.96785939826885	-0.56285221119295
Si 25.51121153345340	-3.93268929975118	0.13153389962599
Si 27.01379090835478	-0.24178381186591	0.06812685478876
Si 19.64083974323241	-8.34712750460462	-0.42519288115010
Si 17.79243728703689	-6.88436000850657	-0.81590347098059
Si 15.56755881149164	-7.64640420492011	-1.00054008871131
Si 13.76206180034263	-6.11766476690090	-1.40901748160512
Si 13.89981547794808	-3.74255436555068	-1.61624998586454

Si	12.03246385834349	-2.27466936228326	-1.99231626655956
Si	9.77898006164584	-2.91340023294200	-2.23146309835772
Si	8.22265099258328	-1.13146230221799	-2.55385377389644
Si	8.28532576271550	1.26251644135821	-2.71757530541878
Si	9.91036865415836	3.01126595548330	-2.63948658440877
Si	12.14787108319384	2.34980624693062	-2.31679367089656
Si	12.63860554085668	0.02905921147621	-2.07585854111863
Si	14.96296836976160	-0.00109290041183	-1.75648435605749
Si	15.81940425851876	2.18334067190804	-1.79428354869016
Si	14.07946005036179	3.77379296157277	-2.14089580375460
Si	14.08998128668135	6.15866650870901	-2.31145247315060
Si	15.92631719969933	7.70796347482299	-2.16237808636430
Si	18.16661142173577	7.00724252781897	-1.79691792207051
Si	20.09313512977847	8.43327789979370	-1.61561833497888
Si	21.94703365434178	6.94819598460532	-1.24255953675040
Si	21.14653173850865	4.72769146770267	-1.19396832794155
Si	18.83094752445284	4.75256232668235	-1.53980384347152
Si	18.11179825756964	2.51169127198229	-1.48682683032137
Si	19.92494412287774	1.00942428073395	-1.11688604791418
Si	24.22572859572107	7.56214481365216	-0.94518449596628
Si	31.34542161064428	-1.64024045125473	0.84576475969028
Si	23.63168316196563	-7.76861323441083	0.13152097780460
Si	21.50621432179875	-6.86601610984173	-0.33872960952548
Si	21.00534888651930	-4.95696717961219	-1.52375156923474
Si	18.67888331347480	-4.91377367169593	-1.60822588704239
Si	17.99324156990152	-2.69757508192543	-1.54565718510750
Si	15.71976186527648	-2.20903764025397	-1.47019421465476
C	20.56780047061981	-4.96498766062301	-3.44020901028369
O	19.08898611250543	-4.85055670538962	-3.42179094684350
H	29.95809488547913	3.97003228451432	3.48145257665517
H	29.52197047713466	-4.26968474574902	4.04919367517579
H	32.25101134256697	1.37588971341690	3.89185649049187
H	26.12826572036606	-6.66710125757063	3.66370443524033
H	26.69793526224446	6.76490886687380	2.67259857662608
H	19.19507242126084	-9.20201144911783	2.93145960022093
H	14.91750587960330	-8.51152809067903	2.27066084450155
H	12.18821243307512	-6.40577137399298	1.62212168888025
H	8.93006427647868	-3.84116668290330	1.01203218760360
H	6.57111250774867	-1.33652850449464	0.37614229979916
H	6.64900731227812	1.94036392731509	0.14245515919553
H	9.10293069187499	4.40399473105987	0.44229930789805
H	12.50098365691561	6.96746393631049	0.59238060318777
H	15.14448719495492	9.16024343386311	0.86134408271948
H	19.65349694894348	9.89072967448497	1.52532064720690

H	24.14615433114808	9.01618943376620	2.17230017786959
H	32.08382955592784	-1.89425625750973	4.12316122127924
H	23.24611380504417	-8.67883854409428	3.43315233990328
H	30.56925141711181	3.65982290271377	-0.53881581205077
H	30.13151415861710	-4.57716118654562	0.02551430321464
H	32.82217716918215	1.09010707187161	0.14303070649636
H	26.76255175819770	-6.97066438010323	-0.22155054845584
H	27.26515874165209	6.48464262549683	-1.16108668298743
H	19.71609561399346	-9.61722057569132	-1.21166669396680
H	15.39033683099419	-8.95537570089659	-1.70510399124486
H	12.72498440564180	-6.76285404655189	-2.27928017167591
H	9.45107246869940	-4.13972804625358	-3.02566592990735
H	7.07233140030802	-1.60211058974849	-3.39436371869596
H	7.15058569607655	1.66584688135038	-3.61279778010123
H	9.61977987601279	4.12588197245032	-3.59617066938169
H	13.04819825949807	6.70151361280636	-3.24434143872931
H	15.70807648692742	8.87056807845977	-3.08263870802668
H	20.24546344141192	9.59504046877567	-2.54850744505681
H	24.73074756577699	8.71694839157178	-1.75637845447268
H	32.65930139229142	-2.18399693409740	0.36626499918099
H	23.95968727818694	-9.07506621387959	-0.52334680987692
H	18.30331227429042	-2.72167217132103	-3.33778237819542
H	20.82103740547079	-5.90323938972236	-3.96130995762064
H	20.97583341281008	-4.11378098914326	-4.01253173237323
H	18.68469261419783	-3.64178984067246	-3.53762870937267

- **TS7 (Hck-H-CH₂OH → Hck-CH₃OH)**

C	20.04909714462925	-5.26115953154477	-3.20631147939818
H	19.35645438935199	-4.07909784695346	-2.86189972549838
H	20.05394058823567	-4.79751569505491	-4.21658925416828
Si	27.33150032123711	2.22717074029488	2.38429095763361
Si	27.05988369417440	-2.38944742383471	2.55954906823172
Si	29.60847169295587	2.73003319037311	2.71983934933299
Si	29.24072325956382	-3.18969137772956	2.93897810678625
Si	31.08031259686432	0.87644143751287	3.02884888224081
Si	19.38059224675257	-1.21401022524407	1.22660687681929
Si	21.41600911058071	2.62862980680635	1.44787835674275
Si	21.12437096198194	-2.77091906028289	1.64036091364713
Si	23.69281698305036	2.28659636648788	1.80118649597727
Si	23.35498502904984	-2.10289535067716	1.89859726485105
Si	25.53364853604173	3.77819655277360	2.01549156861971
Si	25.09187796603926	-6.07540347673206	2.46635139232303
Si	24.32067243176594	0.04450284984948	2.02272616679232

Si 25.63964282144385	6.16586572120567	1.92455779062710
Si 25.07541032201484	-3.70188261351717	2.28254512460015
Si 26.64069822348752	-0.05613222403035	2.37177642618935
Si 19.24047904407052	-8.08800748912830	2.05369486956934
Si 17.36476407772153	-6.64192047584955	2.13718698401727
Si 15.17170557309755	-7.31318800096877	1.52212250339085
Si 13.44418258592010	-5.74351835408917	0.97519047386732
Si 13.70881413448937	-3.42921100761445	0.64276854722838
Si 11.78769766607896	-2.06915826126172	0.29666279362438
Si 9.56322598151683	-2.79672051575398	0.05275794218889
Si 7.97095026250873	-1.04759745735641	-0.27366553691151
Si 8.00694568348246	1.34761571919982	-0.40978760893139
Si 9.61064180260745	3.11070006706052	-0.28768231230369
Si 11.86330330513644	2.49878790444342	0.03396782630648
Si 12.43011996834509	0.20011791604779	0.23282182525945
Si 14.75673412838001	0.12370467314572	0.58918508255466
Si 15.50455981119131	2.33937877720417	0.54276105124157
Si 13.77505115040882	3.93111960519998	0.21198311848790
Si 13.78395092425387	6.31934878825407	0.09298287060271
Si 15.59105751399217	7.89338403789932	0.28961203676232
Si 17.83025629390555	7.20350103222355	0.68260032454750
Si 19.76013189718916	8.61684639944106	0.90358137525429
Si 21.60115005036190	7.11413925970372	1.26824391510812
Si 20.80299633365573	4.89022525509999	1.25623215209471
Si 18.49528447910564	4.94614694733835	0.87994219252751
Si 17.76622610928394	2.71347965356977	0.88551741685887
Si 19.53883654176749	1.16024477068788	1.23279844568618
Si 23.86772953568156	7.75718698790931	1.57550705156120
Si 30.93685812538978	-1.51745332883644	3.11941764551996
Si 23.17486585838851	-7.51041649442651	2.30719381781570
Si 21.03422788398022	-6.49391449572405	2.16230741615567
Si 20.58264145997603	-4.45207199139185	3.23432142067266
Si 18.37618307568923	-4.62352442450296	2.69065533829517
Si 17.67880560912596	-2.78919573731310	1.50338589735346
Si 15.62284792021407	-2.07095926801780	0.72461512823605
Si 27.71966478266088	2.12447991469499	-0.01769381672266
Si 27.45550299901916	-2.50441632347291	0.15796601245305
Si 29.99347638136249	2.62626949786624	0.34139648170671
Si 29.63216945723983	-3.30499009793317	0.55757603797588
Si 31.45623622885164	0.76760076050193	0.67475137091071
Si 19.59939035404302	-1.23933261287637	-1.18157107512656
Si 21.79350335678308	2.52246788932405	-0.95591313752582
Si 21.51507203082882	-2.60892862805000	-0.82862487744592
Si 24.07186722652232	2.17939725649831	-0.59062453907319

