Supporting Information

NHC-Catalyzed Homoenolate Reaction of Enals and Nitroalkenes: Computational Study of Mechanism, Chemoselectivity and Stereoselectivity

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Fig. S1

We took the first proton transfer step (Path-f) as an example to investigate the influence of hydrogen bonding (blue line in Fig. S1).

As shown in Fig. S1, protonation of **Int1-EtOH** by HOAc first occurs to generate the intermediate **Int4** and AcO-EtOH. Subsequently, **Int4** undergoes AcO-EtOH assisted C1-H cleavage via the transition state **TS7-EtOH**. The energy barrier of this path with hydrogen bonding is 15.6 kcal/mol (22.9-7.3=15.6), while the energy barrier without hydrogen bonding is 12.7 kcal/mol (17.7-5.0=12.7). Meanwhile, the presence of hydrogen bond slightly destabilized each of the concerned species. Therefore, the reaction tend to occur in the absence of hydrogen bonding. Based on these, we think that hydrogen bonding induced by solvent will not have a huge impact on our system.

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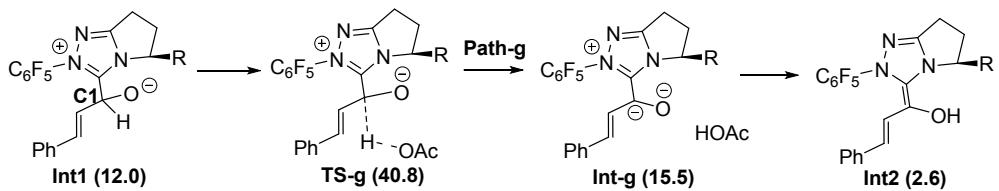
Scheme S1

We also examined Path-g in which C1-H bond of **Int1** breaks first, protonation of O occurs later. From **Int1**, OAc⁻ assisted C1-H cleavage transition state **TS-g** was located to give negative intermediate **Int-g**. Then the in situ formed HOAc protonate **Int-f** to generate **Int2**. The energy barrier of Path-f is 28.8 kcal/mol (**Int1→TS-g**).

Path-g is energetically less favored than Path-f (energy barrier is 12.7 kcal/mol).

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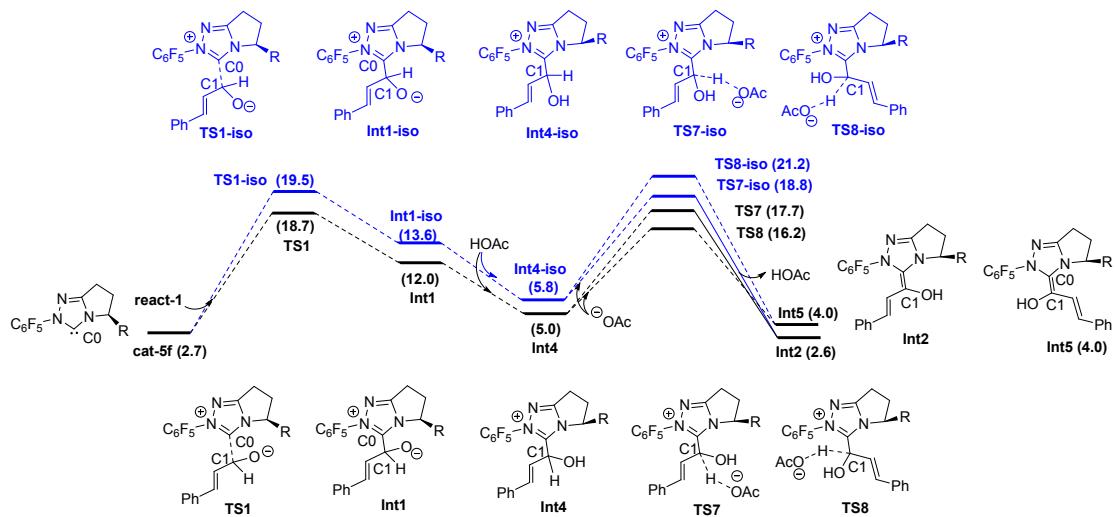
Fig. S2

As shown in Figure S2, the diastereomer of intermediate **Int1** is **Int1-iso**. It is formed via transition state **TS1-iso** with higher Gibbs free energy than **TS1**. Protonation of **Int1** by HOAc gives the intermediate **Int4-iso** and OAc⁻, then **Int4-iso** undergoes OAc⁻ assisted C1-H cleavage via the transition state **TS7-iso** or **TS8-iso** to give the Breslow intermediate **Int2** or **Int5**. The Gibbs free energy of **TS7-iso** and **TS8-iso** are both higher than **TS7** and **TS8**. Therefore, the intermeditaes and transition states shown in our manuscript are the stablest.

Nucleophilic attack transition states of Int2 to react-2
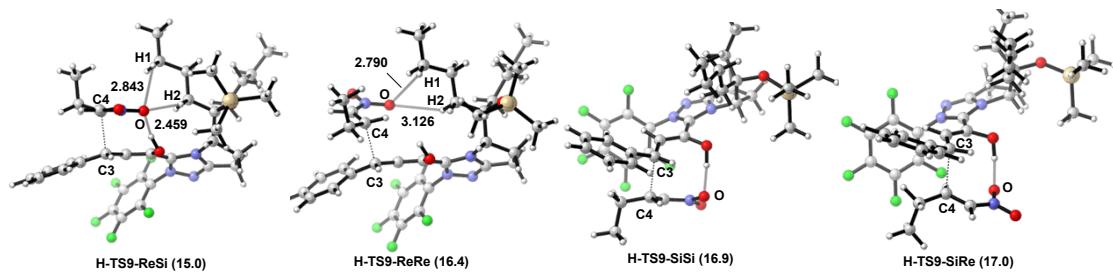
Fig. S3 Nucleophilic attack transition states of **Int2** to **react-2**

Fig. S3 shows four transition states **H-TS9-ReSi**, **H-TS9-ReRe**, **H-TS9-SiSi** and **H-TS9-SiRe** which lead to (3S, 4R) (3S, 4S) (3R, 4R) and (3R, 4S) configuration products with Gibbs free energy of 15.0, 16.4, 16.9 and 17.0 kcal/mol, respectively. Therefore, (3-Re, 4-Si) attack mode leading to *syn*-configuration product (3S, 4R)-**prod-homo** is the most favourable.

Observations on the former two transition states (**H-TS9-ReSi** and **H-TS9-ReRe**) shows that nitro and R group are close to each other with weak electrostatic interactions between O atom and H1,H2 of R group. In addition, shorter distances between O···H1 and O···H2 (2.459Å, 2.843Å) of **H-TS9-ReSi** than **H-TS9-ReRe** (2.790Å, 3.126Å) make the former more favored. In contrast, in the latter two transition states **H-TS9-SiSi** and **H-TS9-SiRe**, nitro is far away from R group. So that no weak electrostatic interaction exists between them, thus these two transition states are more destabilized.

The nitroalkene indeed approaches the Breslow intermediate from the more crowded face in **H-TS9-ReSi** and **H-TS9-ReRe**, because such approaching enables better interactions between O atom and H1, H2 atoms on R group. The steric hindrance can be well compensated by the electrostatic facility.

Open transition state of H-TS9-ReSi
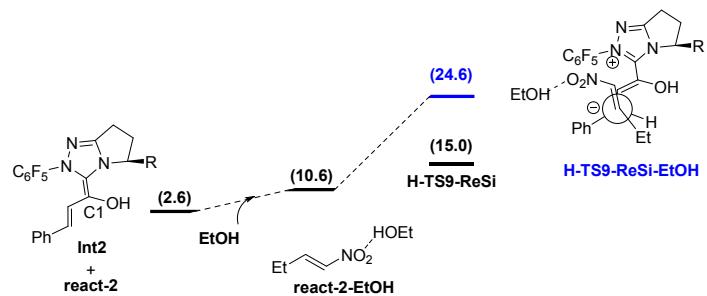
Fig. S4

The calculations indicate that the relative energy of the open transition state **H-TS9-ReSi-EtOH** (Figure S4) is much higher than that of **H-TS9-ReSi** (24.9 vs 15.0 kcal/mol). The observation indicates the intramolecular hydrogen bond can not be easily destroyed by the solvent ethanol, and the open transition state is unlikely in our reaction system.

Another three possible mechanisms Paths 4-6

We also investigated another three mechanisms (Path-4, 5, 6) for enol-keto tautomerisation and attack of OEt to C1 process(Scheme S2 and S3).
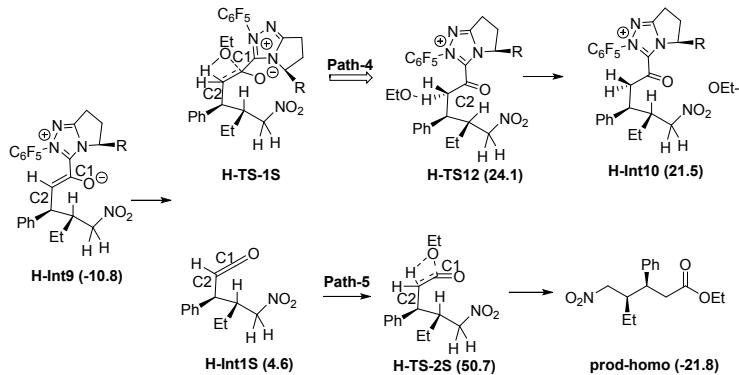
Scheme S2 Path-4 and 5

In Path-4, H-OEt bond addition to C1-C2 double cond occurs via transition state **H-TS-1S**. In the transition state, the attack of OEt⁻ to carbonyl and protonation of C2 are supposed to be synchronous. However, OEt always moves away from the carbonyl group during optimization, thus only C2 protonation transition state **H-TS12** was obtained (i.e. Path-2). It might be attributed to the weak basicity of C2 to capture the proton of HOEt, thus making the OEt in transition state can't accumulate enough negative charge to attack carbonyl.

