

Metal-free catalysis for the Markovnikov hydrosilylation of styrene

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Contents

Table S1~5	Page 2~6
Scheme	Page 7
Figure S1~2	Page 8~9
Coordinates	Page 10~17

Table S1. Absolute (in au) and relative (in kcal/mol) energies of reactants, transition states, and products in hydrosilylation of styrene with phenylsilane in gas phase and THF solvent (values in square brackets).

	E_{zp}^a	E_{sp}^b	E_{tot}^c	E_{rel}^d
R1	0.1346	-309.6492	-309.5146	
	[0.1345]	[-309.6583]	[-309.5238]	0.0
R2	0.1161	-522.9486	-522.8325	[0.0]
	[0.1159]	[-522.9551]	[-522.8392]	
TSX	0.2524	-832.5250	-832.2726	46.8
	[0.2525]	[-832.5418]	[-832.2893]	[46.2]
PX	0.2569	-832.6500	-832.3931	-28.9
	[0.2563]	[-832.6641]	[-832.4077]	[-28.1]

a: zero point energies; b: single point energies; c: total energies of E_{zp} and E_{sp} ; d: relative energies

Table S2. Absolute (in au) and relative (in kcal/mol) energies of reactants, transition states, and products in Markovnikov hydrosilylation of styrene with phenylsilane at fs (field strength) = $\pm 60 \times 10^{-4}$ au along FX directions in THF solvent. (Values in square brackets are those calculated at fs = -60×10^{-4} au)

FX	E_{zp}^a	E_{sp}^b	E_{tot}^c	E_{rel}^d
R1	0.1343	-309.6617	-309.5275	
	[0.1344]	[-309.6611]	[-309.5266]	0.0
R2	0.1159	-522.9571	-522.8412	[0.0]
	[0.1158]	[-522.9567]	[-522.8409]	
TSX	0.2523	-832.5437	-832.2914	48.5
	[0.2519]	[-832.5503]	[-832.2984]	[43.4]
PX	0.2561	-832.6709	-832.4148	-28.9
	[0.2563]	[-832.6683]	[-832.4120]	[-27.9]

a: zero point energies; b: single point energies; c: total energies of E_{zp} and E_{sp} ; d: relative energies

Table S3. Energies of transition states at field-free, FX (-60) and FY (± 60) (in 10^{-4} au).

EEF	F(0)	FY(60)	FX(-60)	FY(-60)
E	-832.2726	-832.2973	-832.2984	-832.2990

Table S4. Absolute (in au) energies of reactants, transition states, and products in Markovnikov hydrosilylation of styrene with phenylsilane at fs (field strength) = 0, -30, ± 60 , -90, -120, -150, and -180×10^{-4} au along FY directions in THF solvent.

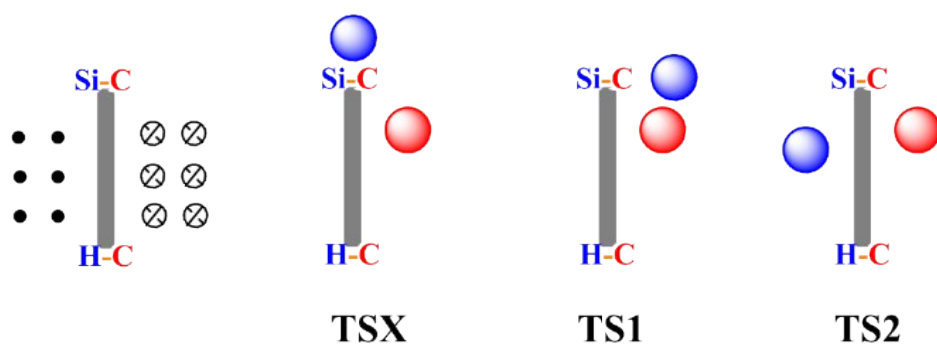
FY	E_{zp}^a	E_{sp}^b	E_{tot}^c
R1	0.1344	-309.6599	-309.5255
{60	0.1345	-309.6587	-309.5242
-30	0.1345	-309.6599	-309.5254
-60	0.1344	-309.6618	-309.5274
-90	0.1343	-309.6646	-309.5303
-120	0.1339	-309.6680	-309.5342
-150	0.1337	-309.6736	-309.5398
-180}	0.1156	-522.9610	-522.8453
R2	0.1160	-522.9546	-522.8386
{60	0.1157	-522.9556	-522.8399
-30	0.1137	-522.9582	-522.8446
-60	0.1150	-522.9624	-522.8474
-90	0.1145	-522.9683	-522.8538
-120	0.1137	-522.9757	-522.8620
-150	0.2516	-832.5489	-832.2973
-180}	0.2528	-832.5450	-832.2922
TSX	0.2527	-832.5516	-832.2990
{60	0.2517	-832.5613	-832.3095
-30	0.2514	-832.5747	-832.3234
-60	0.2502	-832.5918	-832.3415
-90	0.2481	-832.6129	-832.36478
-120	0.2560	-832.6671	-832.4111
-150	0.2563	-832.6657	-832.4094
-180}	0.2564	-832.6696	-832.4132
PX	0.2559	-832.6756	-832.4196
{60	0.2556	-832.6839	-832.4283
-30	0.2540	-832.6977	-832.4437
-60	0.2529	-832.7133	-832.4605
-90			
-120			
-150			
-180}			