Si	23.78790106157469	-2.21231626317360	-0.48809094162285
Si	25.91086936086900	3.67293748207143	-0.35946356333894
Si	25.45093522987820	-6.21832911729141	0.08617115733723
Si	24.73129513823144	-0.05409045590634	-0.35154021238482
Si	26.01191863429085	6.05947438560054	-0.45236973527703
Si	25.47943059203150	-3.84450395910623	-0.07740978387149
Si	27.05193803869293	-0.16601412987553	-0.00880404403418
Si	19.42355921469358	-7.92602924532415	-0.31702493930226
Si	17.70058450737548	-6.29597540416855	-0.26026399588808
Si	15.67794113302512	-7.35501098566627	-0.82126120713889
Si	13.79271826350918	-6.02048378377058	-1.39160874462556
Si	14.02454681746343	-3.66139591864184	-1.72563493076706
Si	12.10847683263324	-2.25423285138928	-2.11020211541053
Si	9.87037750231533	-2.94771361222207	-2.34052246888226
Si	8.28563615826844	-1.18597334275154	-2.63633080569145
Si	8.32330200671767	1.21118522786318	-2.77082595921367
Si	9.91710182824771	2.98933353254471	-2.67671043584034
Si	12.17334807019667	2.37506201955525	-2.37696081928342
Si	12.67935689007384	0.05567430132323	-2.16677980790342
Si	14.99738079874394	-0.02410287770087	-1.80119740357544
Si	15.82900244931162	2.18097364063208	-1.85232688101830
Si	14.10747144994482	3.79929904011079	-2.17150515004322
Si	14.14117001536995	6.19454455711303	-2.28705124997195
Si	15.95543719686767	7.76689884185187	-2.08732545695691
Si	18.19782503426924	7.08090785020847	-1.70985145360881
Si	20.12604931262282	8.49687950617635	-1.47672092126080
Si	21.96561159122118	6.99307655802365	-1.12178970049738
Si	21.15606662963245	4.77320588363063	-1.12725153939614
Si	18.84282075985617	4.81978875438658	-1.49988913129851
Si	18.10683666723319	2.58735813922015	-1.51863994956005
Si	19.91215866107537	1.08528042449797	-1.16257944479703
Si	24.23098822966383	7.64014116429139	-0.80238549951103
Si	31.31868531994525	-1.62734552610954	0.76483050072060
Si	23.46290783148579	-7.52918827064720	-0.08117722801653
Si	21.32770312117500	-6.55202710542658	-0.21839453942655
Si	20.50734713142911	-4.60506500973091	-1.13188390895919
Si	18.28908144621800	-4.04847083753363	-0.47394792693722
Si	18.13282019101817	-2.68206562730960	-2.41314337264636
Si	15.94197753022335	-2.19987691511540	-1.68669281831651
O	19.04084789372943	-6.23700597184100	-3.03284385520582
H	29.95850256171528	3.91092065754159	3.57136746771525
H	29.44638757104505	-4.34164571847968	3.87341855042578
H	32.22679047400375	1.28045704829655	3.90869895332302
H	26.11317785422060	-6.60320543874294	3.42892939341007

H	26.68991105935835	6.76327719752422	2.81327284804860
H	19.31055780495958	-9.32049865877517	2.89809947949301
H	14.59223938294564	-8.47869098538285	2.26582275358117
H	12.15231447248571	-6.10296532143132	1.64508668744366
H	9.06260260539059	-3.91884490206077	0.90895160618821
H	6.64098333901581	-1.44769172427718	0.29409314642928
H	6.68154236903342	1.83656585765808	0.09656239513614
H	9.10257704951667	4.32466157394337	0.42685787968599
H	12.52100111047479	6.93862470884470	0.61464783165489
H	15.12731690532577	9.15291891078079	0.95635620882351
H	19.67180789483407	9.88500094681922	1.69584265331937
H	24.12720091857392	9.01100558040928	2.35457809541374
H	32.02557457908116	-1.99126763829269	4.03696027121769
H	23.36196481434904	-8.74430629550589	3.13653120874439
H	30.61987059545004	3.73119775073297	-0.45174612063945
H	30.10161857301490	-4.53687012853233	-0.15293283448023
H	32.82560495010094	1.10591938218353	0.16258389526741
H	26.62488253469174	-6.94730412324852	-0.49701502574195
H	27.28743888511395	6.59872476396085	-1.02876926470124
H	19.25515886880678	-9.02239764201990	-1.32459828116286
H	15.88802481941005	-8.62300464071160	-1.59117082594098
H	12.82311809266896	-6.75822798463258	-2.26586351590554
H	9.55072616674772	-4.17164693282372	-3.14235725422356
H	7.13902667601586	-1.65662789613649	-3.48209481337159
H	7.17923814693749	1.60931806938288	-3.65690801707487
H	9.58967213270467	4.11180857113065	-3.61238145245897
H	13.10542168611037	6.76535066195355	-3.21066652635522
H	15.73504612252068	8.94452190454724	-2.98781370000331
H	20.29864761545271	9.67789653933320	-2.38154434154457
H	24.72073490174682	8.81955008773131	-1.58703500254822
H	32.63551632223604	-2.16139747912439	0.28244370933015
H	23.61208812705729	-8.78214809146249	-0.88862113636689
H	21.08329624901227	-5.67416584338426	-3.09649626350720
H	19.17429530325672	-6.96623985459718	-3.66569711934647

- **TS8 (Hck-CH₃OH → Hck-H-H-CH₃OH)**

C	20.68180892678644	-1.25535928157066	-5.20635778272478
H	21.47806363671461	-1.73393606946644	-4.60851684297738
Si	27.26569258301226	2.10412121628384	2.27887967483531
Si	26.97781730417211	-2.45928378812145	2.63742045416963
Si	29.55158171423260	2.56879007090666	2.61979671151216
Si	29.12041575364475	-3.32552646918159	3.06451919690952
Si	30.99867420127538	0.70934063420227	3.00777475938446

Si	19.56364432036428	-1.38652329432497	1.19967446315394
Si	21.40208009579070	2.51948187963908	1.28771594220438
Si	21.02979526983660	-3.02544381188538	2.04713753237561
Si	23.65438846131318	2.13888889540752	1.67061153371691
Si	23.18873074335094	-2.22511996165289	1.93134584952323
Si	25.47666557913927	3.64623089224768	1.84785004040758
Si	25.04411407497639	-6.01393707361746	2.82939155345841
Si	24.22636757934725	-0.10673233680916	1.95099832865312
Si	25.58897878728004	6.02792477172507	1.68434058341773
Si	24.95694484285369	-3.69304937855643	2.41702544882323
Si	26.54505013978161	-0.15945449973406	2.34775465593984
Si	19.20750531055538	-8.12401401150043	2.36719033212676
Si	17.35381983834320	-6.63698787774164	2.22237122368133
Si	15.19094571862925	-7.37078193893664	1.58114488824090
Si	13.48073344919513	-5.79321383107406	1.01170416209386
Si	13.75851622086987	-3.47874309822101	0.65326624855602
Si	11.81319229114977	-2.14837488924582	0.32023345587565
Si	9.60064066158436	-2.91700173784309	0.10798391244651
Si	7.98892343530938	-1.18615117599944	-0.22254960797495
Si	7.99061660221700	1.20787627686064	-0.38872528017943
Si	9.55844567428150	3.00683586573299	-0.31468342222029
Si	11.82641890693753	2.43778087047520	-0.02288327349276
Si	12.39808665766871	0.13933759335546	0.21462299867616
Si	14.72294854874056	0.11196317594035	0.56875665142272
Si	15.48565053790063	2.31552892517986	0.43287159665853
Si	13.73017362878474	3.88583479195142	0.10368405588448
Si	13.72124360672053	6.26903076074565	-0.05811716456788
Si	15.57412670442921	7.78827091511618	0.09779708495208
Si	17.79078144984894	7.02830497690753	0.47579095177857
Si	19.70336784507141	8.46967915162575	0.66509189396364
Si	21.57056350168567	7.00491610660841	1.04233809498809
Si	20.79170167511927	4.77466508502694	1.06275632889598
Si	18.48421593073807	4.78106588170959	0.70379663773867
Si	17.77437191318318	2.54046885217083	0.73547442194349
Si	19.57092361621465	0.99637731784472	1.06323099432788
Si	23.84512752386262	7.64106886528878	1.31306315566558
Si	30.84425267468243	-1.67879785156885	3.18931856953081
Si	23.16394609119776	-7.50549017943748	2.86508412731071
Si	20.98331137483486	-6.57965628885264	2.75846648825991
Si	20.30868676770832	-4.51741070768389	3.71628281999571
Si	18.19303251658667	-4.57385191971323	2.92597190667581
Si	17.70390535757423	-2.81798771362956	1.48767683187576
Si	15.64951654047587	-2.06750730120825	0.71415806792285
Si	27.67033962035637	1.90562272502779	-0.11161392766184