Herein, we note that the carbene dissociation occurs in the final step for the above four mechanisms (Path-1 to 4). However, this step can also occur at the first step (Path-5). In this mechanism, intermediate **H-Int9** first undergoes the carbene dissociation step to give the intermediate **H-Int1S** with energy absorption of 15.4 kcal/mol. Then **H-Int1S** experiences addition of H-OEt bond to C1=C2 to directly generate product **prod-homo**. The overall energy barrier of Path-5 is as high as 61.5 kcal/mol (**H-Int9→H-TS-2S**).
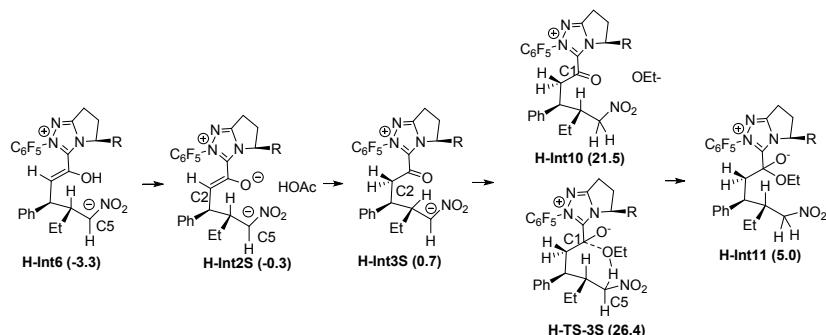
Scheme S3 Path-6

As discussed in Path-1 to 5, protonation of C5 is prior to C2 protonation. Next we investigated another mechanism proposal that protonation of C2 is prior to C5 protonation (Path-6). OAc⁻ in reaction system firstly deprotonate the hydroxyl to give intermediate **H-Int2S** and HOAc with energy absorption of 3.0 kcal/mol. The in situ generated HOAc subsequently protonate C2 atom of **H-Int2S** to obtain intermediate **H-Int3S**. Subsequently, we investigated stepwise and concerted C5 protonation of intermediate **H-Int3S**. For stepwise mechanism, HOEt firstly protonate the C5 atom to give intermediate **H-Int10** and OEt⁻ with energy absorption of 20.8 kcal/mol. OEt⁻ subsequently attack C1 atom of **H-Int10** to generate intermediate **H-Int11**. For concerted mechanism, protonation of C5 and attack of OEt⁻ to C1 atom of **H-Int3S** occurred simultaneously via transition state **H-TS-3S** to directly obtain intermediate **H-Int11**. The energy barrier of this process is 25.7 kcal/mol (**H-Int3S→H-TS-3S**). Therefore, stepwise mechanism is more favored. The overall energy barrier of Path-6 is 24.8 kcal/mol (**H-Int6→H-Int10**).

Path-4, 5 and 6 are all unfavorable compared with Path-3 (20.6 kcal/mol).

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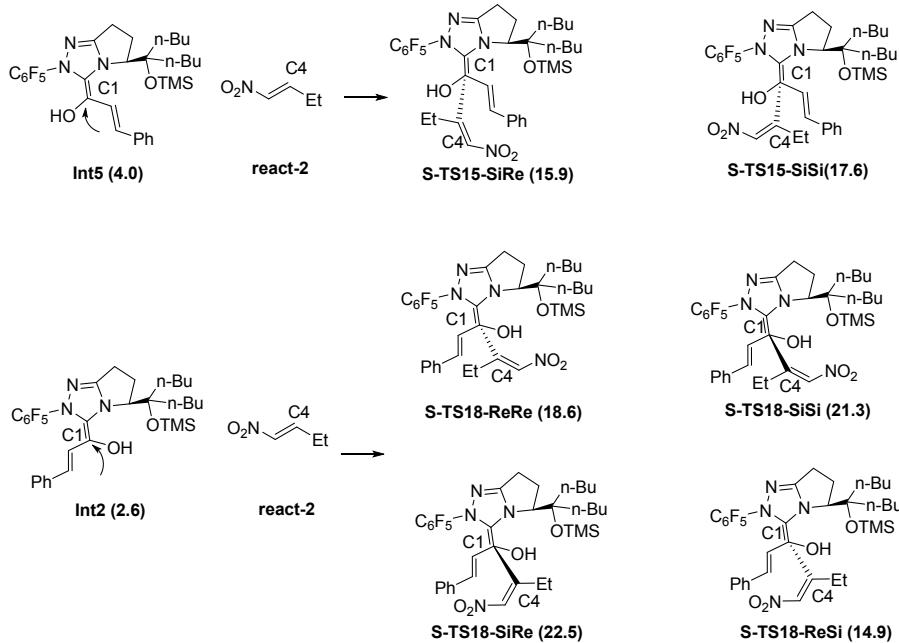
Scheme S4

As to **Int5**, (1-Si, 4-Si) mode transition state **S-TS15-SiSi** was also located. Free Gibbs energy of this transition state is higher than **S-TS15-SiRe**. In addition, (1-Re, 4-Si), (1-Re, 4-Re) mode transition states were can't be located because large steric hindrance between R group on carbene ring and **react-2**.

As to **Int2**, transition states of another three modes (1-Re, 4-Re), (1-Si, 4-Si),(1-Si, 4-Re) are **S-TS18-ReRe**, **S-TS18-SiSi**, **S-TS18-SiRe**. Their Gibbs free energy are 18.6, 21.3, and 22.5 kcal/mol, and they are all higher than **S-TS18-ReSi**.

Gibbs Free Energy Corrections and Electronic Energies in Solvate of related compounds and Transition States

	Thermal Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
react-1	0.109799	-422.7049173
react-2	0.079578	-361.5312236
Prod-homo	0.294219	-939.2855114
Prod-set	0.215236	-784.281767
Prod-set'	0.214732	-784.2833909
5f	0.468679	-1923.484486
Cat-5f	0.453784	-1923.012985
NaOAc	0.020587	-390.7456481
HOAc	0.034577	-228.9919149
EtOH	0.054561	-154.961328
OAc-	0.02178	-228.52681
OEt-	0.040665	-154.4535696
Int1	0.59146	-2345.731036
Int2	0.588776	-2345.743298
Int3	0.587965	-2345.750567
Int4	0.605448	-2346.208415
Int4'	0.603239	-2346.204887
Int5	0.591003	-2345.743337
H-Int6	0.700201	-2707.315651
H-Int6'	0.698277	-2707.313459

H-Int7	0.712345	-2707.780932
H-Int8	0.712345	-2707.780932
H-Int9	0.695058	-2707.322493
H-Int10	0.713368	-2707.783243
H-Int11	0.775333	-2862.284322
S-Int12	0.701724	-2707.304261
S-Int13	0.7011	-2707.291312
S-Int14	0.69728	-2707.299302
S-Int15	0.697711	-2707.294148
TS1	0.587609	-2345.716456
TS2	0.582507	-2345.66235
TS3	-	-
TS4	0.583594	-2345.687789
TS5	0.659669	-2500.640831
TS6	-	-
TS7	0.642326	-2574.729992
TS8	0.641655	-2574.731758
H-TS9-ReSi	0.69548	-2707.281787
H-TS9-SiSi	0.695399	-2707.278803
H-TS9-ReRe	0.692918	-2707.277058
H-TS9-SiRe	0.695036	-2707.278225
H-TS9'-ReSi	0.697397	-2707.283329

H-TS10	0.750459	-2936.30011
H-TS11	0.695865	-2707.300065
H-TS12	0.772147	-2862.250817
H-TS13	0.750978	-2936.312033
H-TS14	0.829089	-3091.287791
S-TS15-SiRe	0.697291	-2707.282177
S-TS16	0.694692	-2707.274333
S-TS17	0.694814	-2707.284739
S-TS18-ReSi	0.693457	-2707.279942
S-TS19	0.695768	-2707.272239
S-TS20	0.695725	-2707.289611
TS-g	0.62665	-2574.225225
Int-g	0.576354	-2345.257971
H-TS-1S	-	-
H-TS-2S	0.287562	-939.1645761
H-Int1S	0.213911	-784.2575567
H-Int2S	0.687186	-2706.845642
H-Int3S	0.699214	-2707.308338
H-TS-3S	0.774214	-2862.249129
S-TS15-SiRe	0.697291	-2707.282177
S-TS15-SiSi	0.697382	-2707.279764
S-TS18-ReRe	0.696625	-2707.277203

S-TS18-SiRe	0.696756	-2707.27115
S-TS18-SiSi	0.695472	-2707.271803
TS4-Ar	0.586224	-2345.674336
TS1-iso	0.588049	-2345.715575
Int1-iso	0.588807	-2345.725802
Int4-iso	0.603239	-2346.204887
TS7-iso	0.642831	-2574.727561
TS8-iso	0.644616	-2574.726806
Int1-EtOH	0.665933	-2500.706726
AcO-EtOH	0.093513	-383.4972857
TS7-EtOH	0.718085	-2729.699935
H-TS9-ReSi-EtOH	0.769653	-2862.24752

Cartesian Coordinates of Intermediates and Transition States

react-1			0.26538200	3.12580600	1.35053400
-3.41226200	0.38909300	0.00000400	0.59760800	1.13963800	2.08578600
-3.88591700	-0.74667000	-0.00000900	-0.68695500	3.30570800	-0.85687100
-4.09049600	1.26493900	0.00000800	-1.10400500	1.44560600	-1.85446200
-1.98594400	0.71178900	0.00000300	-0.19327300	3.91894100	0.29635000
-1.04527600	-0.26168100	0.00000400	0.65683900	3.59056700	2.25220200
-1.73030100	1.76816800	0.00000200	-1.04140600	3.90988400	-1.68844700
-1.40336500	-1.29100400	0.00000600	-0.16186500	5.00295100	0.37126300
0.40498200	-0.10903300	0.00000200	-0.42648300	-0.62907600	-1.11148600
1.19970200	-1.27276400	0.00000200	1.25306500	-0.89975100	1.42988600
1.05008900	1.14569300	-0.00000100	3.32312100	-0.96598500	0.13003900
2.59060200	-1.19031700	0.00000100	4.53351100	-0.72480000	-0.64134200
0.71312500	-2.24505900	0.00000400	5.71386200	-1.05213100	0.24817500
2.43874000	1.22567100	-0.00000300	4.53915700	0.32237400	-0.95890000
0.46310700	2.05938900	-0.00000100	4.50801600	-1.35557100	-1.53508300
3.21403400	0.05965000	-0.00000200	6.64323500	-0.88342600	-0.30736900
3.18654100	-2.09893900	0.00000100	5.72731000	-0.41630300	1.14024800
2.92207500	2.19897600	-0.00000500	5.69044900	-2.10040400	0.56578800
4.29865500	0.12829000	-0.00000400	-1.56027900	-1.08860900	0.65052900
react-2			-2.88047700	-0.64403000	0.00806100
-0.70404300	0.18331200	-0.34169800	-1.46516500	-2.16662400	0.47144700
0.37400700	-0.56872700	-0.09787200	-3.73414200	-1.14716000	0.46996800
-0.57992800	1.26109800	-0.42684200	-3.03657600	0.43364000	0.03691100
0.39273400	-1.64434600	0.01741700	-2.98019900	-1.02874000	-1.44488100
1.68349000	0.02223400	0.04647000	-2.67754300	-2.17803600	-1.76443600
2.61736600	-0.75413500	0.29007100	-3.38686800	-0.18323900	-2.24113200
1.83361800	1.24408600	-0.07152000	-1.64140500	-0.87263000	2.17810000
-2.08539300	-0.36581200	-0.48930800	-2.62132800	-1.80682200	2.89781300
-3.04985600	0.21536200	0.56016600	-1.90174000	0.17148700	2.39285300
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-4.06146600	-0.17020400	0.39297800	-3.66378500	-1.62724900	2.61035600
-2.74262300	-0.06135000	1.57480600	-2.39283100	-2.85983900	2.69051100
-3.08890800	1.30923900	0.50249400	Prod-set		
prod-homo			1.47986200	2.03280200	0.06584800
2.15398500	-0.75733800	-0.49731900	1.73704100	1.33078100	1.04708700
2.07294000	-0.36768400	-1.65043000	0.27595700	2.87718300	-0.02253800
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-2.29486000	2.96965400	3.04400900	2.49242200	-2.51296700	-3.85315400
-3.43605000	5.32838500	0.18882900	2.12916800	-3.68185000	-3.72952700
-1.68735800	4.67885800	-0.86763300	3.59313900	-2.17932500	-4.29199900
-4.19984100	5.22670100	1.35803100	2.55383400	-1.36194400	-1.06214100
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-3.75532300	5.98951200	-0.61243000	2.99084000	-0.65639100	-0.34577300
-5.11156000	5.80850400	1.46453800	3.36148600	-2.05464800	-1.33126900
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2.50606300	3.09545100	-1.47611200	0.57134900	-1.47430500	-0.13569700
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1.77504900	1.22280700	-2.28972000	4.59966400	-1.33573100	-0.78261500
2.52865800	1.28409100	-3.62199700	3.50789100	-0.05456800	-0.61054000
0.75083600	1.58292800	-2.44400800	-2.29394500	-0.04051400	-0.75643100
1.69207600	0.18020300	-1.95534300	-2.04259100	0.56757000	-1.97149300
1.96885400	0.74143400	-4.39280500	-0.19877000	-0.28359900	-1.07528100
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3.51993000	0.82103000	-3.56011800	-5.45860400	-1.38602200	0.65443100
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3.87136400	0.46340400	-0.69070000	-5.67888600	1.00121700	0.36413600
4.08046800	1.95568500	0.25439300	-4.37857200	1.06262200	-0.12293100
Prod-set'			-3.61182700	-0.10017400	-0.23622700
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-0.00351800	0.48612700	-2.28278600	-1.13007000	-1.10267400	0.70928900
1.76553400	1.72361700	-1.27926100	-0.75697700	0.39778600	-2.13150400
0.98081700	2.74319000	-0.86508400	0.25625400	0.72600400	-3.16945400
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2.72899400	4.27714600	0.12115600	1.61296400	-0.97469900	-3.33278700
0.70471700	6.03941300	0.91051600	1.25898700	-0.56108100	-1.22623200
-0.65813900	4.62997600	0.01963900	1.38437200	-1.64039800	-1.13389200
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3.52487400	3.60447800	-0.18476700	3.80648900	-2.87742700	-1.52805100
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-0.08347400	6.72221100	1.21602500	4.58993000	-3.62148200	-1.72853000
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2.29631100	7.25580200	1.71230300	5.41788500	-1.80464300	0.84846200
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1.54383300	-1.42410100	-3.44377000	5.90639500	-0.94830400	1.32896100
3.07759000	-0.10184000	-2.72837100	6.19691100	-2.55547900	0.65550500