a: zero point energies; b: single point energies; c: total energies of E_{zp} and E_{sp} .

Table S5. The number of imaginary frequencies of reactants, transition states, and

products in Markovnikov hydrosilylation of styrene with phenylsilane, and the frequency values (cm^{-1}) in brackets are those of transition states at different field strengths.

	R1	R2	TSX	PX
F(0)	0	0	1 (-1076.6i)	0
FX(60)	0	0	1 (-1130.7i)	0
FX(-60)	0	0	1 (-877.23i)	0
FY(60)	0	0	1 (-613.6i)	0
FY(-30)	0	0	1 (-1067.1i)	0
FY(-60)	0	0	1 (-1061.5i)	0
FY(-90)	0	0	1 (-1048.2i)	0
FY(-120)	0	0	1 (-1046.5i)	0
FY(-150)	0	0	1 (-1046.1i)	0
FY(-180)	0	0	1 (-1045.1i)	0



Scheme S1. Addition models of Markovnikov hydrosilylation of styrene with phenylsilane.

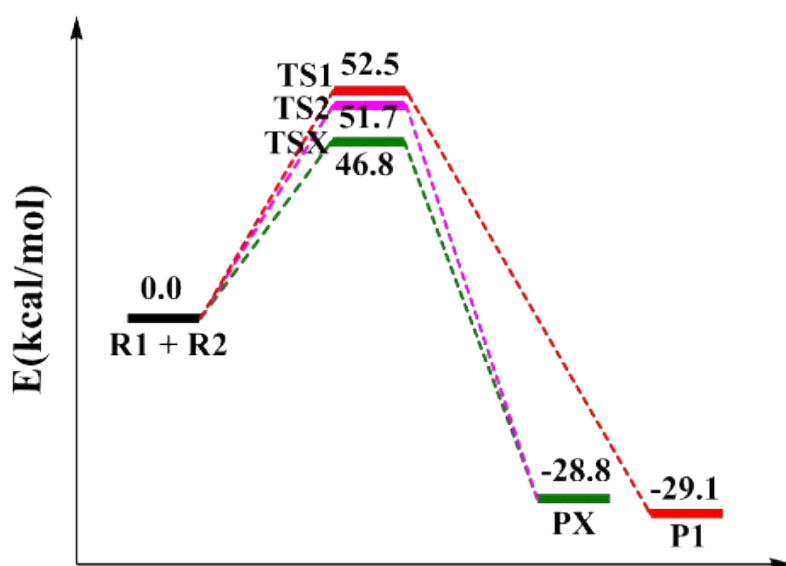


Figure S1. Relative energies (in kcal/mol) of Markovnikov hydrosilylation of styrene with phenylsilane through three pathways.