Si	27.35737239985916	-2.70049304992083	0.23990832283946
Si	29.95294460508137	2.37401426257361	0.25036502966949
Si	29.51141510328313	-3.53878122613121	0.68773479477606
Si	31.38513976371424	0.50666822276451	0.66195559178816
Si	20.13171053375777	-1.41895037289732	-1.16374017250325
Si	21.80162412518910	2.38021494083959	-1.10117512213514
Si	21.75518112972178	-2.98908936606754	-1.95713257306100
Si	24.05208353172872	1.92115846520655	-0.70813987925947
Si	23.53022793852572	-2.42853184654725	-0.47738516609989
Si	25.86590249811287	3.45213625839302	-0.52262321732081
Si	25.40410762672464	-6.31719989849171	0.46690690393044
Si	24.64946265148001	-0.33375644657895	-0.40645970803197
Si	25.94106577074932	5.84392331600492	-0.69100014619716
Si	25.31945688508610	-3.96200130172317	0.05753670456799
Si	26.96870392927694	-0.37260825524359	-0.02263141946756
Si	19.58453892432586	-7.90694678306588	0.01719272962599
Si	17.76609061386949	-6.40918907946615	-0.14839338983073
Si	15.73107556699884	-7.41925125842533	-0.75863503003843
Si	13.84009808426243	-6.10504373853867	-1.35129879847860
Si	14.02763723783225	-3.75343418537000	-1.71230170284371
Si	12.10493618238733	-2.35644686444166	-2.08786216947655
Si	9.88071537837371	-3.09622291206278	-2.28785080274774
Si	8.27776429737762	-1.34948895576048	-2.58739799199478
Si	8.27213614717715	1.04648097026722	-2.75230187240420
Si	9.82589151196001	2.86143663523999	-2.70758746760439
Si	12.09482677146919	2.28601589458212	-2.43629479811453
Si	12.59480992848824	-0.02926012010362	-2.18673873878846
Si	14.90871404796965	-0.02840732460938	-1.82592075527655
Si	15.78403996815252	2.14136596398337	-1.96116652535365
Si	14.02458888968320	3.71827478600574	-2.28344031819803
Si	14.05151007471885	6.10497827738657	-2.43943956411831
Si	15.91489707431840	7.62016768000182	-2.28080106596020
Si	18.14177755547868	6.87797200054225	-1.91729023742914
Si	20.05365914851709	8.31849314826159	-1.71662511880411
Si	21.91414052526154	6.84287157041286	-1.35062287448510
Si	21.14054882042617	4.61562035194648	-1.31514175594078
Si	18.82389946445427	4.62713319295054	-1.67586441601882
Si	18.09116434469137	2.39281647111020	-1.66921265330334
Si	19.94679919669462	0.92841252299872	-1.33371976960491
Si	24.19083479382559	7.45999957926365	-1.06313526477352
Si	31.22553130894471	-1.88265554444348	0.84118823755210
Si	23.38381962047862	-7.56695919907053	0.46868117607037
Si	21.35448877502346	-6.38782375257692	0.39224181498021
Si	20.91204555838168	-4.16075113492646	-0.08454213484037

Si	18.54674336427433	-4.23658040042845	-0.28814392971636
Si	18.15616986479165	-2.54827865546515	-1.83278412938703
Si	15.85403914575295	-2.18387898608633	-1.70360950594002
O	19.46353654253897	-1.13015235461410	-4.43749812414805
H	29.91458532838903	3.77499668527492	3.43000805380289
H	29.28193628961825	-4.44349294593265	4.04796861777672
H	32.14503015680421	1.14312477835699	3.87404841548751
H	26.07960008559200	-6.38787293605583	3.84775320289749
H	26.65897917887549	6.63552500579563	2.54239824936121
H	19.07928343596483	-9.39666824469531	3.14186580288297
H	14.58312885103179	-8.53233802352508	2.30698006987045
H	12.17020400861816	-6.11865881177994	1.66213870499915
H	9.12466213787970	-4.03418890416523	0.98386091135459
H	6.66882796275820	-1.59275776821034	0.36281897547726
H	6.66388876302572	1.68088878078485	0.12857032024371
H	9.03541046012687	4.21741278206255	0.39424174440237
H	12.47404222306160	6.90410943889854	0.48052630817513
H	15.16072977440976	9.07017973067308	0.75455488181784
H	19.58202202197673	9.74834367208604	1.43577398423872
H	24.11807589225466	8.91182416248265	2.05908764200530
H	31.92564063509124	-2.12566534823443	4.12882880416496
H	23.47923528554324	-8.67385713792943	3.75167268189278
H	30.60777322812812	3.44081012183155	-0.57201859659618
H	29.97233713614154	-4.80416659846828	0.03201787237601
H	32.76302897793028	0.81056310192030	0.15015689500881
H	26.56802608540551	-7.09038563526769	-0.07855708405476
H	27.21343590138001	6.37268701493101	-1.28541897126654
H	19.71044718495320	-9.00669104466560	-0.99027165336781
H	15.93526722348810	-8.67953653706471	-1.54019324143173
H	12.88243196570461	-6.85599984218680	-2.22690049192239
H	9.56972237644466	-4.33240046460787	-3.07340464970651
H	7.12743698499352	-1.84790714875303	-3.41165981733167
H	7.10473530059378	1.40782048194103	-3.62324448776128
H	9.46459845791363	3.96493519948090	-3.65269979059534
H	13.02163111667898	6.66985693720718	-3.37233423983981
H	15.71639031891710	8.78871715814302	-3.19802745815537
H	20.20010396415486	9.48649969371593	-2.64275111349994
H	24.69570753409354	8.61130807059619	-1.87937493304627
H	32.53729460105134	-2.44619152451535	0.37872666607755
H	23.33992929752957	-8.83105295319791	-0.33366803169125
H	20.43767809085655	-1.88191207314176	-6.07654306051659
H	20.99908715072094	-0.25646549554349	-5.54949171449926
H	18.92730326036368	-2.38747581451323	-3.83583640593765
H	18.56492008329730	-3.14651494687901	-3.49673242844614

H 19.63971966069318 -0.57072717493100 -3.64190993892481

• **TS9 (Hck-H-H-CH₃OH → Hck-H-CH₃-H₂O)**

C	21.64921887424387	-5.86119399564514	-2.74094530272491
H	22.28364406753719	-5.61052446100333	-3.61117622481655
H	22.31479400945860	-6.19048940201549	-1.92701620415086
H	20.98202955106888	-6.69281845163259	-3.02091955254817
Si	27.22952116529551	2.29247324552422	2.41801728539811
Si	27.08316851643318	-2.25994904788834	2.55320168273434
Si	29.49033053311263	2.81539333827938	2.82573394822489
Si	29.23814963142135	-3.09251266028100	2.98678415175930
Si	30.99583727086781	0.99250573574843	3.15987463940823
Si	19.71566114262123	-1.32309053093083	0.66920448382278
Si	21.40879137290385	2.63979209212676	1.27006368446647
Si	21.10756214064302	-2.96455256255981	1.65761828121037
Si	23.64590870136413	2.26229141216093	1.69611564925145
Si	23.26185419832397	-2.15949193119586	1.75457631094232
Si	25.41507234909315	3.80145802531949	2.01270886097122
Si	25.14759527738159	-5.81925908426290	2.72958310569852
Si	24.22851707520529	0.01563976823615	1.90087034807446
Si	25.55891613456499	6.18325320388289	2.00121005575440
Si	25.10156486346867	-3.52429605491240	2.23330311386305
Si	26.53868001636904	0.02130468614277	2.37438399727859
Si	19.15626014579264	-7.65105705850965	2.01913119524492
Si	17.34016649584792	-6.11276802203678	1.66296480825135
Si	15.32556954351850	-7.21976052974029	1.04608720261809
Si	13.57977436353734	-5.68303191842505	0.51812414302626
Si	14.01629390927630	-3.38053020737878	0.29194854383159
Si	12.03888432587697	-2.07284665539061	0.15439333746884
Si	9.82918957354536	-2.86338839921115	0.01169764090996
Si	8.17392442691992	-1.14336850168774	-0.09250805416732
Si	8.12375218865894	1.25550730820883	-0.07126812805822
Si	9.67196314682176	3.06422776882756	0.07192653932954
Si	11.95739595002203	2.50843826636488	0.19159102319078
Si	12.58764665208350	0.21432163712512	0.20256641526812
Si	14.93269402341451	0.18241441408655	0.38873966262601
Si	15.59125197640313	2.41855528167622	0.47783417244841
Si	13.82309921302528	3.99402576492018	0.35766170221811
Si	13.74835432419840	6.37947016655154	0.40680520532185
Si	15.55695062389968	7.93699400490111	0.65174355859792
Si	17.78410217097703	7.17790791523795	0.94078714747991
Si	19.68449228423067	8.61602281833019	1.21563275620811
Si	21.56002659417803	7.13392960565864	1.43073549668544