5.89259700	-0.63493100	-1.95551500	-5.49643900	1.07331600	0.10703500
6.34721200	0.27962000	-1.55401800	-4.18424200	1.00555900	-0.34752300
6.70146900	-1.35845100	-2.12256400	-3.46906900	-0.19494000	-0.31396500
5.46079200	-0.38914800	-2.93372900	-1.06701400	-0.70818600	-0.09781200
-3.86955800	2.24424500	-0.47236400	-0.62743500	-0.09933400	-2.23571700
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-7.45852000	-0.27914300	1.23246400	0.60795800	1.07069100	-3.52906800
-5.97819900	-2.55797800	1.02709200	0.09537000	-0.46554000	-4.22909300
-3.44756000	-2.44616200	0.04849100	1.63761700	-0.68491500	-2.64789500
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2.69688100	-0.00781800	2.43398700	1.78834900	-1.66432800	-3.10893800
2.19157100	-1.62898600	1.09262900	1.34111300	-0.87988900	-1.12494200
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2.47638100	-0.86845600	3.68647400	2.22696600	-0.01412300	-0.15847900
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3.21259200	-0.33420500	4.91813300	4.75227900	-3.96062100	-0.72329900
1.39933400	-0.92765000	3.90105200	3.47811900	-3.26982500	-1.73374800
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3.03095400	-0.96585900	5.79622300	4.87132100	-1.79797300	2.08563900
4.29679900	-0.30272200	4.75059700	6.00636500	-0.56133100	1.51339500
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1.88496500	1.65955900	-0.09512700	5.97966500	-1.09863700	-1.73807800
3.06582400	2.57233200	0.27432900	6.42393900	-0.10742500	-1.58162400
1.05634000	1.82477200	0.60545700	6.79676800	-1.83191600	-1.72488500
1.52525700	1.99668900	-1.07461000	5.54237600	-1.11151300	-2.74435100
2.63407800	4.04010900	0.39920300	-3.60853600	2.11936700	-0.81466600
3.53392100	2.25358300	1.21191200	-6.16397900	2.23330600	0.06768100
3.83736100	2.48854800	-0.50063100	-7.36873300	-0.00214300	1.06655200
3.80550400	4.98992600	0.66313400	-6.00552300	-2.36435500	1.15613000
2.11789000	4.34736400	-0.52199100	-3.47291600	-2.50693800	0.22831100
1.89629200	4.13599300	1.20889300	1.96681300	-0.49019700	1.29030400
3.46414000	6.02851200	0.75376400	2.60769800	0.30528700	2.43560400
4.32944200	4.73074100	1.59228600	2.28996600	-1.53914900	1.35481700
4.54036900	4.95240700	-0.15137900	0.88111200	-0.50715100	1.44275000
Cat-5f			2.39508200	-0.37221900	3.79709300
4.70244600	-1.50412700	-0.41595500	3.68359800	0.42982400	2.26249800
3.58954400	-0.24360500	-0.54769300	2.17719000	1.31444100	2.47350500
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-1.90504200	0.11835500	-2.13686800	1.31825400	-0.51494200	3.96820600
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3.06223800	2.48826300	-0.09133300
1.05607400	1.75045800	0.26339800
1.59862600	1.66275000	-1.39882000
2.59948100	3.94568400	-0.22744400
3.48463700	2.34085100	0.90869700
3.87794800	2.30283300	-0.80117200
3.73359600	4.95463000	-0.02786600
2.14883000	4.09530300	-1.21959300
1.80179800	4.14426000	0.50295100
3.37151700	5.98645500	-0.11614100
4.19205500	4.84796200	0.96391700
4.52641900	4.81644700	-0.77454300

NaOAc

-0.60748500	0.68025000	0.02611700
0.65648200	0.64392300	-0.11954200
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-1.36299700	-0.64129600	0.00389100
-2.38202000	-0.52836100	0.38290400
-1.41343700	-1.00573100	-1.03026400
-0.83079900	-1.39702100	0.59074900
0.66835700	2.89345600	-0.04244700

HOAc

-0.42119400	0.51292600	-0.05909000
0.77376100	0.44970100	-0.28723400
-1.04973700	1.68307300	0.18420600
-1.36750600	-0.65255700	-0.00505600
-1.79872000	-0.73174500	0.99943400
-2.19421200	-0.49806100	-0.70681700
-0.83725400	-1.57364400	-0.25103100
-0.38113400	2.39599200	0.14080000

EtOH

-1.22631200	-0.22155900	0.00000700
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0.14134100	1.19537200	-0.88673800
1.15914800	-0.39982500	-0.00001400
1.98854300	0.10612700	0.00010600

OAc-

-0.46561300	0.59920600	-0.04754000
0.76662800	0.37726100	-0.23100600

-1.00189300	1.73085800	0.12421400
-1.38275800	-0.63943300	0.00086100
-1.19281000	-1.20204700	0.92523400
-2.44354000	-0.36859800	-0.02516300
-1.16233300	-1.31551600	-0.83418100

OEt-

-1.18023100	-0.20748900	0.00000000
0.20703500	0.48670300	-0.00000100
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-2.01706000	0.50894200	-0.00000300
0.17084700	1.20553400	0.88087400
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Int1

-5.14362700	1.89197200	-1.26430600
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1.05288800	-1.37831300	-0.93956200
0.42925300	-2.33371400	-1.73340900
-0.91924800	-0.63863400	-1.23837300
3.46309100	-1.20507400	-1.29156600
4.76787000	-1.42439800	-0.87033500
4.99729300	-2.06074500	0.34663200
3.92895400	-2.46676800	1.14156900
2.62539800	-2.23339800	0.71762500
2.38315400	-1.59753200	-0.50068300
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-0.76023700	-1.83429200	-1.90532700
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-2.49592700	-3.02449700	-2.31147900
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-2.76527700	-0.84594200	-2.67484800
-3.83692600	-1.02682700	-2.60032700
-2.58363200	-0.27449500	-3.58886400
-2.25919400	-0.01434400	-1.45435300
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-3.23460300	-0.02739500	-0.20900000
-3.99921900	2.83224700	-2.43381800
-3.08355700	3.18090500	-1.94066200
-4.52301600	3.72424500	-2.80478700
-3.71002900	2.23791500	-3.30900100
-5.62286800	3.02902500	0.16103100
-4.75603700	3.39572600	0.72241700
-6.30254800	2.53764300	0.86779700

-6.14792500	3.90827900	-0.23805400	4.77978500	2.40494700	-0.82439900
-6.70141600	1.35639100	-2.17458900	6.13545200	3.61074000	1.29683900
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-6.47260000	0.72180000	-3.04004700	4.27824100	1.90704200	-1.64988200
1.60952400	-2.64152000	1.47798500	6.68923500	3.63955400	0.01465100
4.16064500	-3.08210100	2.30586200	6.65996400	4.07496800	2.12843800
6.24781600	-2.28013200	0.75496500	6.43831900	3.03063200	-2.04098500
5.79771500	-1.01906100	-1.62075800	7.64707000	4.12355100	-0.15812200
3.24744300	-0.56890300	-2.44709500	-0.15365300	1.62420400	-0.01668200
-2.68243800	0.91994700	0.87381400	Int2		
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-3.37546000	0.03954700	2.72873400	3.25539400	-1.83992300	-1.17119800
-3.39125700	2.13088200	4.52276800	4.64040300	-1.94406400	-1.21252200
-1.69040100	1.83775100	3.21440600	5.35336400	-2.12740700	-0.03102000
-2.83057500	3.05032400	2.64919300	4.68155900	-2.18925300	1.18573800
-2.90653700	2.89531900	5.14267800	3.29711100	-2.06118900	1.21568000
-4.45971900	2.37737000	4.46814400	2.55972900	-1.87510000	0.04309000
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-3.43796100	-1.47249600	0.32584100	-0.70141400	-2.72657800	-0.39616300
-4.79572000	-1.78458400	0.97819800	-1.93032700	-3.49594900	-0.75503700
-2.62925300	-1.68332100	1.03716300	-2.41889600	-3.90468400	0.13460600
-3.31756200	-2.19003600	-0.49158300	-1.68572900	-4.33956700	-1.40700300
-4.82739500	-3.19447800	1.58500800	-2.78788400	-2.41747600	-1.47751100
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-5.58484900	-1.70155100	0.22058200	-2.68558400	-2.53997200	-2.55942900
-6.19123100	-3.56203600	2.17679900	-2.22407400	-1.01755800	-1.07811400
-4.55530500	-3.93042200	0.81421800	-2.15528800	-0.36152900	-1.94429500
-4.05744200	-3.27207400	2.36616500	-3.09416700	-0.26937900	0.01202100
-6.18332300	-4.57402400	2.60019900	-4.14405100	0.74383900	-3.40129000
-6.47868100	-2.86933600	2.97835000	-3.20742800	1.30572600	-3.30148500
-6.97874400	-3.52894700	1.41265200	-4.73618200	1.24008600	-4.18292700
0.60448600	0.85233800	0.26853600	-3.89912700	-0.26030700	-3.76794600
0.50907800	0.39092600	1.53287400	-5.54332800	2.47620000	-1.29747600
1.93638600	1.47366600	-0.15339100	-4.64474600	3.08558300	-1.14589900
2.90267200	1.74363400	0.73484400	-6.14272500	2.52262300	-0.38012700
2.03204800	1.75459900	-1.20297800	-6.12912200	2.95568700	-2.09425300
2.70395700	1.48158400	1.77373100	-6.75643100	-0.23462200	-2.08183400
4.19949900	2.38219400	0.45976900	-7.36296400	-0.27263500	-1.16792300
4.90829700	2.98422800	1.51617800	-7.36074700	0.25084000	-2.85942700