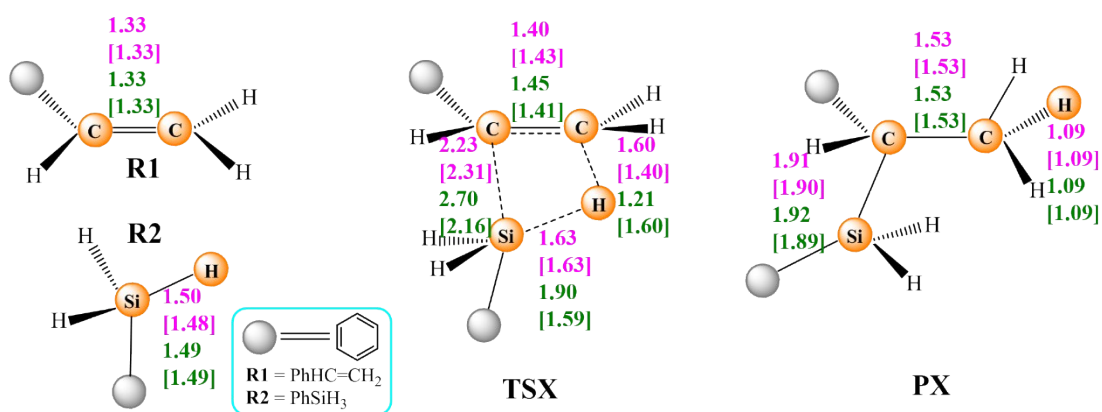


Figure S2. The structures of stationary points along potential energy surface in Markovnikov hydrosilylation of styrene with phenylsilane at fs (field strength) = $\pm 60 \times 10^{-4}$ au along FX and FY directions in THF solvent (bond lengths are given in Å; FX, red; FY, green. Values in square brackets are those calculated at negative directions.)

Coordinates of transition states

F(0)			
C	-0.003873742137	0.019151656662	0.006353747123
C	1.406018943247	-0.006568461144	-0.007416193106
H	1.943800549126	0.306873276788	-0.896578116974
C	-0.818841708722	0.442796171471	-1.149337099026
C	-0.333066279854	0.475923450789	-2.459905851021
C	-2.148692580942	0.818482189509	-0.935515485794
C	-1.145275599568	0.875763214663	-3.511497146340
H	0.689399120351	0.185839865110	-2.670731357168
C	-2.960078185654	1.218060881850	-1.986046063945
H	-2.548846837726	0.794962452485	0.072478567193
C	-2.462789432348	1.249080774910	-3.282780114639
H	-0.743099680298	0.893948238093	-4.517820917935
H	-3.987324686750	1.503364547334	-1.790934216079
H	-3.095426198853	1.560113425370	-4.105329884062
H	1.932299819824	0.164281423941	0.924756482365
Si	0.525576974682	-2.181106062312	0.023561015870
H	0.303424004297	-1.985526267765	-1.439984422776
H	1.941226225332	-1.406252139417	-0.115713858058
H	0.543421365011	-1.945149478561	1.501625491922
C	0.194846356220	-4.059051522273	0.080501970338
C	-0.055863098257	-4.778550714017	-1.089952499397
C	0.190422667311	-4.753466728102	1.292150799909
C	-0.301439231993	-6.144985690073	-1.055544032792
H	-0.062614010440	-4.261191351934	-2.045444593343
C	-0.051773826487	-6.119976092084	1.337559436278
H	0.377076388326	-4.216706179253	2.218431409107
C	-0.298708494091	-6.816484687236	0.160788916025
H	-0.496174960873	-6.686303055376	-1.974234065506
H	-0.051063487214	-6.642398505250	2.287275886730
H	-0.490055777410	-7.882894730531	0.192280511975
H	-0.474408594849	0.170265095907	0.969743684609

FX (60)			
C	-0.017815763591	0.019159989551	-0.005203695670
C	1.385162813520	0.023168978198	0.005832187270
H	1.933228603791	0.352304580167	-0.870779304326
C	-0.838748806762	0.463229113673	-1.158472259573
C	-0.333162561934	0.591803320631	-2.453484522137
C	-2.185565268788	0.757411930306	-0.940783623631
C	-1.150938577059	1.010033607044	-3.493997532461
H	0.703581633727	0.351594185853	-2.662149926222