Si 20.79982717106149	4.90479383344360	1.24593243929976
Si 18.48416638250803	4.91879907468879	0.96085091929447
Si 17.86552647738993	2.65831305649432	0.78428227021584
Si 19.65420667775883	1.06721521923699	0.93056145891501
Si 23.81605206177653	7.80578330360391	1.73564716462624
Si 30.91089031167981	-1.40448071421274	3.22616903304797
Si 23.13592292296945	-7.10341152363196	2.81782557190443
Si 20.89469385828521	-6.35257138184508	2.98340349155847
Si 19.85710148455594	-4.29919978986835	3.13026138300870
Si 17.57310554662462	-4.06636598920140	2.85139379378303
Si 17.98270266269112	-2.84931404292124	0.86816860399293
Si 15.90846756539665	-1.97198330833131	0.27662511802725
Si 27.68013704009693	2.21942853042225	0.03041923672072
Si 27.51231386811025	-2.38088145483966	0.16709654721064
Si 29.94058289052164	2.73818566778833	0.45634790034904
Si 29.68374242352750	-3.17583208201349	0.60883434644289
Si 31.43726506313412	0.91220072662144	0.81563925189515
Si 19.90249788278949	-1.07602236788425	-1.70628639314605
Si 21.81843343806852	2.70128437498006	-1.11984658779460
Si 21.89920699845686	-2.29357029395647	-2.15120119441140
Si 24.05971397989241	2.19015445021247	-0.68760545168613
Si 23.70014747594742	-2.22315084542502	-0.61801927654815
Si 25.84469204846615	3.73688042263599	-0.35909409988660
Si 25.32244640617596	-6.03277742866186	0.33016333727900
Si 24.69212234871523	-0.07095317922037	-0.44622547460494
Si 25.90487668248764	6.14035711048946	-0.38455679261351
Si 25.53969362571580	-3.72188092614601	-0.12320937873536
Si 26.99981310793928	-0.06669912134107	0.00407152052893
Si 19.65570780336240	-7.03114684644878	-0.18288979230189
Si 17.67965211878108	-5.93633132983016	-0.73525804955342
Si 15.80465997180002	-7.19886157444186	-1.31379167560122
Si 13.90117274114346	-5.86439534687463	-1.86196514717985
Si 14.15184928899525	-3.48528501262790	-2.10332519715831
Si 12.19156026986396	-2.09371009443685	-2.27522790054275
Si 9.96924978941551	-2.85299983931533	-2.40267825469139
Si 8.33257227329590	-1.11686973361107	-2.47453911808783
Si 8.29886101477507	1.28528048192967	-2.45076795453121
Si 9.82359664605311	3.12577868343176	-2.33508402073832
Si 12.11416509076820	2.57660538586306	-2.23387584468142
Si 12.64499068586023	0.25149291238100	-2.21316504369402
Si 14.97904535753672	0.24875293796975	-2.01886695963378
Si 15.81051572982862	2.44488701823356	-1.93499225738545
Si 14.03207787913634	4.03664562364188	-2.04268808602144
Si 14.01892740630092	6.42821395562769	-1.98597371926634

Si	15.86114686101240	7.96057144024085	-1.73589293617321
Si	18.10460294935389	7.22578850323366	-1.46272912605444
Si	20.00055719911534	8.67317251621400	-1.17389674561585
Si	21.87646879604718	7.18528693215585	-0.97372222668146
Si	21.13810619516537	4.95055674276443	-1.13489661127800
Si	18.80598490793369	4.96762285113525	-1.42608669994372
Si	18.11935738347266	2.73408040157597	-1.63987746702880
Si	19.96740423774751	1.25276454637558	-1.45901403216000
Si	24.15180454830353	7.78075707586770	-0.64970029521127
Si	31.34821823916415	-1.48470694840285	0.88052619490399
Si	23.04100782016420	-6.65947676859620	0.51616929352299
Si	21.09434787107588	-5.25695809591770	0.72406212091426
Si	20.68393261537588	-4.28561929369955	-2.32421665900547
Si	18.54203527351769	-3.86395211857600	-1.28740422372188
Si	18.12983750768511	-2.19967913695128	-2.93725323034353
Si	15.96566834782234	-1.88861357518577	-2.11408210248256
H	29.80136803552859	3.99494352641793	3.69428120921568
H	29.41136139841526	-4.25333314409812	3.91712344432347
H	32.10573455137580	1.41723758019210	4.07587190321236
H	26.21971519859231	-6.17573177785632	3.71239366461769
H	26.64590563897967	6.70733078037163	2.89165464729753
H	18.88299910015067	-9.04952228379818	2.47162154449343
H	14.81989851815752	-8.43894301960682	1.75604725961926
H	12.26337938850030	-5.95796493645960	1.17889815122142
H	9.41505223510460	-4.05021123077701	0.82607358572020
H	6.89493611053241	-1.62355257495267	0.52854971705288
H	6.81517597249420	1.66291085253127	0.54028007122006
H	9.18588636376764	4.20713234497680	0.90872459623388
H	12.49764138261699	6.92268613716078	1.03118707827254
H	15.13408726520434	9.15396951286940	1.41692810611518
H	19.58794596070240	9.82101217225195	2.09994478318746
H	24.06798704009917	9.02654715624027	2.56695473923884
H	31.97987809453432	-1.86959566737531	4.17027640650947
H	23.37833269391071	-8.47630995706735	3.36327888627989
H	30.57252503858294	3.86412576606863	-0.30194481768262
H	30.18749277163473	-4.39558228905339	-0.09936804604883
H	32.81187609759584	1.28268571731502	0.34158302162866
H	22.45435872242314	-2.03141563732627	-3.52845546518043
H	26.08708207293247	-7.10862406873439	-0.38447166542899
H	27.17442366876105	6.71382168656247	-0.94267145844045
H	20.45361866220378	-7.86523255002112	-1.13895923735587
H	16.08051017688613	-8.41368005353747	-2.14426684551944
H	12.94723172965522	-6.59055221922253	-2.76378988191222
H	9.62608859448645	-4.02989456134056	-3.26313478377398

H	7.13830457663602	-1.55509946164038	-3.27069965933478
H	7.08647835877776	1.69966851977156	-3.23294534985097
H	9.37771196516238	4.29155297328205	-3.16292296664504
H	12.96558117890822	7.07236632777029	-2.83838752347725
H	15.64395719512187	9.19669071323397	-2.55517497652897
H	20.11706200910000	9.91686078281839	-1.99999255790219
H	24.67835632182020	8.97130034108456	-1.39266133829630
H	32.68074628592610	-1.99610011789885	0.41838816723626
H	22.61687324272896	-7.75604467909656	-0.41190618738599
O	20.10923635926268	-4.03834631723869	-4.10028344009983
H	20.77822094034587	-3.54942394071310	-4.62648007080141
H	19.16862803615551	-3.31950400254947	-4.03518136539437

- **TS10 (Hck-H-CH₃-H₂O → Hck-H₂O-CH₄)**

C	20.87056969765533	-5.21737606811643	-3.00610394453043
Si	27.38330912482451	2.44664408587331	2.38167235206974
Si	27.19927165779959	-2.13481840919427	2.46952360246701
Si	29.65457004541884	2.94356191997016	2.76200684476295
Si	29.34942594377548	-3.00087705185991	2.86607179543649
Si	31.12702747531583	1.08598452143028	3.05712179244194
Si	19.81833275666122	-1.00211404943996	1.15524727320187
Si	21.49290271593011	2.83075480974221	1.39291553594602
Si	21.24824500944777	-1.96501742736644	2.74727271717798
Si	23.74789009523382	2.36672179000197	1.72693183246722
Si	23.31125254770362	-1.94414861964662	1.72336748178407
Si	25.52837106273701	3.91912650030181	2.01191455524088
Si	25.37646314546410	-5.65749262578188	2.44439361129175
Si	24.46383757228190	0.13272116113156	1.77040321960275
Si	25.63390053709491	6.30855451651842	2.01745247511784
Si	25.16756944777471	-3.33568056510391	2.14003233721604
Si	26.75638508801221	0.16624722113050	2.30263286904975
Si	19.48075614049851	-7.59871404229895	1.93217404241255
Si	17.67308447643712	-6.06480677942242	1.72140409445605
Si	15.57239345201386	-7.01631259014518	1.13656593806983
Si	13.86865938182856	-5.42451844746858	0.58831402313729
Si	14.19322969906867	-3.11556256671199	0.26489164726883
Si	12.17280933938100	-1.88500152216369	0.04017439962145
Si	9.99654931870266	-2.74941827456799	-0.17362796958626
Si	8.29945734754638	-1.07993174160769	-0.38234816556858
Si	8.18505998611913	1.31640698031632	-0.42080152233890
Si	9.67368781014754	3.17369133111809	-0.26725418154788
Si	11.96973953542954	2.69593432012626	-0.04041257159031
Si	12.65852208228254	0.41979015780934	0.06144747501217