-6.57329200	-1.26816000	-2.40172100	4.04464800	1.83744800	1.39206000
2.67218400	-2.11090300	2.39716200	5.61619400	4.78142400	0.72872100
5.36975100	-2.36491800	2.32103200	5.04997800	6.15798100	-0.83518600
6.68394300	-2.24341000	-0.06684200	5.91435400	3.21195300	2.18082400
5.28862100	-1.89705800	-2.38339000	6.44508600	5.38726300	1.08524000
2.58482200	-1.69086500	-2.31932800	-0.31804500	2.04304700	-1.32701500
-2.49665000	1.12864700	0.28863200	Int3		
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-2.49784900	1.68744200	-0.65603300	-4.00233300	-0.32516800	-0.27743200
-1.44455700	0.99059900	0.56224800	1.82473500	-1.61678800	-0.94789700
-2.52273100	3.39773400	1.43296000	1.24811000	-2.85623000	-0.48941000
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-3.01593900	1.51896000	2.35981300	2.55351700	-2.57653600	-3.12217000
-3.10433900	4.27089300	2.54791700	3.51849700	-2.71026500	-4.11457600
-1.43539200	3.30663600	1.57058400	4.70909400	-1.99635800	-4.02349000
-2.66624200	3.89899200	0.46455000	4.93305300	-1.16147200	-2.93440200
-2.64255100	5.26586600	2.55888800	3.97094400	-1.06027500	-1.93539000
-4.18608500	4.40913800	2.42269300	2.76227700	-1.76386600	-1.99922800
-2.94088100	3.81879600	3.53475400	0.72593600	-0.61047400	-1.15115500
-3.20999100	-1.11178400	1.31475000	0.03874700	-2.56016700	-0.18414500
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-4.44962500	-1.75001900	3.44664900	-2.31307200	-2.61778700	-0.34389500
-4.72288100	0.08481800	2.34857600	-3.14845200	-2.55104900	0.35318900
-5.35012100	-1.33326900	1.52968600	-2.67249400	-3.13936600	-1.23456100
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-3.61395700	-1.37694800	4.05638700	-2.60750700	-0.02153500	-0.09626700
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1.90931800	1.19583800	-0.29462300	-5.02632400	2.04548000	-2.34311000
2.33178600	2.42044800	-0.72454600	-6.21298300	1.84366200	-1.04070600
2.43978000	0.70469900	0.51712800	-6.58649700	1.28830000	-2.67703200
1.80105700	2.88558200	-1.55363700	-6.49279300	-1.44409700	-0.91626300
3.45134700	3.19297100	-0.19708300	-6.91680100	-1.05381700	0.01769300
3.77071200	4.43091700	-0.79932900	-7.30887900	-1.50549500	-1.64818100
4.25389300	2.77911200	0.89148000	-6.14662400	-2.46686900	-0.72113300
4.83303500	5.21090500	-0.34628900	4.22018700	-0.25400600	-0.89362200
3.17006100	4.77668400	-1.63818900	6.07969600	-0.47333800	-2.84371900
5.31590900	3.55926100	1.34156000	5.63299800	-2.10811500	-4.98442200

3.29541500	-3.50198200	-5.17359900	3.00514800	3.15807400	6.51052400
1.39901600	-3.24093500	-3.27145700	0.46875500	-0.46366700	-2.21335100
-2.24228300	1.29671900	-0.81706800	Int4		
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-1.15166000	1.37883900	-0.85370300	1.10510200	-1.11517700	-1.04213300
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-1.41001500	0.60021100	1.58722400	-2.30284200	-2.14182700	-3.14576700
-2.08845700	-1.00093300	1.77172200	-1.37098500	-1.13166100	-4.25190800
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-2.09931600	1.20992100	3.91766900	-3.20530600	0.02509100	-0.23733600
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1.23128000	0.73910100	-0.59984500	-3.54832100	3.12736200	-2.55833900
1.43904500	1.65500400	-1.39688500	-5.48294000	2.94102300	0.97891700
1.48501300	0.82886200	0.84275000	-4.61104600	3.10934900	1.62148100
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1.31714400	-0.06517900	1.43320700	-5.97855500	3.91282300	0.84474200
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2.18989800	2.26259600	2.80138000	-7.27829400	1.31760800	-1.28205300
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2.88188300	3.88729300	4.48348900	1.46152700	-2.82984200	1.12511100
2.67268300	4.32445200	2.38519100	3.93822400	-3.61906500	1.92874000
2.38126100	1.61174400	5.13780800	6.14046300	-2.71976000	0.60547200
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2.77816100	2.91102100	5.47681600	3.40730200	-0.21098100	-2.29661100
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3.01106000	1.61088800	0.91337100	4.93154400	-2.97066600	1.53586600
1.77594800	2.20697700	-0.71540000	6.44217900	-2.05717600	1.35288100
3.03977200	1.00404400	1.81684800	6.29605200	-3.67719600	0.66190800
4.23881100	2.37212900	0.63819700	6.62002700	-1.68801700	-1.91391500
5.24290100	2.40431400	1.62317100	7.28475800	-0.93630900	-1.46979000
4.46577800	3.06198700	-0.56879400	7.21413800	-2.59578200	-2.08153900
6.42786100	3.11166700	1.41962500	6.30286900	-1.31398800	-2.89543300
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3.71917800	3.03846900	-1.35770600	-6.19109700	2.79112900	0.56990700
6.63506700	3.79746500	0.22124100	-5.94749400	1.08521400	-1.53594200
7.18879500	3.12466200	2.19572100	-3.48159900	0.18782900	-2.27083800
5.80788400	4.29174300	-1.71053400	2.79759200	-0.55359500	1.19548600
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Int4'			3.29228000	-1.00162100	3.65165200

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4.18270600	-0.69555700	4.85901300	4.34213200	0.65686500	-0.75905600
2.24669400	-0.76639300	3.89888800	5.66830100	0.98349000	-0.50408000
3.32090200	-2.08069200	3.44239200	6.47032100	0.10671000	0.21909700
3.86593600	-1.26194500	5.74336900	5.93232600	-1.08092400	0.70353500
5.22961600	-0.95474900	4.65557600	4.59481400	-1.37996900	0.47225900
4.15087000	0.37050800	5.11864500	3.76856700	-0.51583500	-0.25605100
3.33148700	1.57686200	-0.14200100	1.26562600	-0.12449500	-0.44668100
4.70984200	2.14606300	0.23355800	1.02029700	-2.00954000	-1.63412400
2.57197700	1.96683700	0.54788300	0.14731500	-2.85612600	-2.49764200
3.08735500	1.99180400	-1.12445500	-0.01812700	-3.84184800	-2.05265400
4.69396900	3.67956000	0.30423700	0.60486300	-3.01508800	-3.47843500
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5.44384100	1.82934000	-0.51700900	-2.04644800	-2.61492400	-2.54804600
6.06799800	4.27807300	0.61796700	-1.15210700	-1.44212100	-3.51744500
4.33037000	4.08444600	-0.65158600	-1.11941600	-0.98630900	-1.39401200
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H-Int6			-2.59678400	2.33482600	2.31090100
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1.27475000	4.44823100	2.92551500	5.95661600	-0.48797400	-1.08471500
3.00804300	4.17223400	1.66300400	3.35762200	-0.27831900	-1.84721400
2.49441200	2.72093700	2.50604800	-2.41180000	-0.12044900	0.90904500
1.85736600	4.74009400	3.80794300	-3.14086400	-0.11777000	2.26048800

-2.44031100	0.89053200	0.48095900	2.87055800	2.17074700	-0.78502300
-1.35736600	-0.33467700	1.10930200	3.47119900	4.37916200	1.24606700
-2.60490000	0.98033900	3.19125500	3.95636400	2.42928300	1.54381200
-4.21879400	0.02149200	2.11868000	4.71081300	2.68105500	2.55538000
-3.01049600	-1.08787100	2.75632600	3.83945900	1.15082800	1.18487900
-3.30422900	1.00584200	4.55302900	2.46609200	4.19979900	-1.33827500
-1.52506000	0.83365700	3.33782900	3.83920000	4.39959900	-1.98838500
-2.71521500	1.96044200	2.70520600	2.14077200	5.13712700	-0.86845800
-2.89181900	1.79109500	5.19851200	1.73075000	3.97696400	-2.12071500
-4.38002100	1.19562900	4.44564900	3.80522300	5.20261600	-2.73485900
-3.18782000	0.04939600	5.07919700	4.60345900	4.66389000	-1.24804500
-2.90078400	-2.57936100	0.36166400	4.17391000	3.48629800	-2.49710100
-4.20549200	-3.07602000	1.00613200	H-Int7		
-2.07650800	-2.68051000	1.07895800	-5.32398400	0.54701200	-1.78954700
-2.67442300	-3.27187500	-0.45477500	-4.62029700	-0.48170400	-0.64447600
-4.05483300	-4.48771700	1.59017800	0.89260000	-2.39141400	-0.42378600
-4.53954900	-2.39574200	1.79715400	0.19664200	-3.57046400	-0.59966900
-4.99973100	-3.08268300	0.24984900	-1.11127500	-1.79915200	-0.88819600
-5.35209600	-5.02014400	2.20511900	3.18429600	-2.16256100	-1.24551500
-3.71557000	-5.17560100	0.80196400	4.55568600	-2.25142600	-1.04122000
-3.26377600	-4.48444400	2.35386700	5.04150200	-2.65916900	0.19904200
-5.21657000	-6.02932100	2.61334600	4.16397300	-2.97073500	1.23439200
-5.69938100	-4.37605500	3.02331900	2.79304300	-2.86911200	1.02677500
-6.15585200	-5.06904500	1.45915700	2.29537100	-2.45606700	-0.20955300
0.89988200	0.14482300	0.02118500	0.11119500	-1.30150600	-0.61271100
1.62524800	-0.09854900	1.14123200	-1.00771200	-3.17013300	-0.89834100
0.55421500	1.35432800	-0.46803200	-2.26783200	-3.82388000	-1.34280100
0.98528500	2.62426900	0.20614400	-2.75310200	-4.34487400	-0.51201600
0.01004100	1.39196200	-1.40662300	-2.06626400	-4.56217900	-2.12301600
1.12062400	2.37764600	1.26288900	-3.08675100	-2.60956900	-1.86623100
-0.06337000	3.72639700	0.15277100	-4.14428600	-2.69389000	-1.61942200
-0.30717400	4.48907000	1.30595700	-2.99689100	-2.55587300	-2.95405100
-0.80397500	4.02451100	-1.00303700	-2.48031300	-1.30978800	-1.25003100
-1.25252000	5.51749000	1.30747900	-2.34942600	-0.53512900	-2.00253300
0.25008000	4.27197100	2.21449700	-3.33170200	-0.69809700	-0.06532700
-1.75238500	5.05042400	-1.00436700	-4.11900100	1.18273400	-3.09569200
-0.64215200	3.45915100	-1.91663100	-3.29342900	1.76795500	-2.67405200
-1.98126000	5.80192800	0.15081700	-4.66575200	1.84500400	-3.78171400
-1.42225300	6.09094600	2.21547300	-3.68994900	0.37702000	-3.70356200
-2.31270700	5.26125100	-1.91199000	-6.14372900	2.01475500	-0.93874600
-2.72172500	6.59774700	0.14954200	-5.41737500	2.71116200	-0.50387400
2.45882800	0.51655700	1.20021000	-6.82820500	1.69795400	-0.14209400
2.45939800	3.06206000	-0.30232800	-6.73637100	2.57855000	-1.67247500
3.33887400	3.37404300	0.86284900	-6.63945900	-0.51802400	-2.61067400