C	-3.003089895762	1.174733037718	-1.980517027039
H	-2.601973467354	0.651459916609	0.054913948069
C	-2.488512576850	1.303492629892	-3.263186504897
H	-0.744019981425	1.100325694402	-4.494745093840
H	-4.047159899202	1.390573241280	-1.789750085739
H	-3.129925654074	1.621901239909	-4.075607485767
H	1.895516792393	0.150010550082	0.953249876588
Si	0.476801055839	-2.152337710924	-0.024360275391
H	0.365911819404	-1.935437762461	-1.500609279748
H	1.948602235272	-1.464808953057	-0.134613167155
H	0.573375275956	-1.961829220963	1.463443152447
C	-0.187950327948	-3.933505102837	0.014531329481
C	-0.594074922263	-4.569888327118	-1.161106862452
C	-0.391762598918	-4.597553554225	1.226649197746
C	-1.186907611764	-5.825230377333	-1.130083827511
H	-0.477114073372	-4.061972779682	-2.114646213636
C	-0.981394196193	-5.853801230735	1.267814960125
H	-0.116218292954	-4.109698108315	2.158027265261
C	-1.382674797588	-6.466515013447	0.086868774749
H	-1.528072121202	-6.291122358652	-2.047027680121
H	-1.159799348085	-6.343441377885	2.218091171693
H	-1.874345169765	-7.431573025424	0.117271350670
H	-0.508179467389	0.123998777834	0.955108753311

FX (-60)

C	-0.018124450377	0.028788575577	0.012172285219
C	1.405496267747	-0.030444341781	-0.017848008300
H	1.934375091362	0.285098045177	-0.912969808523
C	-0.824260667164	0.425555798729	-1.140929378174
C	-0.349299902412	0.397522947623	-2.460791387732
C	-2.154303256003	0.832032722597	-0.946762515204
C	-1.159886274732	0.764067757305	-3.524591264374
H	0.671705401908	0.100044951037	-2.665628819701
C	-2.962340514678	1.198963515818	-2.010888890665
H	-2.546348119390	0.868600768856	0.064800563184
C	-2.472818260574	1.166132104899	-3.312718744337
H	-0.752360541048	0.739894118450	-4.528721783985
H	-3.982036198629	1.519779226171	-1.821244627285
H	-3.097190453304	1.462084173333	-4.148016359838
H	1.938564390043	0.196397650422	0.899791684554
Si	0.560095987791	-2.202211875764	0.050040273542
H	0.238203323208	-2.025750353557	-1.395468049750
H	1.924922854262	-1.323859557843	-0.096801343336
H	0.468843444236	-1.941783954924	1.515968223885

C	0.600509973320	-4.102072546437	0.103967469361
C	0.563340240034	-4.855385324490	-1.072372010580
C	0.756528053435	-4.779552548929	1.315859467328
C	0.681486520568	-6.238545722454	-1.042641777849
H	0.467622938888	-4.350899090456	-2.030094463031
C	0.875350510569	-6.162258015806	1.355584716541
H	0.815080026563	-4.215889537643	2.242969146055
C	0.841168656403	-6.891824856169	0.173450919257
H	0.682211181054	-6.805043515455	-1.966762414665
H	1.026875115866	-6.669135536014	2.301453935633
H	0.968197601701	-7.967890925379	0.198167484787
H	-0.469217450644	0.220038147108	0.977730957979

FY (60)

C	0.000206948525	0.005228645130	0.011100880400
C	1.445940235983	0.000833126606	-0.030468387589
H	1.900224968856	0.531789088053	-0.869023828384
C	-0.818495699727	0.300638744228	-1.134594164768
C	-0.318866602730	0.325716413836	-2.455686782707
C	-2.201846917618	0.553258210159	-0.984935860085
C	-1.145457364766	0.581751199885	-3.539632087377
H	0.725229068480	0.099393616391	-2.638880016077
C	-3.018592682712	0.808423654864	-2.070077534014
H	-2.633773822913	0.509271775781	0.009957346033
C	-2.501436326458	0.830812000009	-3.365033265641
H	-0.725170058713	0.556358157432	-4.539588654136
H	-4.080084208331	0.966192144263	-1.909572907843
H	-3.149287165497	0.995765149515	-4.217675131377
H	1.925382897680	0.277783267689	0.907787959958
Si	0.781011417619	-2.581516303509	0.020381865766
H	0.417500495469	-2.116267212203	-1.323519140403
H	1.944024986856	-1.090347175962	-0.201128418790
H	0.796498166581	-2.041424118244	1.386644749926
C	0.901922311829	-4.410996119353	0.085016851794
C	0.827233405242	-5.186482959536	-1.082984769486
C	1.122460766270	-5.056158931922	1.312523219475
C	0.959802992640	-6.563224753612	-1.021825751557
H	0.660196191159	-4.711678013093	-2.044642930845
C	1.252711784571	-6.432924091620	1.371027023876
H	1.186786365918	-4.478435447984	2.229494650452
C	1.174400721452	-7.184560408329	0.203604045668
H	0.898828324926	-7.158578995386	-1.924221372595
H	1.416914957840	-6.927782439666	2.320075968207
H	1.279975466790	-8.261691347159	0.249801332098