Si 14.99602247259440	0.45209083698424	0.35742749098767
Si 15.60399385243843	2.70790709804775	0.38064588027385
Si 13.79828220906710	4.22574962570933	0.15666255116256
Si 13.79903614554916	6.61467008796664	0.15794590539616
Si 15.64170852031486	8.13522842202817	0.42244360039832
Si 17.87952301183500	7.41759976561423	0.77623357468697
Si 19.78480625481024	8.84998416324082	1.08014429299614
Si 21.64845622868940	7.36534967499510	1.39885387702436
Si 20.91490543823145	5.11807403159615	1.29128034599744
Si 18.61351510271511	5.17978161671919	0.89542474499434
Si 17.86570524353590	2.96976457745083	0.77195877787582
Si 19.60963927296607	1.38648699606048	1.08145303689959
Si 23.92003060921753	7.97214077639799	1.73214234468777
Si 31.02439977038570	-1.31305937334765	3.10279005133887
Si 23.46603008406355	-7.08506196539195	2.39647039667093
Si 21.29530727430209	-6.10796592832113	2.36297280370444
Si 20.28964068664086	-4.02864081325850	2.69072419854230
Si 17.98192154969634	-4.08373848629911	2.99750020806222
Si 18.06416030525307	-2.60135796966313	1.14766080455313
Si 16.06450390210592	-1.67279795908320	0.33790042652125
Si 27.80265612526050	2.39587474585137	-0.01565543816872
Si 27.61659898659756	-2.22384338365960	0.07411231472454
Si 30.07344476661417	2.88650450679340	0.38785663079874
Si 29.77562851717074	-3.06473507541527	0.48603221897400
Si 31.53800601888654	1.02520618897333	0.70775510959251
Si 20.27594177778527	-0.84850879757284	-1.20330366367240
Si 21.92840283647493	2.86696033628061	-0.99953980217370
Si 22.01074447753602	-2.11834163376539	-2.22903083290558
Si 24.16937805734229	2.34746999360055	-0.65724163922513
Si 23.77861769507827	-1.99738707812866	-0.67854189130706
Si 25.95399024612040	3.89800837404069	-0.36130203816172
Si 25.71380122342842	-5.85442611442657	0.07169835165120
Si 24.86668220099108	0.10384054836352	-0.60001309260462
Si 26.02527198682235	6.29489691174487	-0.36091812997043
Si 25.60320776344372	-3.49514702345012	-0.22120118131017
Si 27.15359665361926	0.09962943026219	-0.07605650542449
Si 19.85405259480231	-7.45268791267361	-0.41431564029149
Si 18.01258132349355	-5.97628020962519	-0.66250428492326
Si 16.02118103283101	-7.06429533018795	-1.22613461007648
Si 14.16244691313888	-5.68917321499204	-1.78992974820723
Si 14.38016920378428	-3.32047260191934	-2.10856346087080
Si 12.41676080740768	-1.95067980178777	-2.37894503462904
Si 10.22875953064578	-2.78709982166347	-2.58162005328226
Si 8.54528000703553	-1.10321619778362	-2.75767987648930

Si	8.44477710872612	1.29610297416803	-2.79219217691316
Si	9.91515568811674	3.17840423818170	-2.66621139933581
Si	12.21793448135207	2.71035861478657	-2.46174732163473
Si	12.80513537083778	0.40200191242979	-2.35313204845180
Si	15.12359503003709	0.47931658413171	-2.03864473593218
Si	15.90861731921222	2.68924757375020	-2.01812192448353
Si	14.09229051311624	4.21957046943217	-2.23683980024183
Si	14.13652087029395	6.61402255050449	-2.22811974800090
Si	16.00332229362224	8.11590749100840	-1.95854521920679
Si	18.25060981626411	7.40857023297205	-1.61287879578495
Si	20.16166670181799	8.83902436260606	-1.30268694635281
Si	22.02042443833708	7.34890044537981	-0.99485409889241
Si	21.27074226512323	5.11511662336608	-1.08761261480361
Si	18.96206975309349	5.15738431970758	-1.49479099028210
Si	18.20514834467540	2.93852087625734	-1.63796389619737
Si	20.05425984037830	1.47471266666047	-1.29600918064046
Si	24.29256429530178	7.94479267420907	-0.64612437885871
Si	31.44084854110469	-1.37386267094595	0.75395853465548
Si	23.69839320082525	-7.11611372972074	0.00889441707486
Si	21.65541869222439	-5.96872388731024	-0.01855399287370
Si	21.00218166112786	-4.05143201940772	-1.14594064281748
Si	18.69326895499465	-3.78790301126364	-0.84580766156119
Si	18.41989822886056	-1.95355468109229	-2.21380572335497
Si	16.13025316849342	-1.65281998281313	-2.11172205523545
H	20.56574456758732	-4.80837010898991	-3.98836721078780
H	21.79790930952555	-5.80025756555327	-3.12742555674714
H	20.04421396897278	-5.86515184682578	-2.64976350032684
H	29.99307281399433	4.10839845600321	3.64024248373857
H	29.53233438656984	-4.16947475756878	3.78495636576766
H	32.26092636888188	1.48497223774900	3.95596227428847
H	26.39787755109872	-6.06006876889542	3.46375534714388
H	26.69715565130776	6.84307193405569	2.93126847740178
H	19.39681314225595	-8.87389721713175	2.70842675582457
H	14.95833401312869	-8.16954405761585	1.87257055352546
H	12.55243035068831	-5.70821066221411	1.24685696077513
H	9.58479237316443	-3.93039904150283	0.64975803874158
H	7.01264261448903	-1.58117417055316	0.20432099131861
H	6.84392335406867	1.69839808278563	0.13318826582942
H	9.12058412146203	4.32116353667588	0.51948166121957
H	12.54660495470443	7.21166822533874	0.72750580896713
H	15.19553752219566	9.37413129333604	1.13840421820082
H	19.64758377812341	10.08151312937866	1.92187830745272
H	24.20748638578367	9.18181073108588	2.56881610190918
H	32.10654386552900	-1.78644268951699	4.02820209285583

H	23.61127927937358	-8.31122833468442	3.24380512594700
H	30.71701584732290	4.00596367612694	-0.37098271794193
H	30.26221761943430	-4.27786514477816	-0.24569156916157
H	32.91387819028713	1.38725304588728	0.22930653817254
H	26.85448592124586	-6.59327132534209	-0.56128959935116
H	27.31239586842289	6.85367024512182	-0.89327026667413
H	20.04182733333075	-8.55707945871737	-1.40926561804001
H	16.24762011177814	-8.29703731403027	-2.04576911386261
H	13.17913583828929	-6.39730200931540	-2.67428953008986
H	9.96177008209875	-3.99323245579907	-3.42815895263128
H	7.39841940022078	-1.60003738628111	-3.58793444530367
H	7.25184839546554	1.65750995720774	-3.62823684567026
H	9.47528997157635	4.31077664399914	-3.54164227789413
H	13.11328868668926	7.25808712746528	-3.11632334251060
H	15.79579579961145	9.34325189057932	-2.79381055584816
H	20.32620792266670	10.06097763088533	-2.15333268558465
H	24.81225500441182	9.14062224636239	-1.38524936799852
H	32.77302867060614	-1.87783707161417	0.28148525340336
H	23.67674496634831	-8.35296515517317	-0.83536872789039
O	19.25800887209078	-2.18176615698308	-3.97659289414811
H	19.05332031240278	-3.02187503807954	-4.43876654162367
H	20.27124223338368	-2.14139582149922	-3.83009675842955
H	21.39776162816313	-3.82697727925654	-2.78573459875298

- **TS1' (Hck-CO₂ → Hck-H-CO₂)**

Si	-7.83070408868863	2.39055339798264	-1.27453886983298
Si	-7.79836815989990	-2.22255455401925	-1.34631446882452
Si	-10.10877925090220	2.98296756526658	-1.33189083234016
Si	-10.02531848193864	-2.97813024627840	-1.41322743784150
Si	-11.66896671432361	1.17643900911029	-1.39374688750776
Si	-0.34347889399076	-1.25987873547959	-1.24206426332890
Si	-1.83430345827371	2.57483021915677	-1.16067913670294
Si	-1.99422239220083	-2.27778417568232	-2.60188942062041
Si	-4.13113056996163	2.20436727077521	-1.16256814348666
Si	-3.85647420327960	-2.11942192755006	-1.21185736206740
Si	-5.89353882798032	3.80363856482526	-1.18367356637209
Si	-6.00596451567767	-5.88235230438486	-1.35083615249479
Si	-4.93739953262380	-0.00296226070782	-1.10548728638044
Si	-5.91618011319189	6.19613807749775	-1.17124021348845
Si	-5.79121613461426	-3.52127190619776	-1.26664282889986
Si	-7.28088121051243	0.07997525711806	-1.27149643636114
Si	-0.11212526882317	-7.93407277069783	-1.36930768622606
Si	1.72724634704152	-6.43449787980454	-1.29207050092874