-7.34207200	-0.93112600	-1.87592300	3.63910900	3.33877900	-1.86303700
-7.22429300	0.07213000	-3.32840900	5.83351100	1.29898100	0.58623500
-6.19597400	-1.35925200	-3.15794300	3.99675400	0.63963100	1.47139400
1.95236600	-3.15617100	2.02169100	6.44006300	2.08309200	-0.39789100
4.64027000	-3.36128700	2.41933700	6.10035200	3.43157000	-2.04860500
6.35598800	-2.74464100	0.39815000	6.44356900	0.71260700	1.26879500
5.40569100	-1.95935600	-2.02852800	7.52304300	2.11165100	-0.48493900
2.71779700	-1.76702900	-2.43095700	-0.20585100	1.72781800	-1.40450500
-2.69872700	0.62830500	0.41274400	1.46420200	2.96894900	0.95239200
-3.41857200	1.37534900	1.54681500	1.40721900	4.38882400	0.40011100
-2.61004700	1.29337600	-0.45476900	0.43144700	2.63929700	1.10549600
-1.67551100	0.41732100	0.74569000	2.36413400	4.75075200	0.01832000
-2.86342600	2.79185500	1.75332000	0.44106100	4.56483800	-0.75307500
-4.49237000	1.44036400	1.33760700	0.52414200	5.60991300	-1.38631500
-3.31462600	0.81689100	2.48534500	-0.40824800	3.69732800	-0.98817900
-3.55679700	3.54480300	2.89190100	2.16494800	2.95360700	2.32729900
-1.78499500	2.73434800	1.95945000	1.36754200	3.62098500	3.45363500
-2.96621200	3.36344700	0.81994900	3.15329900	3.42199900	2.24509000
-3.14144600	4.55251600	3.01513800	2.34436300	1.90782200	2.60298100
-4.63251500	3.65025700	2.70148100	1.90133700	3.51764500	4.40570000
-3.44009700	3.01876500	3.84825800	1.21466300	4.69315200	3.28420500
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-4.77774000	-1.64781900	1.92881100	1.04173800	5.10777300	1.13877300
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-3.44857800	-2.73987800	0.68933000	-5.32398400	0.54701200	-1.78954700
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-5.64137800	-1.80809900	1.27240900	0.19664200	-3.57046400	-0.59966900
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-6.19480200	-1.68385000	4.37691500	4.16397300	-2.97073500	1.23439200
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-0.16445000	0.77582000	-1.62564900	0.11119500	-1.30150600	-0.61271100
1.55486100	0.58740800	0.07091800	-1.00771200	-3.17013300	-0.89834100
2.09894100	1.98250000	-0.10423200	-2.26783200	-3.82388000	-1.34280100
1.98424000	-0.04993500	0.83505700	-2.75310200	-4.34487400	-0.51201600
1.76318400	2.32763800	-1.08646400	-2.06626400	-4.56217900	-2.12301600
3.62729300	1.99839800	-0.17368500	-3.08675100	-2.60956900	-1.86623100
4.25121800	2.77354300	-1.16374700	-4.14428600	-2.69389000	-1.61942200
4.44193900	1.25803400	0.69801900	-2.99689100	-2.55587300	-2.95405100
5.64269400	2.82266100	-1.27307000	-2.48031300	-1.30978800	-1.25003100