H	-0.480517503909	0.072288633992	0.979308389345
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FY (-30)

C	0.008442308191	-0.021959751252	-0.001923037855
C	1.415762332882	0.026455437801	-0.003378791939
H	1.951105429828	0.346223902871	-0.891022500639
C	-0.820256731001	0.390372430267	-1.159331510463
C	-0.327435431003	0.476763948099	-2.462942911080
C	-2.159833328087	0.716058354820	-0.937358746027
C	-1.146468503248	0.886509258132	-3.505265992991
H	0.707987273569	0.237742455984	-2.674485285572
C	-2.978746609209	1.125238164510	-1.978985076731
H	-2.559006746147	0.662292736406	0.069753394410
C	-2.475443315783	1.212349077737	-3.270101034398
H	-0.738015893785	0.964833788111	-4.505973946973
H	-4.010913241458	1.387409989232	-1.779151383593
H	-3.109194206896	1.546033780117	-4.082702856362
H	1.930799426995	0.199294299629	0.934086694062
Si	0.602684057316	-2.142484937104	0.013733903255
H	0.417295803477	-2.002930385179	-1.466367156082
H	2.022052446744	-1.409898617694	-0.110866057027
H	0.631514340903	-1.961827747555	1.504964860828
C	0.218530581523	-4.031779087026	0.073614671676
C	-0.048699666847	-4.749358329138	-1.093523677389
C	0.183790944432	-4.722557627053	1.285966786158
C	-0.338399303474	-6.107851514071	-1.056616345248
H	-0.035276051253	-4.233283928248	-2.049849010792
C	-0.102186651150	-6.081154966131	1.336750449490
H	0.379409799087	-4.185360068081	2.210325555635
C	-0.364579346736	-6.775655942661	0.161831046682
H	-0.547752609101	-6.643681610268	-1.975937193631
H	-0.126692268196	-6.596382697044	2.290669600265
H	-0.592760875611	-7.835372889396	0.196644307551
H	-0.469616965950	0.116255474184	0.960183244783

FY (-60)

C	-0.001313808555	-0.055046940028	-0.009116132827
C	1.403778284573	0.045511308956	-0.000194032514
H	1.935481822028	0.375847372745	-0.885918998788
C	-0.833489334070	0.353757422157	-1.169526093709
C	-0.336632673316	0.454378807970	-2.469701119948
C	-2.170217490529	0.682724993207	-0.941959659011
C	-1.151408895385	0.886374078755	-3.506268677258
H	0.701294005238	0.225204098367	-2.681072754433

C	-2.984839794091	1.114735563174	-1.978277784509
H	-2.566873684956	0.631176692213	0.066223055771
C	-2.478196281609	1.218495413336	-3.266408237254
H	-0.738699556357	0.991178285837	-4.502687774198
H	-4.011048003376	1.395610466377	-1.774021982678
H	-3.104123233434	1.584013370291	-4.071245250123
H	1.909200002131	0.223680015174	0.941381776834
Si	0.642500293072	-2.121271083745	0.008433106230
H	0.481541598403	-2.028036226578	-1.481048683623
H	2.061521610310	-1.405093577571	-0.107081796724
H	0.679490842660	-1.982225735785	1.506922834915
C	0.235796050673	-4.026906760805	0.071808896489
C	-0.038614938552	-4.746329315491	-1.092339856282
C	0.188856722447	-4.716063893170	1.284470081345
C	-0.346236252527	-6.101567437893	-1.053477426171
H	-0.018700333821	-4.230427249307	-2.048926385277
C	-0.114539573451	-6.071423379775	1.339657903621
H	0.386767987459	-4.176219055669	2.207030649477
C	-0.383724383999	-6.767297034617	0.166470740712
H	-0.564117740048	-6.634429053597	-1.973281615416
H	-0.150863755881	-6.580735800581	2.297082005598
H	-0.629587045177	-7.823924753561	0.204140987117
H	-0.484906435162	0.076604409798	0.951674219731