Si	3.88535431928579	-7.39935900844147	-1.43635889459956
Si	5.80554751284439	-5.96441912411681	-1.43638713224455
Si	5.72732319212199	-3.58728799675510	-1.36263912548751
Si	7.73812751039843	-2.28306118709212	-1.37020741093712
Si	9.95509331003609	-3.07275737153551	-1.41594435703701
Si	11.63744823523782	-1.37770016587563	-1.39094015097159
Si	11.73748246499013	1.02065977774662	-1.33689807358913
Si	10.23116370762721	2.87332925542763	-1.28149362795384
Si	7.93461866483159	2.34924171886470	-1.26064492178368
Si	7.30075811480449	0.05063614999564	-1.29336661864487
Si	4.95813043098114	0.13356956057733	-1.28447249710668
Si	4.22749008596695	2.34868876625578	-1.19801938690803
Si	6.06865618716798	3.86000308729525	-1.19414439177382
Si	6.10799322430869	6.24635122551628	-1.15741983421641
Si	4.24170471565561	7.76135614061656	-1.12565471884895
Si	1.98283744373592	7.02659417072442	-1.13307021073544
Si	0.08836895828028	8.49976523536980	-1.11471186836388
Si	-1.83422690528522	7.06146072331829	-1.13074991421909
Si	-1.12619881535955	4.81143723933652	-1.13843187084582
Si	1.21308512047224	4.79122579984597	-1.14194697516202
Si	1.90400712857101	2.54859380316570	-1.18188230416537
Si	0.01612525432796	1.08478456608757	-1.17013617683044
Si	-4.09866918242047	7.76820664812388	-1.13175267037210
Si	-11.64963191515221	-1.22485301603610	-1.42901873837229
Si	-4.10822954831453	-7.32629630713956	-1.37574366399269
Si	-1.93235790335196	-6.38258387508421	-1.29946248181778
Si	-1.09976704818729	-4.30312425725183	-1.93374580028597
Si	1.09873276078931	-4.51853786410328	-2.43395235214753
Si	1.66332873746670	-2.59162747339215	-1.26594178786018
Si	3.94659424617552	-1.99175876081214	-1.29404305923940
Si	-7.89854349644816	2.37143274664849	1.15906751375564
Si	-7.88741571402016	-2.25466637132266	1.08797879540041
Si	-10.18218107038371	2.95175096592192	1.07944627061928
Si	-10.11369184535476	-3.00843546014522	1.00298617882025
Si	-11.74214537419938	1.14312645457994	0.99067232717943
Si	-0.19267588305268	-1.22739080657156	1.21085750635492
Si	-1.85533095925885	2.56324325475995	1.27079011679854
Si	-1.97545782739726	-2.46539653675082	2.07753041252190
Si	-4.16466495347370	2.22129263253300	1.25846583517188
Si	-4.08809749210257	-2.11663093205356	1.24813880487272
Si	-5.95642387269042	3.79360505363460	1.22720917117609
Si	-6.04564318859355	-5.98093638176613	1.05192392825539
Si	-5.00325190808684	0.03524633268650	1.29972669564240
Si	-5.95343227792742	6.18493540014023	1.23941066457298

Si	-5.91809848141265	-3.61264325850266	1.13250420316471
Si	-7.34025898935718	0.05573324396475	1.14202966189145
Si	-0.10138700707624	-8.11128041337597	1.01214205886848
Si	1.80953087019116	-6.68742039939984	1.10416998365018
Si	3.99835965796438	-7.54743607828372	0.95811135635362
Si	5.86650618769195	-6.04445376232684	0.97323487275189
Si	5.78375758892831	-3.66540254464486	1.03642147587532
Si	7.78235903792360	-2.34262467559939	1.06589286932086
Si	9.99885613218918	-3.12934699394834	0.99905292611030
Si	11.67789009942355	-1.43157011109305	0.99585701682408
Si	11.77621930819577	0.96660924225623	1.04783401310874
Si	10.27327339851164	2.82177455319298	1.12922459202081
Si	7.97509505176896	2.30327473208061	1.17290874595992
Si	7.34966159483493	-0.00135029120771	1.12350523282219
Si	5.00559391744935	0.09884294080998	1.13139833515338
Si	4.26245032924076	2.31259949544316	1.22852814214811
Si	6.10762756889188	3.81923536454477	1.21385798415804
Si	6.12162788338581	6.20818775487997	1.25015950978580
Si	4.25080451407067	7.72521477083433	1.28295526862114
Si	1.98522778357447	7.00803586310121	1.28769190261109
Si	0.08723641669928	8.48196362086154	1.29915330300574
Si	-1.84004322370208	7.04315466961917	1.29214430976215
Si	-1.11929287373914	4.79409353144605	1.26741652705347
Si	1.22217578617896	4.77167619877282	1.26887534078021
Si	1.93899621498352	2.53663943507471	1.25520561490649
Si	0.02918457952082	1.10909327753552	1.25363149376436
Si	-4.11427057513736	7.73783534372506	1.27794099626965
Si	-11.73589659073956	-1.25744773516267	0.95630534679689
Si	-4.17142460468531	-7.47032818210532	1.01601113999357
Si	-1.96971928345486	-6.62890386265389	1.11657634509653
Si	-1.15502870924242	-4.66412671301252	1.99025188246559
Si	1.17602923160394	-4.65574893053438	1.98134868178383
Si	1.76581694466717	-2.59305868907181	1.12121126399717
Si	4.03901778123958	-2.04511559949655	1.13212144662007
C	0.68291718841457	-4.54564655143212	3.88325582965355
O	-0.79849218851448	-4.58978191084344	3.81068796598826
O	1.20791462578455	-4.39614356922694	4.94248164578296
H	-10.52483958017002	4.15608741447881	-2.16409671170825
H	-10.39353749724268	-4.14409478411768	-2.27758783681629
H	-12.90702043665164	1.60525327894317	-2.12524336340481
H	-7.13857482208147	-6.39380887035392	-2.18836234463278
H	-7.07437528983559	6.78052825039158	-1.92432978938193
H	-0.17146003340535	-9.06345142126342	-2.34835603293277
H	4.05600421226353	-8.59112223303452	-2.32718487618222

H	6.92636520999952	-6.53758856914047	-2.25101702564458
H	10.29828705958868	-4.24312567382824	-2.28449053655200
H	12.85370441296273	-1.85140484724429	-2.13103508134321
H	12.99662609602061	1.41875198694328	-2.04953234031448
H	10.69219976719976	4.03871613834773	-2.10070045583343
H	7.25802553386934	6.85517245368371	-1.90278019733591
H	4.55361559336970	9.00697269924657	-1.89843645559334
H	0.09833086682271	9.73200926854706	-1.96628601595549
H	-4.44039712124919	9.00026457312867	-1.91341272914296
H	-12.86703050558739	-1.66415570175028	-2.18806166024874
H	-4.24250553588016	-8.52505693391363	-2.26186057936488
H	-10.66597815457416	4.09736795971028	1.91357903851223
H	-10.52522528911827	-4.19706117864981	1.81545378776323
H	-13.02076900878006	1.55918744785764	1.65711141268730
H	-7.17812765714103	-6.57051193735792	1.83762348942068
H	-7.12025277031186	6.78849244980745	1.96381222094944
H	-0.14407859415452	-9.35648880357989	1.83897583447636
H	4.25770199330393	-8.81982058262098	1.70285534461930
H	7.02233046418827	-6.64787212197195	1.71411304804468
H	10.37247596959686	-4.33755868800651	1.80075792189736
H	12.91818218672474	-1.93610148400831	1.67295463091110
H	13.05812016397790	1.33225353155732	1.73696689552949
H	10.77383716076730	3.94749713190665	1.98012706401258
H	7.27172053493515	6.81034225339192	2.00123507996790
H	4.58233542969742	8.94345953646514	2.09073745383134
H	0.10572504080022	9.70021763090606	2.17076120739610
H	-4.46844413152222	8.94953340275759	2.08588310230225
H	-13.00458182822083	-1.71200006573645	1.61567516850727
H	-4.40694542795596	-8.73798884545112	1.77624237948870
H	-1.89034115718900	-2.58054840346821	3.87042268364576
H	-1.41506769645949	-3.42941444265067	4.03788627258004

- **TS2' (Hck-H-CO₂ → Hck-CO-H₂O)**

Si	-7.81567634192895	2.37551282666428	-1.22590325375717
Si	-7.76946812032619	-2.22801916254905	-1.29624959930486
Si	-10.10311928398762	2.94036811213797	-1.23136555701172
Si	-9.98691237954486	-3.01400313552707	-1.31624982440036
Si	-11.65358921095508	1.12349513279537	-1.25433699601101
Si	-0.32065183954190	-1.23537610325525	-1.32509654029921
Si	-1.81655629507090	2.60380923489700	-1.22741263308326
Si	-1.96401260280559	-2.28508758312582	-2.66860145624000
Si	-4.11323279253236	2.21358755583124	-1.21337333406548
Si	-3.81651392979721	-2.11540004437012	-1.26973369445333