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-4.11900100	1.18273400	-3.09569200	-0.16445000	0.77582000	-1.62564900
-3.29342900	1.76795500	-2.67405200	1.55486100	0.58740800	0.07091800
-4.66575200	1.84500400	-3.78171400	2.09894100	1.98250000	-0.10423200
-3.68994900	0.37702000	-3.70356200	1.98424000	-0.04993500	0.83505700
-6.14372900	2.01475500	-0.93874600	1.76318400	2.32763800	-1.08646400
-5.41737500	2.71116200	-0.50387400	3.62729300	1.99839800	-0.17368500
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-6.73637100	2.57855000	-1.67247500	4.44193900	1.25803400	0.69801900
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-7.34207200	-0.93112600	-1.87592300	3.63910900	3.33877900	-1.86303700
-7.22429300	0.07213000	-3.32840900	5.83351100	1.29898100	0.58623500
-6.19597400	-1.35925200	-3.15794300	3.99675400	0.63963100	1.47139400
1.95236600	-3.15617100	2.02169100	6.44006300	2.08309200	-0.39789100
4.64027000	-3.36128700	2.41933700	6.10035200	3.43157000	-2.04860500
6.35598800	-2.74464100	0.39815000	6.44356900	0.71260700	1.26879500
5.40569100	-1.95935600	-2.02852800	7.52304300	2.11165100	-0.48493900
2.71779700	-1.76702900	-2.43095700	-0.20585100	1.72781800	-1.40450500
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-1.67551100	0.41732100	0.74569000	2.36413400	4.75075200	0.01832000
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-1.78499500	2.73434800	1.95945000	1.36754200	3.62098500	3.45363500
-2.96621200	3.36344700	0.81994900	3.15329900	3.42199900	2.24509000
-3.14144600	4.55251600	3.01513800	2.34436300	1.90782200	2.60298100
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-3.44009700	3.01876500	3.84825800	1.21466300	4.69315200	3.28420500
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-5.64137800	-1.80809900	1.27240900	0.39140900	-3.49251800	-0.45467600
-6.07285200	-2.65850100	3.88693100	-1.01119500	-1.80714100	-0.79756600
-4.68097100	-3.70258200	2.60549500	3.27320600	-1.82378100	-1.10965400
-3.92276900	-2.55463400	3.70018900	4.64832600	-1.82435900	-0.91530100
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-2.04680100	-3.89731200	-1.22471800	-5.04265100	-0.67486500	2.18458900
-2.53674900	-4.40307700	-0.38698000	-5.67537000	-1.88741900	1.08604800
-1.79305400	-4.65863200	-1.96665100	-6.26290700	-2.63793700	3.70455200
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-6.59166900	2.47501800	-1.99485700	4.29705500	1.54709000	0.09301000
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-6.02038600	-1.48635000	-3.36209400	4.11155800	0.83585300	0.89200500
2.14088400	-3.05143200	2.11255100	5.84367000	2.54338400	-1.48404600
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-4.53944900	1.43047500	1.15736600	-0.40227100	4.90441700	0.56629400
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-5.76841200	0.25277500	-1.13140200
-5.14648600	-0.97766000	-0.14541500
0.33618000	-2.94701700	0.07835100
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-2.54353900	-4.91244000	-1.94752500
-3.58716600	-3.00036200	-1.52575300
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1.22303500	2.94183500	4.70987600	2.21163600	-3.66947300	-1.72383800
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H-Int11			-2.91388500	3.41558600	1.44780000
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1.47038500	1.67104100	3.03383500	6.32553100	-0.37639800	-0.05368600
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S-Int12			3.46304400	1.33994300	-2.74018300
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S-Int13			-3.17015100	0.79152600	3.04388700
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2.62580200	3.22784700	-1.00915100	-6.39623800	-2.87687400	-1.56183900
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-4.60001300	1.72585300	0.63267300	3.92025600	2.34884300	-3.51810500
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-5.01994200	4.27388100	0.95955700	2.42614000	-3.16204800	-4.30252500
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3.42301600	-1.25871800	2.98838700	5.84106000	5.60411800	0.92110800
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H-TS9-ReRe			-2.67695800	3.15269500	1.29747400
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H-TS9-SiRe			-2.71195200	2.78987800	2.24306700
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H-TS9'-ReSi			-3.11903300	1.14131300	3.04593200
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5.11337000	-1.51809800	-0.56997500	-4.98492600	1.12823100	4.18039800
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4.54403600	-3.40551500	0.82160300	-2.82045600	-2.56429800	0.35726200
3.20423400	-3.24006200	0.49072100	-4.08461500	-3.14726500	1.01082300
2.80264200	-2.21752700	-0.37009500	-1.99328600	-2.58247700	1.07826700
0.59171600	-1.02717100	-0.54532500	-2.53981200	-3.25790300	-0.44101100
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-1.39142900	-3.02580700	-2.73760000	-4.46835300	-2.48520900	1.79380900
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-3.37668700	-2.06625500	-2.66451300	-3.02549000	-4.46438000	2.36402300
-2.16377500	-1.18288900	-3.59489700	-4.85803800	-6.13724900	2.68153600
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-5.88323500	-5.26657600	1.53027400	2.76474700	-2.63905900	-0.05069100
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1.88424300	-0.01517300	1.14109600	-0.41435100	-3.83906400	-0.62634700
0.32969700	1.38824600	-0.06396400	-1.57443600	-4.69401800	-0.99442800
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-0.41404100	1.43166900	-0.85332300	-1.27507200	-5.46968100	-1.70391600
1.34053500	2.45030800	1.46066600	-2.54873500	-3.65567200	-1.61951800
-0.09080800	3.80395500	0.59314400	-3.58341800	-3.85441400	-1.34335800
0.16300200	4.77385200	1.58634700	-2.47488500	-3.70011000	-2.70892100
-1.11596400	4.07862400	-0.33720100	-2.11698100	-2.23132000	-1.14632100
-0.57368300	5.95533800	1.65314000	-2.08113000	-1.52942100	-1.97679500
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-1.85407600	5.26008600	-0.26736600	-4.06022200	-0.23097500	-3.24915900
-1.34222400	3.36591800	-1.12533600	-3.33748100	0.51470100	-2.89789200
-1.59034200	6.20680700	0.72698400	-4.68513200	0.25817200	-4.00963200
-0.35580300	6.67989900	2.43418900	-3.50704000	-1.03150000	-3.75515100
-2.64121200	5.44136600	-0.99552100	-6.23521900	0.53347000	-1.21452200
-2.16833200	7.12566400	0.77963200	-5.63526500	1.39017100	-0.88651700
2.66825500	0.59495900	0.98118700	-6.86370900	0.21881800	-0.37202400
2.56077800	3.11950900	-0.65760900	-6.90778100	0.89143400	-2.00638300
3.51757500	3.48684600	0.29171100	-6.30625400	-2.22774500	-2.56075700
2.62768000	2.10425000	-1.03181100	-6.92354200	-2.67428300	-1.77092900
3.68177800	4.50749500	0.61379400	-6.98754500	-1.82112800	-3.31977300
4.26621200	2.56646500	0.96241400	-5.73292100	-3.03579900	-3.03225800
5.10916800	2.93925100	1.83154000	2.53676500	-3.31496100	2.20289700
4.13758100	1.30661700	0.70569300	5.22976200	-3.16510500	2.57218800
2.06520400	4.15000200	-1.63880600	6.83690000	-2.39493000	0.51188300
3.05265400	4.33097200	-2.80727000	5.76992200	-1.79992900	-1.92027300
1.91525700	5.11138300	-1.13411800	3.07903400	-1.97332300	-2.29811200
1.09435200	3.84416200	-2.04247700	-2.61063100	-0.16983500	0.29492100
2.66069200	5.06231500	-3.52464100	-3.46463400	0.60064200	1.31442400
4.02744200	4.68803300	-2.45606900	-2.58383000	0.39585200	-0.64386300
3.21266800	3.38757900	-3.34333600	-1.57880500	-0.20079300	0.66502300
H-TS10			-3.11408700	2.09421700	1.35692800
-5.18167600	-0.88069300	-1.87833000	-4.52717000	0.49121100	1.06963600
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0.83141600	-4.04781200	-0.30584800	-2.06180900	2.21564700	1.64893700
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3.60056700	-2.26650700	-1.10540300	-3.73098200	3.95225100	2.31576400
4.97333000	-2.17114900	-0.91481500	-5.05899400	2.81542200	2.03942600
5.51979900	-2.47935600	0.32888800	-3.90445900	2.52333900	3.35030800
4.69821900	-2.87029800	1.38266200	-3.06852400	-2.51798300	1.23910800
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-2.23133900	-2.21291100	1.88029200	-1.76271200	6.04917800	0.54247100
-2.86825500	-3.55555700	0.95469700	-0.49599000	5.96655700	0.86819400
-4.22240600	-3.41715500	3.31973200	-2.37321000	5.20361100	-0.12166100
-4.66917500	-1.53632400	2.36355900	-2.44265700	7.30018600	1.06872400
-5.17816400	-2.94096900	1.44269100	-1.89329300	8.19281100	0.74936800
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0.70068300	-0.39063200	-0.72001700	0.29024300	-3.53329500	-1.52120100
-0.06118100	0.11481200	-1.73266700	-0.94511600	-1.69481900	-1.47909000
1.63303500	0.28084300	-0.01258000	3.31885900	-1.97720100	-1.90632900
1.99117300	1.70781000	-0.31508100	4.69071300	-2.14338600	-1.76603900
2.11352600	-0.22999700	0.81367500	5.18707700	-2.92045100	-0.72226100
1.69684100	1.88304800	-1.35366400	4.31764500	-3.51581900	0.18733900
3.49455800	1.96784300	-0.26845300	2.94634600	-3.33144100	0.05134500
4.05995200	2.81608400	-1.23439000	2.43654800	-2.55819800	-0.99260200
4.34839300	1.39967500	0.69047800	0.29024900	-1.28771100	-1.13615100
5.42678700	3.10164200	-1.23574200	-0.90320000	-3.04380700	-1.71741300
3.42085000	3.25103500	-1.99923500	-2.22083100	-3.53384000	-2.21628800
5.71751500	1.67832000	0.68804900	-2.76731700	-4.03965400	-1.41537200
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6.26283100	2.53260200	-0.27283500	-2.89239300	-2.19276500	-2.62945400
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7.32843400	2.74693300	-0.27475800	-2.28497000	-1.09163200	-1.71546800
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1.68719100	4.60590700	-0.47881900	-7.68992400	-2.05260500	-1.19024000
0.06123400	3.80450900	-1.40654500	-6.34562600	-1.70994300	-2.28424600
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2.57370500	3.72402100	1.81482000	-5.50928200	-4.22538400	-0.26652400
2.17223400	2.09578400	2.32482800	-4.81034900	-4.72158800	0.41851300
1.25735900	3.73871600	3.92636500	-6.50183500	-4.66287800	-0.09344300
0.29610900	4.51026700	2.65636400	-5.21526000	-4.48179400	-1.29158500
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-1.00165700	-1.08715400	3.21946200	4.49001300	-3.11135700	-0.12936600
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2.23549000	1.82830000	0.16775900	-2.74105100	-4.52887700	-0.27585000
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2.49715900	2.19957500	-0.83490600	-3.05955700	-2.88829000	-1.75220200
3.52812100	1.73662400	0.97081800	-4.12330100	-2.98202700	-1.53584600
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3.53081600	1.24396100	2.28609000	-2.50220900	-1.53323400	-1.21633200
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4.71695000	1.15743000	3.01652300	-4.23738100	0.36516900	-3.51487800
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-6.07205200	2.67634300	-2.15295800	0.91626500	4.98342900	-2.40266800
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4.22293000	-1.76351500	3.23439900	3.80391600	3.70655400	-3.65694900
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H-TS14			-3.30186400	2.12803000	2.86414100
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S-TS15-SiRe			-3.07403200	0.43841200	3.25670900
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6.37816900	-1.15336300	2.26661100	3.12159500	4.77385800	2.54519400
5.82397300	-3.21518200	0.57320200	2.53878100	7.00922900	1.61763500
3.29038100	-3.60044000	-0.31274500	1.87109400	-0.60011800	-2.28057900
-2.54442700	0.79294800	0.18783100	2.46269900	0.39397000	-3.29187400
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-1.49288000	0.76656000	0.49896100	3.45785000	1.36436800	-2.70787300
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1.36310100	-1.84124000	-3.04548400	-3.67425800	-2.03624500	-3.05683500
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3.04471200	-0.11954800	-4.06287500	1.35054900	0.00030400	-1.22394400
TS-g			2.08309800	1.59162500	-3.40654300
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4.05102400	-1.46544600	2.17871000	4.03252400	-3.64612100	-2.56897700
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Int-g			-2.00313800	1.25612000	3.44629800
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H-TS-2S			1.20215800	3.66196800	-1.90042100
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H-Int3S			-2.61914500	2.41714000	2.18110900
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0.22215400	-3.62938300	-0.66950900	-1.61756500	2.15774900	2.55265400
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4.03565500	-2.59796500	1.61391000	-3.58070800	-1.84424800	0.91439700
2.71129900	-2.39063900	1.24856500	-4.95897900	-1.78430400	1.59525800
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2.83051400	-3.31626700	-2.25956400	1.48283200	2.83734100	0.84661100
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2.33271500	2.71787500	2.12845600	3.91143800	-2.02546400	3.25491400
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H-TS-3S			-3.11624800	3.09996900	2.10156800
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3.10268900	4.96301000	-1.76288900	-5.14085000	0.92984600	0.53492600
4.30931800	3.64858100	-0.54310800	-6.13342200	-0.53239000	0.70412800
2.93268700	4.34689600	0.28998600	-6.55468500	0.69545800	-0.49675400
3.63563500	5.88169500	-1.48791300	-5.75913600	-1.91735600	-2.27130400
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1.13810000	0.31673400	1.41446300	-5.19984500	-2.42927400	-3.06435000
1.93250700	-1.01821800	-4.34569500	2.49981800	-0.88673200	2.50486800
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S-TS15-SiSi			-3.07885600	0.50084700	3.24667700
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5.91863500	-0.62425300	0.22951800	-4.86224000	-0.10267000	4.35183800
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3.85002500	1.89215200	-1.37580800	2.96757000	-3.40474900	0.29865900
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2.68563900	4.41405400	-2.71815500	-1.44614100	1.43618400	0.44396800
S-TS18-ReRe			-2.49034100	4.00522700	0.21592900
-5.19382300	0.21776600	-1.52917000	-4.19997100	2.74518200	0.60808200

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-5.18406100	-2.04562800	1.08483700	N -0.82442900	-1.18881100	-0.83273300
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C	-2.17945300	-0.68157700	-1.24178900	H	-5.72825300	-1.55366800	4.43142400
H	-2.00820500	0.16981600	-1.90176200	H	-6.22720000	-2.91182700	3.41080900
C	-3.13481900	-0.21022400	-0.06624400	C	0.81823500	0.73754500	-0.08769500
C	-4.36596900	1.22217200	-3.22193600	O	0.37841700	1.21176800	1.01566700
H	-3.52273000	1.88391500	-2.98984000	C	0.94746300	1.57758000	-1.32154400
H	-5.02430100	1.76813100	-3.91178200	C	0.70024400	2.90166000	-1.30187100
H	-3.97668000	0.35245900	-3.76469900	H	1.29430300	1.06736500	-2.21863800
C	-6.04267400	2.27870700	-0.87439900	H	0.36343500	3.32789100	-0.35810700
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H	-6.72165100	2.77943100	-1.57879700	C	1.28446900	3.49190500	-3.69437500
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H	-7.35694900	-0.71273200	-1.29724300	H	0.10697300	5.48962000	-1.20391700
H	-7.46564900	0.11524200	-2.85797600	C	1.36843400	4.43902200	-4.71126400
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F	2.42587100	-0.48977900	1.86669300	C	0.99971700	5.76847100	-4.47451500
F	4.83330400	0.72313000	1.32473900	H	0.25975400	7.17246300	-3.01162500
F	6.56027800	-0.63660800	-0.27721100	H	1.72460300	4.14106200	-5.69418500
F	5.70067000	-2.71862600	-1.81898600	H	1.06746700	6.50446300	-5.27139800
F	3.06238300	-3.34046400	-1.88346100	H	2.14991100	0.38441200	0.06927500
C	-2.72622000	1.21448700	0.35717700				
C	-3.41469900	1.83347900	1.58173500	TS1-iso			
H	-2.87389500	1.87245500	-0.51101100	Si	-4.94698900	2.29390900	-0.26458800
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H	-4.50620800	1.79639500	1.48151500	N	0.70212400	-1.28816600	-2.29556400
H	-3.16043200	1.25523700	2.47907100	N	-0.77078800	-0.05324800	-1.19390800
C	-3.59355400	3.92115000	3.05127500	C	3.55207500	-1.22110800	-1.30042000
H	-1.87825000	3.32342700	1.87991500	C	4.75909400	-1.76601000	-0.87683700
H	-3.23798000	3.88851200	0.91929300	C	4.80784900	-2.51192600	0.29726300
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H	-2.22248700	-0.98015300	1.72980000	C	-1.53345600	-0.55507400	-3.38582000
H	-2.89128200	-2.23390600	0.70464400	H	-2.07170800	-1.49350300	-3.55371200
C	-4.13962300	-2.32564400	3.14618400	H	-1.10844400	-0.24472100	-4.34417200
H	-4.64916500	-0.37754900	2.37396100	C	-2.42699600	0.54985800	-2.74577600
H	-5.18057200	-1.70580500	1.35861000	H	-3.48881500	0.36016600	-2.90473200