FY (-90)

C	0.008181133260	0.010462013212	0.024544721021
C	1.418985285363	0.029206967487	0.013995597589
H	1.950171931152	0.335502887824	-0.881237827383
C	-0.792469730215	0.514288325210	-1.123963701307
C	-0.340849146864	0.470662695320	-2.443326124291
C	-2.016864921042	1.126190188507	-0.856743608351
C	-1.085550296258	1.045865495421	-3.462627307758
H	0.617777946445	0.021849780169	-2.679485246188
C	-2.759333834418	1.705164257908	-1.876149214852
H	-2.366129155884	1.200963161486	0.167295326003
C	-2.295635983464	1.668392842722	-3.183576732086
H	-0.701313863169	1.044002116222	-4.475826451598
H	-3.683091381267	2.220483163380	-1.642894641430
H	-2.853489506782	2.156861812863	-3.972898632082
H	1.950119982393	0.166969342960	0.948348000001
Si	0.516927503021	-2.067179026346	0.040183455051
H	0.344854695197	-2.011343896627	-1.450999583393
H	1.984704402913	-1.473531208091	-0.111982661191
H	0.607665891439	-1.960385011726	1.540531756404

C	-0.023646073678	-3.960274501191	0.127390610141
C	-0.352115104020	-4.675341990087	-1.025811761502
C	-0.103944716674	-4.636199080561	1.346029754516
C	-0.741366733186	-6.009585275279	-0.971968737847
H	-0.312277465867	-4.167881114519	-1.986623967240
C	-0.490356610256	-5.970073245257	1.418616718612
H	0.131640174675	-4.097834552616	2.260911496989
C	-0.810259711998	-6.661735329870	0.254836676486
H	-1.004431631833	-6.533843545841	-1.885743266974
H	-0.556420802831	-6.463099374347	2.383702002380
H	-1.127775460436	-7.699682484484	0.305879755786
H	-0.448469821454	0.180407586567	0.993043597435

FY (-120)

C	-0.040961256878	-0.011717326815	0.011270942862
C	1.372344656571	0.027117434455	0.011067568146
H	1.903344244268	0.343833859787	-0.880959066299
C	-0.829417657119	0.506082894489	-1.141512292384
C	-0.375865185294	0.448312905791	-2.459655691627
C	-2.022843603245	1.174718782491	-0.870707136220
C	-1.087862774773	1.069217921779	-3.475928108086
H	0.568252602021	-0.032128582934	-2.694142704054
C	-2.730687944957	1.801171161864	-1.887184637175
H	-2.365550187718	1.269676982581	0.153887402329
C	-2.264681137912	1.751891719200	-3.193236689734
H	-0.697128728178	1.067458770861	-4.486656890760
H	-3.621641488515	2.370168353647	-1.650863266068
H	-2.788910023570	2.284908869770	-3.976854899946
H	1.895577896943	0.168606909718	0.949634998373
Si	0.490515469636	-2.064531658152	0.035322837801
H	0.325061303164	-2.052372366150	-1.458753580057
H	1.956333183453	-1.472740385410	-0.117333303245
H	0.587690702601	-1.987304071873	1.537826420041
C	-0.030819176388	-3.987735918475	0.133758674886
C	-0.360588559276	-4.715833359944	-1.011770528275
C	-0.081589961903	-4.665493198354	1.353873702526
C	-0.721190305041	-6.058562570352	-0.950634587251
H	-0.345504584492	-4.208011256258	-1.973501251795
C	-0.437220053912	-6.007967593554	1.435846698894
H	0.153224089338	-4.117579306824	2.263699507954
C	-0.758002463552	-6.711649612680	0.278262573306
H	-0.989199538068	-6.587878171164	-1.861109159096
H	-0.480996539748	-6.497399151706	2.404948188184
H	-1.055506533703	-7.756611207109	0.336633907151