Si	-5.88587474647776	3.80482125331769	-1.18962029767790
Si	-5.99272119657219	-5.86014905740033	-1.36796852620921
Si	-4.88833261740891	-0.00063397993132	-1.21310305835197
Si	-5.91461117715219	6.19781725335888	-1.16441304119682
Si	-5.75110934357586	-3.50845575203354	-1.27802928183862
Si	-7.23567822094454	0.07143583819762	-1.24432135983551
Si	-0.10795809360911	-7.90601880619288	-1.42534559318281
Si	1.71085449902944	-6.37146813155886	-1.36656166336366
Si	3.85389417535696	-7.38642768299241	-1.40263898439083
Si	5.78892840360757	-5.97092310161914	-1.39378739729091
Si	5.68878484948841	-3.59507464450320	-1.33469552088247
Si	7.70123991605670	-2.29568292018988	-1.32225284286380
Si	9.90721568428506	-3.11627582908661	-1.33514556815969
Si	11.61179281579162	-1.44436263593660	-1.29718911983009
Si	11.73103585886292	0.95283129060574	-1.25734496983475
Si	10.23960280379025	2.81818862089925	-1.23466538078409
Si	7.93408014683555	2.32887466785756	-1.24155598504635
Si	7.26605388171343	0.04009815452383	-1.26907251237441
Si	4.92187075301532	0.13389675287016	-1.29405152410779
Si	4.23189454477707	2.36402846009929	-1.22996093075465
Si	6.08230281314667	3.86118893456523	-1.20535093940661
Si	6.11998724776874	6.25052396891285	-1.17470040185901
Si	4.25899201681742	7.77612557001239	-1.15177200387341
Si	1.98972583026066	7.06847021195355	-1.16386961063651
Si	0.09144059116185	8.54213507891379	-1.13910721873382
Si	-1.83175096857722	7.10139850035563	-1.16135506343453
Si	-1.12202523330926	4.84889901746152	-1.18790491288771
Si	1.21658981302454	4.83605902486699	-1.19675444337100
Si	1.91217198791688	2.59612583982545	-1.24064269352467
Si	0.03995835821344	1.11313433835451	-1.25275257744494
Si	-4.10596708052752	7.78475563776547	-1.14385954697679
Si	-11.62714436300272	-1.27763565717871	-1.28822791524007
Si	-4.09406684500622	-7.30344071596342	-1.43157967242508
Si	-1.92063977564385	-6.35517885352259	-1.41406985217216
Si	-1.05214599970269	-4.29102852179537	-2.06080017599876
Si	1.15167135286709	-4.51946327548818	-2.65497005722992
Si	1.64043063460230	-2.64259248653909	-1.35855660323204
Si	3.91158224785521	-1.99774776255579	-1.29065009258460
Si	-7.83325949483460	2.35161752977774	1.20861214220188
Si	-7.79092269657304	-2.27063025866261	1.13931841721860
Si	-10.12215866262267	2.91320556618068	1.18015810603360
Si	-10.00989164121991	-3.05173047372904	1.10077188764406
Si	-11.66767535434851	1.09096518563842	1.13101727703464
Si	-0.30292776948945	-1.21761230076168	1.10598420484727

Si	-1.82539831735075	2.57736384893019	1.20296585632192
Si	-1.92362679292611	-2.32927285774315	2.39040743433172
Si	-4.12370828675352	2.19184612929939	1.21038827496800
Si	-3.89227982112358	-2.13696750991626	1.16585317869421
Si	-5.89930757592662	3.78183510926211	1.22210415323492
Si	-5.99074625225798	-5.94285193438252	1.03563618535203
Si	-4.92442465978166	-0.01238521869925	1.19062847242500
Si	-5.92024733605196	6.17487224425660	1.24521365931454
Si	-5.78369798633223	-3.58026565463006	1.12579074433475
Si	-7.26921491803216	0.04008854306046	1.17077503053547
Si	-0.12952308875399	-8.06381337003062	0.95558538654890
Si	1.75640388548031	-6.63321739052622	1.03362791584813
Si	3.94536193917244	-7.49279450799398	0.99470341660104
Si	5.83422660924413	-6.02935389887936	1.01679016247381
Si	5.71582805584340	-3.65649355492233	1.06213682699303
Si	7.71513940883025	-2.33818761632548	1.11264532017542
Si	9.91921987967322	-3.15978999385484	1.08138498322903
Si	11.61918006410839	-1.48271952995064	1.09088708830793
Si	11.73802375726234	0.91473686731041	1.12791600321794
Si	10.25057438020281	2.78315932507592	1.17648656325410
Si	7.94480170788057	2.29643444528608	1.19301163551623
Si	7.29278027508075	0.00161811133416	1.14701973237690
Si	4.94768407042874	0.10925399159612	1.11750760787979
Si	4.24298282870434	2.33489630999395	1.19642761700650
Si	6.09324583289069	3.83097256838626	1.20298064227464
Si	6.12560281740412	6.22047901481641	1.23338492925174
Si	4.26201626332882	7.74343475416204	1.25693610319873
Si	1.99256285486679	7.03618875566014	1.25455682826615
Si	0.09387041385912	8.50969433509883	1.27339424867530
Si	-1.83068799418271	7.07021765220072	1.26116881765500
Si	-1.12067063982481	4.81847978801927	1.21772470181567
Si	1.21839784742222	4.80399061766681	1.21568303424421
Si	1.92481294733721	2.56688894853972	1.19573933716801
Si	0.04096556944526	1.10873557647426	1.17030450788595
Si	-4.10530307180131	7.75489207333560	1.26421368842359
Si	-11.64478615748432	-1.31048898277841	1.09807317837566
Si	-4.11256116879323	-7.42325046683901	0.95819531362201
Si	-1.92973959132254	-6.52005217103355	0.99944026012309
Si	-1.33265436554764	-4.56047653217144	2.09086253408355
Si	1.04164908786209	-4.60372388098915	1.91307029290559
Si	1.67899786813500	-2.53442730084312	1.03909081982584
Si	3.96722732854989	-2.03935766591288	1.13282850065749
C	1.53319854003829	-4.56054814277670	3.69803518780338
O	-1.66631185984277	-4.75493848487376	3.93563447537934

O	1.87833572513206	-4.50172348467371	4.79778189876428
H	-10.55239830573225	4.10761909997755	-2.05501640774341
H	-10.35695008821974	-4.18220578088555	-2.17745295400755
H	-12.91191709665756	1.54840229377856	-1.95342664398669
H	-7.13183983892812	-6.37665689103202	-2.19384005222471
H	-7.08321945077231	6.78657600132993	-1.89839799284495
H	-0.12040203934318	-9.05789875712993	-2.37811283698778
H	4.03199634602978	-8.60588222113118	-2.25377062397960
H	6.91275167790252	-6.54968960051250	-2.20014988943388
H	10.24675739459629	-4.29729084378343	-2.19086189507807
H	12.83158190247253	-1.93685091642309	-2.01893536883747
H	13.00327374396182	1.33508468160618	-1.95529773963861
H	10.72818274076083	3.97278690252327	-2.05323775782887
H	7.27493401200772	6.85849181929141	-1.91354034802978
H	4.59318313745463	9.01698076233949	-1.92341396713428
H	0.10620122127742	9.78022257239488	-1.98253268436233
H	-4.46729383520441	9.01274107025793	-1.92361406215082
H	-12.86349393982558	-1.72394981954534	-2.01204189936374
H	-4.23895565182861	-8.51244019285197	-2.30180779311294
H	-10.59771054081824	4.05666158463641	2.02242616246910
H	-10.39982673499691	-4.24392322780359	1.91975826861475
H	-12.93487847128700	1.49492492125955	1.82677274941922
H	-7.10298942139870	-6.53582833882106	1.84881911789837
H	-7.08842160999867	6.75600542452839	1.98606034450801
H	-0.18107174394775	-9.28074298992398	1.82365120280304
H	4.12820243343572	-8.75579533354727	1.77767208877109
H	6.96572209163660	-6.63721264383872	1.79103111256119
H	10.26680849655151	-4.36827554542859	1.89487035197475
H	12.84308989494926	-1.99709688252636	1.79020179159229
H	13.01457708158643	1.27194968966409	1.83142189280376
H	10.75322705866058	3.90995354285154	2.02486078177732
H	7.28126013386072	6.81301778798862	1.98367656127571
H	4.59614107893006	8.96262345881554	2.06246702301213
H	0.11125514588228	9.72420158052770	2.15046636343014
H	-4.46021279119398	8.96420515395996	2.07553679125284
H	-12.89244014531688	-1.77254648563422	1.79217385859368
H	-4.26991031182506	-8.69019087998551	1.74217151341080
H	-1.88508617964499	-3.53193140725595	3.90898755912946
H	-2.47829661826637	-5.26230213086129	4.15781602476165

- **TS3' (Hck-CO → Hck-HCO-H)**

Si	23.02498747635740	-3.35792277764018	4.30974485038770
Si	23.02044902716309	-7.99698087448726	4.67926666578721