H	-2.18893700	1.51372200	-3.20349000
C	-2.08954300	0.62182900	-1.22427900
H	-1.92200900	1.64599800	-0.89761100
C	-3.17686400	-0.00985000	-0.27503700
C	-3.67755400	3.63849400	-0.63838800
H	-2.81294700	3.60391500	0.03532700
H	-4.15108500	4.62155200	-0.50573700
H	-3.30652500	3.59501400	-1.66963800
C	-5.56465000	2.52453500	1.50247800
H	-4.75772300	2.48531300	2.24337400
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C	-6.40244600	2.42447500	-1.45216100
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H	-6.07852800	2.34581200	-2.49763700
F	1.34248200	-2.38857200	1.33283200
F	3.70191900	-3.42740500	2.17460100
F	5.96585100	-3.03203100	0.70930400
F	5.87293500	-1.56946500	-1.59027600
F	3.52912400	-0.49631700	-2.42160800
C	-2.72162200	0.15123900	1.19290400
C	-3.62317900	-0.43145100	2.29110600
H	-2.56056300	1.22010900	1.38343600
H	-1.73795600	-0.32376500	1.28549900
C	-3.12589200	-0.06412900	3.69661200
H	-4.65352900	-0.07654800	2.17069000
H	-3.65578500	-1.52507400	2.20600800
C	-3.99094600	-0.65512100	4.81314500
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H	-5.02896900	-0.30553600	4.74034700
H	-4.00716900	-1.75192100	4.76824300
C	-3.44414700	-1.49852600	-0.64032200
C	-4.86478200	-2.03283700	-0.39213100
H	-2.71925700	-2.11449200	-0.09262100
H	-3.23433700	-1.65930200	-1.70265600
C	-4.97410600	-3.53442900	-0.69169900
H	-5.18227000	-1.85081500	0.64010500
H	-5.56934700	-1.48689700	-1.03145200
C	-6.39435000	-4.07754200	-0.51013200
H	-4.63913100	-3.72783200	-1.72130700
H	-4.28619700	-4.08927100	-0.03728200

H	-6.44298100	-5.15180800	-0.72722100
H	-6.74859100	-3.93177600	0.51861300
H	-7.10326100	-3.57186500	-1.17846200
C	0.53791300	1.30709600	0.92867100
O	-0.11784700	2.30396400	0.47595200
C	2.04545300	1.36490600	0.98272100
C	2.73584300	2.39746400	0.47268200
H	2.53615800	0.54720500	1.50645500
H	2.16005500	3.17912200	-0.02200500
C	4.18938300	2.60792600	0.49846500
C	4.71907000	3.74264100	-0.14465700
C	5.08955200	1.72895400	1.13457600
C	6.09180800	3.99078200	-0.15951500
H	4.04025200	4.43382300	-0.63917200
C	6.45999300	1.97714800	1.12107800
H	4.71531600	0.84771200	1.64774000
C	6.96951500	3.10826300	0.47335800
H	6.47489800	4.87404900	-0.66444700
H	7.13567200	1.28614600	1.61911500
H	8.03957400	3.29862900	0.46525500
H	0.14488400	0.76621000	1.81084500

Int1-iso

Si	-5.71114200	0.65875600	-1.35897400
O	-4.56616000	-0.21236900	-0.47282900
N	1.09425000	-1.47377500	-0.74077100
N	0.48011600	-2.59543700	-1.29204700
N	-0.93189500	-0.89703900	-1.05174100
C	3.46059000	-1.12839700	-1.27225800
C	4.80452400	-1.28778700	-0.95495600
C	5.16246200	-1.92903900	0.22816600
C	4.18319900	-2.40089400	1.09777200
C	2.84170800	-2.23179800	0.77572900
C	2.46928700	-1.58363100	-0.40274500
C	0.25144400	-0.42794900	-0.59618500
C	-0.74498000	-2.19380100	-1.46676000
C	-1.97839800	-2.77460300	-2.05723900
H	-2.44138200	-3.47783400	-1.35618600
H	-1.76807200	-3.31613000	-2.98266000
C	-2.84479700	-1.50768200	-2.28075300
H	-3.89490500	-1.70290500	-2.07692800
H	-2.75336900	-1.18586200	-3.32118400
C	-2.29997600	-0.36780400	-1.36036900
H	-2.14247200	0.55176100	-1.92403500

C	-3.19805800	-0.03408700	-0.08898000	C	0.50397900	1.04766200	-0.19791000
C	-5.02910600	1.32693600	-2.98704000	O	0.04892900	1.80305900	-1.20913600
H	-4.25001800	2.08518700	-2.84165600	C	1.94538000	1.28343800	0.25345900
H	-5.84252800	1.80545300	-3.55013600	C	2.72142200	2.19679000	-0.34782400
H	-4.61510700	0.53546600	-3.62290100	H	2.27307100	0.74550000	1.14243800
C	-6.45776500	2.08360600	-0.37504500	H	2.29396500	2.70002800	-1.21383500
H	-5.75279400	2.90624700	-0.20940400	C	4.08603500	2.60355600	0.01838900
H	-6.83722900	1.75931800	0.60170400	C	4.75248800	3.54172900	-0.79281500
H	-7.31004500	2.49433600	-0.93441700	C	4.77247700	2.10096300	1.14264800
C	-7.05088700	-0.62493000	-1.67895800	C	6.05139700	3.95921300	-0.50093200
H	-7.43970400	-1.03241700	-0.73702100	H	4.24002400	3.94309300	-1.66438000
H	-7.89739200	-0.18257700	-2.22037800	C	6.06938600	2.51748300	1.43473500
H	-6.67970600	-1.46705100	-2.27633400	H	4.28693500	1.38164000	1.79649700
F	1.90385700	-2.68473100	1.61140200	C	6.71742000	3.44834400	0.61497600
F	4.53501400	-3.01623800	2.23145800	H	6.54208700	4.68425700	-1.14566000
F	6.45121600	-2.08737700	0.53237400	H	6.57801300	2.11595700	2.30787500
F	5.75258100	-0.83687500	-1.78240200	H	7.72927600	3.77078800	0.84640600
F	3.12532900	-0.50856100	-2.40420400	H	-0.07616700	1.13100800	0.76302100
C	-2.93670600	1.44209000	0.30356800				
C	-3.46189100	1.93992000	1.65569400	Int4-iso		
H	-3.35962800	2.06317600	-0.49807000	Si	5.14741700	-2.04268900	-0.79896000
H	-1.86272500	1.63274500	0.25406400	O	4.43659500	-0.51671500	-0.62793100
C	-3.20498300	3.44132700	1.85279000	N	-1.17402600	1.03402400	-0.97462600
H	-4.53725800	1.74489200	1.74990700	N	-0.62272600	1.68502000	-2.06148800
H	-2.96985600	1.39124100	2.46942400	N	0.78640700	0.21076500	-1.18132400
C	-3.67137200	3.95554700	3.21730000	C	-3.60151600	1.03254400	-1.24717000
H	-2.13103900	3.64451800	1.73354400	C	-4.86045900	1.48345800	-0.87071300
H	-3.71145100	4.00589300	1.05672000	C	-4.98504700	2.35680700	0.20779000
H	-3.48046100	5.03024500	3.32649700	C	-3.85926000	2.77256200	0.91441200
H	-4.74787500	3.79339200	3.35835600	C	-2.60273000	2.31873000	0.53167200
H	-3.15025100	3.44243600	4.03606900	C	-2.46766900	1.43655800	-0.54125800
C	-2.90269500	-1.05607500	1.04349600	C	-0.34201600	0.11180000	-0.45400000
C	-4.02205100	-1.32015300	2.06254000	C	0.55676400	1.14304500	-2.16908000
H	-1.99572500	-0.72891700	1.56816400	C	1.67338400	1.21742500	-3.14799600
H	-2.65785900	-2.02523100	0.59163300	H	2.20388300	2.17100800	-3.06811700
C	-3.58466100	-2.31902100	3.14403700	H	1.29727800	1.13558700	-4.17113000
H	-4.34716300	-0.39264100	2.54517400	C	2.54292400	-0.00278600	-2.73369900
H	-4.89738900	-1.71999500	1.53692600	H	3.60716100	0.21996500	-2.79316900
C	-4.70097400	-2.65492300	4.13668700	H	2.33441800	-0.83901600	-3.40540800
H	-3.23373100	-3.24485500	2.66505500	C	2.14767600	-0.41932000	-1.28207500
H	-2.72119700	-1.91187400	3.68977300	H	2.00644500	-1.49391400	-1.19993300
H	-4.35984100	-3.37175600	4.89387900	C	3.19378500	0.02747000	-0.17951300
H	-5.05107000	-1.75760300	4.66322600	C	4.00105200	-3.30298500	-1.60840300
H	-5.56678800	-3.09744000	3.62714700	H	3.13950200	-3.55754400	-0.97913100

H	4.55873500	-4.23448200	-1.77846900
H	3.62541200	-2.96740300	-2.58233000
C	5.75105200	-2.74056900	0.84505000
H	4.93154400	-2.97066600	1.53586600
H	6.44217900	-2.05717600	1.35288100
H	6.29605200	-3.67719600	0.66190800
C	6.62002700	-1.68801700	-1.91391500
H	7.28475800	-0.93630900	-1.46979000
H	7.21413800	-2.59578200	-2.08153900
H	6.30286900	-1.31398800	-2.89543300
F	-1.52348200	2.72111800	1.20533600
F	-3.98925700	3.61003700	1.94676600
F	-6.19109700	2.79112900	0.56990700
F	-5.94749400	1.08521400	-1.53594200
F	-3.48159900	0.18782900	-2.27083800
C	2.79759200	-0.55359500	1.19548600
C	3.70433900	-0.22636100	2.39162100
H	2.71629600	-1.64278700	1.09204600
H	1.79446500	-0.19143000	1.44055400
C	3.29228000	-1.00162100	3.65165200
H	4.74953800	-0.45505600	2.15503100
H	3.65905200	0.84754400	2.61120300
C	4.18270600	-0.69555700	4.85901300
H	2.24669400	-0.76639300	3.89888800
H	3.32090200	-2.08069200	3.44239200
H	3.86593600	-1.26194500	5.74336900
H	5.22961600	-0.95474900	4.65557600
H	4.15087000	0.37050800	5.11864500
C	3.33148700	1.57686200	-0.14200100
C	4.70984200	2.14606300	0.23355800
H	2.57197700	1.96683700	0.54788300
H	3.08735500	1.99180400	-1.12445500
C	4.69396900	3.67956000	0.30423700
H	5.05716500	1.74736900	1.19247800
H	5.44384100	1.82934000	-0.51700900
C	6.06799800	4.27807300	0.61796700
H	4.33037000	4.08444600	-0.65158600
H	3.97197100	4.00363400	1.06777000
H	6.02742900	5.37376200	0.65351000
H	6.44467100	3.92869900	1.58809600
H	6.80684200	3.99808500	-0.14393300
C	-0.64585700	-0.88496100	0.65241500
O	0.08008300	-2.04504600	0.27326100
C	-2.12477000	-1.14868900	0.86249100