H	-0.500938133760	0.161630541319	0.978219189625
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FY (-150)

C	-0.099097214432	-0.027631609515	-0.007597801416
C	1.317524578470	0.016253942842	0.000949850701
H	1.849216482464	0.340448782490	-0.888483896225
C	-0.871452917530	0.510254112554	-1.162721116014
C	-0.417140237238	0.438264309666	-2.480380521665
C	-2.026075129242	1.242392967639	-0.886024030010
C	-1.090007517873	1.110106999945	-3.491417412939
H	0.508891007054	-0.077501289373	-2.714817216111
C	-2.691321234997	1.922630604170	-1.897148007892
H	-2.360589124377	1.356756962998	0.139298334695
C	-2.224502777634	1.859718076450	-3.202357984749
H	-0.693471277175	1.106517434152	-4.499945958910
H	-3.540660907734	2.550351727896	-1.655747172038
H	-2.708727010792	2.440480185937	-3.977942402515
H	1.834387837212	0.160536775965	0.943080931060
Si	0.442027104333	-2.066907867146	0.026784009660
H	0.278599119701	-2.099477715458	-1.467559654700
H	1.906486362196	-1.475396239678	-0.128935009431
H	0.544646526315	-2.015879416996	1.529786544689
C	-0.047586652358	-4.027275690095	0.141054018178
C	-0.367373803932	-4.777234085974	-0.994790031250
C	-0.064368849926	-4.702762775528	1.364969396968
C	-0.684731137259	-6.131036864576	-0.922195028571
H	-0.378918151707	-4.273918435468	-1.959456436876
C	-0.375127773983	-6.055979367418	1.460525754807
H	0.162967309757	-4.139819883841	2.268065319155
C	-0.685908479505	-6.780078370618	0.311050548690
H	-0.948132340317	-6.672575606211	-1.828183246641
H	-0.392374076761	-6.538178924647	2.435142924151
H	-0.951701590386	-7.834740216313	0.379985165704
H	-0.560241122925	0.150964476492	0.958459129062

FY (-180)

C	-0.205323227314	-0.040345809559	-0.034135831060
C	1.216122385538	-0.014824640423	-0.014938609959
H	1.750645007630	0.315751206830	-0.901105463800
C	-0.946135331553	0.534051640844	-1.190485359845
C	-0.502928143223	0.419015454873	-2.510243588585
C	-2.015853352670	1.385511229475	-0.906391579657
C	-1.099836354072	1.167826652269	-3.514981286093
H	0.372293624028	-0.180298476885	-2.746107137310

C	-2.598355107633	2.146763531162	-1.911269634858
H	-2.331851019155	1.537798917799	0.120009625232
C	-2.140774605783	2.041429427218	-3.217329728626
H	-0.706253038228	1.133272346112	-4.524245836610
H	-3.366603725523	2.869993352815	-1.664789709791
H	-2.551351993336	2.687385167852	-3.984306418330
H	1.726181987124	0.130016226512	0.931445394902
Si	0.331976314429	-2.083806726890	0.014799355828
H	0.163685077948	-2.164345018114	-1.476065579437
H	1.793981353559	-1.487815385929	-0.146073057930
H	0.433354795943	-2.052723959070	1.516585482060
C	-0.085378763814	-4.095655439809	0.151577437983
C	-0.376068022303	-4.883079464637	-0.969799312232
C	-0.036457809194	-4.764792449374	1.381097811344
C	-0.609909304585	-6.253246231151	-0.878529590198
H	-0.433542751033	-4.391736319079	-1.939614748979
C	-0.260975224823	-6.133682707464	1.497195271080
H	0.174309275901	-4.178233210392	2.273822056803
C	-0.543491398406	-6.892765156178	0.360351152457
H	-0.851682401712	-6.819388659390	-1.777352427848
H	-0.222633727690	-6.604397291179	2.478050779969
H	-0.744609287773	-7.962791854340	0.445393345952
H	-0.667298232648	0.144396646058	0.930887187907