Si 25.25294709510019	-2.65821672334572	4.59175520060556
Si 25.26095186657534	-8.60141342050131	5.08420470663230
Si 26.83069780004395	-4.40539109903106	4.98776044361855
Si 15.22210525584637	-6.66159470896139	3.08950006099319
Si 17.09507815111285	-3.05591288949227	3.30684895509998
Si 17.13407399890617	-8.06307035132234	3.46902047775171
Si 19.35006083361783	-3.53544794017020	3.70176912829143
Si 19.37332197412704	-7.88404339606060	4.08748067042380
Si 21.12666475804005	-1.95829744728800	3.85249286126135
Si 21.04730974143439	-11.84706089474581	4.62049506216348
Si 20.22193676987743	-5.70687949716582	3.94674858089702
Si 21.23801846570878	0.42231367358829	3.68046140313167
Si 21.12988833398914	-9.46535190679384	4.43792684326737
Si 22.51843335265194	-5.68124213654282	4.40723957742709
Si 14.99925476421640	-13.86794721321289	3.79120502720649
Si 13.16177092048022	-12.38070874522509	3.37758362071701
Si 10.89783163266635	-13.04061823944575	3.09505819560475
Si 9.11247983536026	-11.47756934597836	2.70651940620032
Si 9.17402870431011	-9.09631587796202	2.52972920497762
Si 7.26901526627917	-7.67173450696922	2.18364757700308
Si 5.03081547358071	-8.34805610687945	1.90314201711201
Si 3.45282119406528	-6.59122826865826	1.54635450495673
Si 3.45976030112973	-4.19641368500084	1.37323659727403
Si 5.04278158745741	-2.41312341015397	1.48058078932686
Si 7.28320397761817	-3.03842098032153	1.85610868837168
Si 7.80477638962894	-5.35285799680970	2.08593110905086
Si 10.13331536025999	-5.34768162644987	2.35919891390718
Si 10.96954091610258	-3.15918683392939	2.38326225375931
Si 9.20883719926520	-1.60536164706854	2.01037165553348
Si 9.32451260077300	0.77788508834081	1.86115506171745
Si 11.22452614218266	2.24720227223153	2.03771740964702
Si 13.45586583736049	1.51659677532048	2.42431123169569
Si 15.40201384844409	2.91626887025882	2.60929754326101
Si 17.24206297035141	1.42268493280979	2.99730354451163
Si 16.47016845396899	-0.80668597330779	3.02917227963545
Si 14.15162783163751	-0.72602980910306	2.65690490578909
Si 13.27273306109345	-2.89952598085778	2.69586633753131
Si 15.10589493072575	-4.33987065915407	3.18103564606827
Si 19.51138814634138	2.05005921269467	3.28773753028880
Si 26.82536727992195	-6.79842389559865	5.19122068770783
Si 19.13567590682347	-13.28584274185840	4.40050668215648
Si 16.94995913097800	-12.47840799181194	3.94286462194992
Si 16.27837047836901	-10.23150484414331	3.66391206186792
Si 13.96209071300605	-10.16671988193002	3.30199226277182

Si	13.24112237177770	-7.94962585726115	3.03652275745626
Si	10.96527792440267	-7.52929402221769	2.64176097306845
Si	23.39814244250065	-3.56414388340413	1.91096719295960
Si	23.42371059631679	-8.17726137339572	2.28377592050516
Si	25.62962540157969	-2.87488422398920	2.21860738528246
Si	25.65973876853339	-8.78303051945184	2.71484938713132
Si	27.22022364693217	-4.60515602628215	2.64159077328554
Si	15.55912246088535	-6.85874784227241	0.60133028515709
Si	17.45034075571802	-3.24639523551623	0.91327827498518
Si	17.52336309208000	-8.31000701648980	1.02147636624066
Si	19.71715585415547	-3.72718039044323	1.29258811009694
Si	19.75756397942583	-8.13291724571667	1.70442806787815
Si	21.50051022410808	-2.15144350580503	1.48677070808577
Si	21.44642501874333	-12.03011799478560	2.24937213145803
Si	20.53692037192299	-5.91785633123511	1.56873308984629
Si	21.60269698711354	0.23206146955036	1.30749549503614
Si	21.54566478473371	-9.65330000393623	2.08393204276570
Si	22.84027937061511	-5.88019907065149	2.00863040391018
Si	15.36561555933395	-14.09508010240977	1.41663700009262
Si	13.52816563661663	-12.59680958061448	0.99398581154929
Si	11.25396031090151	-13.23053934335242	0.71756506115397
Si	9.46587742228357	-11.65945001902866	0.32948758575105
Si	9.49610422213207	-9.27347205035307	0.15610571550780
Si	7.60424264149084	-7.83882377976073	-0.22665979063031
Si	5.36200314333855	-8.51374719204924	-0.47964936260264
Si	3.77709398722072	-6.76068046988100	-0.81199311745335
Si	3.79316268696015	-4.36656518375554	-0.98306917454568
Si	5.38509006390357	-2.58841405992362	-0.89900331434677
Si	7.63252396611857	-3.20992958957063	-0.54970152131848
Si	8.17481508355540	-5.52301847580617	-0.30646011436619
Si	10.49901475146293	-5.52808529265185	-0.01353614163148
Si	11.31944864569203	-3.33211255319393	-0.02069776949463
Si	9.55422630318006	-1.77163371238953	-0.36523342565183
Si	9.67315665836013	0.61200712067111	-0.51581740998087
Si	11.57755736078669	2.07805110739521	-0.34195050569534
Si	13.81204765752362	1.34997994042264	0.04013946583292
Si	15.76132689062942	2.74637545536114	0.22852781778368
Si	17.59923195816186	1.24397663603829	0.60761751038784
Si	16.81712279499193	-0.98651254119300	0.65856398730733
Si	14.50121066261673	-0.89159173153460	0.27764982201160
Si	13.61927524267421	-3.05778895719608	0.29147028659721
Si	15.42938272107762	-4.51603236457043	0.77957711250413
Si	19.87193299955543	1.86012560443130	0.91166293806198
Si	27.23306147976737	-6.99529172333112	2.84878276114066

Si	19.53166702626538	-13.47676468592943	2.03000462923837
Si	17.32298323933895	-12.70867507242380	1.57129552816237
Si	16.64055388593930	-10.45982034624140	1.29587485110113
Si	14.32010969295432	-10.37527300769949	0.93298843531568
Si	13.57004913377440	-8.15650797661343	0.64303155422501
Si	11.30179776975118	-7.72451043047000	0.24453789676933
H	25.52734776186050	-1.41193202249811	5.37500921137218
H	25.54927052990154	-9.69162726532422	6.06906360389364
H	27.95000890190473	-3.90046927460892	5.85021657870066
H	22.02575637870258	-12.43649799110007	5.59257678181755
H	22.30822965363938	1.02409920358863	4.54251117081463
H	14.83881507717610	-15.00435485337829	4.75425674841261
H	10.42201838296533	-14.20072505723508	3.91628638116656
H	7.84070501073603	-12.00231927851707	3.30446772516956
H	4.50138845339231	-9.45970366311419	2.75502186685924
H	2.11860799994316	-6.98659265268413	2.10759730521709
H	2.12438093545291	-3.72006534183167	1.86455221387718
H	4.51769085717467	-1.18811148935195	2.16252660444574
H	8.10259167796326	1.47754195619084	2.37805715883016
H	10.81699137641686	3.54239566961306	2.67280762808226
H	15.32068580393169	4.20041228521884	3.37636897019106
H	19.78665711794820	3.31900419697889	4.03594635639383
H	27.93777092487961	-7.15691587580412	6.13244705628771
H	19.24629239695575	-14.46760995323182	5.31571032409461
H	26.16345464086709	-1.77687741740618	1.35157691691885
H	26.19854891145039	-10.00927831545842	2.04594866148449
H	28.56330218340207	-4.19698663128061	2.11128984607200
H	22.67006818350395	-12.74158595089547	1.75345129565298
H	22.88941608937660	0.73080392195272	0.71862446876722
H	15.43505581632141	-15.39632849274241	0.67728280442583
H	10.98309499203762	-14.50867453478954	-0.01745044239286
H	8.41701497787058	-12.31464429609133	-0.52016526703932
H	5.07412938969613	-9.74393497611277	-1.28300556730072
H	2.63543069864035	-7.25502443865431	-1.65077153998660
H	2.65758768140754	-3.98265390323302	-1.88567413058871
H	5.09382253229693	-1.48544980479477	-1.86871114333510
H	8.66656173523441	1.21496818002807	-1.45032844433013
H	11.39422825966952	3.26419305642368	-1.24009462797080
H	15.92911227640309	3.90892923810959	-0.70117083721772
H	20.39796409817036	3.00113997308617	0.09457083189018
H	28.58503819509670	-7.47042216769592	2.40395037694006
H	19.94798825551998	-14.77573746473228	1.40814607794904
C	15.97366497156777	-6.90484932181836	-1.48929509091669
O	15.48080098432163	-6.38059965701708	-2.41125203929720

H	17.15375804906923	-7.72247010205898	-1.40626063407123
H	17.74859643227713	-8.12373553666769	-0.74418754454584

- **TS4' (Hck-HCO-H → Hck-CH₂O)**

Si	22.97517763902816	-3.29880363519759	4.39709527436728
Si	22.69766926676217	-7.92841777749961	4.74195071672389
Si	25.26786035023741	-2.82104185138253	4.64952525030311
Si	24.86527017434694	-8.76947056599444	5.08878984093750
Si	26.70648326943396	-4.69873441491077	4.99092272287835
Si	15.14311924032290	-6.66886873465172	4.19872046747468
Si	17.02581476028774	-3.00843021386616	3.49488735038318
Si	16.74352111161825	-8.04917831486638	4.95916767517981
Si	19.30333310149097	-3.33040233244578	3.86847358625901
Si	18.88679326371659	-7.60089209446537	4.18387563157138
Si	21.13064936670259	-1.81154967043778	3.98935327149966
Si	20.75706472015620	-11.53549476352959	4.69303522233246
Si	20.03962223424917	-5.54213611324890	4.06216102235400
Si	21.20047118072040	0.56982831628676	3.79371307539842
Si	20.66337507523063	-9.16498577647052	4.50641101371290
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