C	-2.76209900	-2.17590900	0.27917900
H	-2.62162800	-0.48448100	1.56301300
H	-2.19008900	-2.81551000	-0.39106600
C	-4.17112400	-2.55872600	0.44524400
C	-4.64420500	-3.68262400	-0.25713000
C	-5.07645000	-1.85634600	1.26558900
C	-5.97248200	-4.09393400	-0.14786100
H	-3.95789700	-4.23470900	-0.89514400
C	-6.40257300	-2.26739000	1.37395500
H	-4.74544100	-0.98579300	1.82461200
C	-6.85744600	-3.38723900	0.66861700
H	-6.31480400	-4.96520000	-0.70012600
H	-7.08589900	-1.71292800	2.01208700
H	-7.89337400	-3.70376900	0.75640700
H	-0.24374500	-0.45351600	1.58059900
H	0.05797600	-2.65696900	1.02996000

TS7-iso

Si	-4.86572300	1.82824100	-1.53003500
O	-4.36232200	0.29085400	-1.04366500
N	1.12928600	-1.71788200	-0.86271000
N	0.46936000	-2.71167700	-1.59327700
N	-0.80805100	-0.90717900	-1.31766100
C	3.46985800	-2.34671300	-1.11813900
C	4.68878600	-2.73200400	-0.57293500
C	4.82705600	-2.82663100	0.80945000
C	3.74963900	-2.54089500	1.64344400
C	2.52765900	-2.17874100	1.08882000
C	2.37901100	-2.05031900	-0.29526600
C	0.38858600	-0.56626800	-0.75337100
C	-0.67357200	-2.16583300	-1.86509700
C	-1.81512200	-2.51033700	-2.75937700
H	-2.42143200	-3.32269000	-2.34951100
H	-1.44602900	-2.84084200	-3.73425000
C	-2.57197200	-1.15335900	-2.84219300
H	-3.65359900	-1.28448200	-2.86171400
H	-2.28008000	-0.63547700	-3.76005400
C	-2.13347800	-0.28880500	-1.62020300
H	-1.95473100	0.74357200	-1.90293500
C	-3.19459900	-0.29001600	-0.44259500
C	-3.51112600	2.85053900	-2.35574100
H	-2.65928200	3.05230100	-1.69550000
H	-3.93200500	3.82324700	-2.64659800
H	-3.12875800	2.37880800	-3.26907200

C	-5.58687300	2.81718800	-0.09569200
H	-4.83183100	3.12193800	0.63820300
H	-6.37011800	2.26106800	0.43403000
H	-6.04845600	3.73531200	-0.48548200
C	-6.23378900	1.46235700	-2.77067300
H	-7.02961700	0.85347600	-2.32323700
H	-6.69384200	2.39252700	-3.12935400
H	-5.85385800	0.92175500	-3.64671600
F	1.49146300	-1.93646700	1.89634300
F	3.88492100	-2.64752500	2.96929600
F	5.99689800	-3.19073800	1.33702100
F	5.72849600	-3.00480500	-1.36828700
F	3.35304400	-2.24475700	-2.44391300
C	-2.69905300	0.54800400	0.75684200
C	-3.60843500	0.58374500	1.99620100
H	-2.51952600	1.57277900	0.41373800
H	-1.72265000	0.15437800	1.06221200
C	-3.07874000	1.52158400	3.09035000
H	-4.61948500	0.89866900	1.71354500
H	-3.70201100	-0.42290200	2.42204100
C	-4.02559500	1.63354800	4.28876900
H	-2.10053900	1.15749800	3.43296700
H	-2.90335900	2.52105400	2.66852100
H	-3.62039100	2.30460300	5.05628000
H	-5.00494700	2.02740400	3.98758700
H	-4.19298700	0.65564600	4.75892300
C	-3.55856100	-1.73742900	0.00657300
C	-5.01371600	-1.99203900	0.43743100
H	-2.88155900	-2.01437900	0.82486400
H	-3.35733700	-2.44517900	-0.79974500
C	-5.20852800	-3.42276700	0.95951500
H	-5.33247400	-1.28349400	1.20880000
H	-5.67661400	-1.83016800	-0.42136900
C	-6.65887100	-3.72928800	1.34268400
H	-4.87493200	-4.13914700	0.19451600
H	-4.55889000	-3.58419400	1.83187300
H	-6.76617300	-4.75643200	1.71282600
H	-7.01435800	-3.05424900	2.13203000
H	-7.33113100	-3.61412400	0.48270100
C	0.80562200	0.71873400	-0.24536200
O	-0.11424300	1.73306400	-0.60832600
C	2.22715200	1.10922400	-0.42202400
C	2.62737700	2.37450500	-0.66383000
H	2.97141100	0.33591100	-0.26284900

H	1.86442500	3.13401400	-0.81904000
C	4.01245300	2.85165100	-0.76328900
C	4.24029200	4.18242100	-1.16853000
C	5.14101900	2.05622700	-0.47259600
C	5.53182800	4.69528700	-1.28861200
H	3.38599100	4.81725200	-1.39402100
C	6.43094300	2.56791200	-0.59445500
H	5.01079000	1.02961400	-0.14075300
C	6.63691300	3.89006000	-1.00391500
H	5.67412900	5.72604500	-1.60451500
H	7.28266900	1.93255900	-0.36301900
H	7.64503500	4.28595000	-1.09485400
H	0.73877900	0.69610000	1.16704500
H	-0.21926600	2.28546100	0.20837500
C	0.45076100	2.14602200	2.65581100
O	0.01588900	2.97032500	1.82776900
O	0.74376000	0.90851600	2.37766900
C	0.71467700	2.55304600	4.08903800
H	1.78854200	2.74718400	4.20636000
H	0.16681300	3.46407700	4.34066800
H	0.44817800	1.74915300	4.78111500

TS8-iso

Si	-5.04253000	-0.36048000	-1.49872300
O	-3.78037400	-0.46947000	-0.39501300
N	1.87398800	-1.41979500	-0.50455500
N	1.48894400	-2.50719400	-1.29031000
N	-0.13673700	-0.99550900	-1.12263400
C	4.24029800	-1.14973000	-1.00539000
C	5.56871100	-1.07966000	-0.60342700
C	5.89008200	-1.22945600	0.74169900
C	4.88592200	-1.45437900	1.67967000
C	3.56023800	-1.52504900	1.26928300
C	3.21982700	-1.35248600	-0.07397300
C	0.91246600	-0.43990300	-0.44896600
C	0.28331800	-2.19879600	-1.65255500
C	-0.75529700	-2.80030800	-2.53753700
H	-1.18165800	-3.70342800	-2.09204700
H	-0.33748600	-3.07335000	-3.51019300
C	-1.77753800	-1.63498500	-2.63650200
H	-2.79801500	-1.99537300	-2.75505900
H	-1.53700700	-1.02193500	-3.50992800
C	-1.59312700	-0.76017200	-1.36265300
H	-1.75408800	0.29347700	-1.58238500

C	-2.53077600	-1.10562200	-0.12835500			
C	-5.71061500	-2.03547500	-2.05675900			
H	-5.00302600	-2.61556500	-2.66052100			
H	-6.60487000	-1.87412600	-2.67495300			
H	-6.01361800	-2.65564100	-1.20409900			
C	-4.55004000	0.67985900	-2.99447100			
H	-3.80823200	0.19383200	-3.63874600			
H	-4.14342500	1.65160300	-2.68638800			
H	-5.43530000	0.88015400	-3.61365100			
C	-6.38304400	0.54374600	-0.53446900			
H	-6.04305100	1.53116300	-0.19767000			
H	-7.27542700	0.69571500	-1.15596400			
H	-6.69138300	-0.02192100	0.35396300			

Coordinate listing:

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.53077600	-1.10562200	-0.12835500	C	1.15797600	0.91486200	-0.00021100
C	-5.71061500	-2.03547500	-2.05675900	O	1.89523400	0.95562400	1.20813100
H	-5.00302600	-2.61556500	-2.66052100	C	0.13328400	1.95665300	-0.16323200
H	-6.60487000	-1.87412600	-2.67495300	C	0.00262300	3.02565800	0.65285400
H	-6.01361800	-2.65564100	-1.20409900	H	-0.45044000	1.90068200	-1.07961400
C	-4.55004000	0.67985900	-2.99447100	H	0.61159600	3.05536500	1.55435700
H	-3.80823200	0.19383200	-3.63874600	C	-0.88822400	4.17520300	0.46078800
H	-4.14342500	1.65160300	-2.68638800	C	-0.98718200	5.13434600	1.48941500
H	-5.43530000	0.88015400	-3.61365100	C	-1.65572500	4.38663800	-0.70455100
C	-6.38304400	0.54374600	-0.53446900	C	-1.81850100	6.24758500	1.36775100
H	-6.04305100	1.53116300	-0.19767000	H	-0.40136100	4.99636600	2.39579200
H	-7.27542700	0.69571500	-1.15596400	C	-2.48725900	5.49759600	-0.82480500
H	-6.69138300	-0.02192100	0.35396300	H	-1.59780100	3.67990400	-1.52798700
F	2.61258800	-1.75514300	2.17876100	C	-2.57554300	6.43643700	0.20921000
F	5.20165800	-1.61202600	2.97076200	H	-1.87268400	6.96960200	2.17909300
F	7.16388300	-1.15939900	1.13402600	H	-3.06658400	5.63621800	-1.73466900
F	6.53281100	-0.84460900	-1.50329200	H	-3.22285800	7.30378000	0.10931700
F	3.94613900	-0.99615400	-2.29892600	H	2.09508800	1.34335700	-0.96327700
C	-1.95679600	-0.44556700	1.15646200	H	2.73190900	1.45119300	1.00382900
C	-2.96148900	-0.02804300	2.24426600	C	4.03297300	2.18580900	-1.01669800
H	-1.41889300	0.46415200	0.87465300	O	4.11834000	2.17506600	0.22747900
H	-1.21051800	-1.12611800	1.58637400	O	2.99319900	1.78742700	-1.68787500
C	-2.25003300	0.52770100	3.48664900	C	5.20320200	2.63570000	-1.86352100
H	-3.63066100	0.74069300	1.83892700	H	5.74231600	1.74435800	-2.20934600
H	-3.60104400	-0.86400900	2.54485200	H	4.86166800	3.18277600	-2.74681700
C	-3.22042200	0.95875100	4.58972900	H	5.88920100	3.25236200	-1.27816000
H	-1.56366000	-0.23386000	3.88469200				
H	-1.62162600	1.38194200	3.19681000				
H	-2.68414300	1.34816800	5.46395500	Int1-EtOH			
H	-3.89995800	1.74675300	4.23990100	Si	-5.17805900	1.00327900	-2.01359600
H	-3.83816200	0.11671200	4.92822300	O	-4.53314500	-0.15631000	-0.96716300
C	-2.70793100	-2.63473700	0.03331200	N	0.98021100	-1.92797400	-0.38671200
C	-3.56183600	-3.13640600	1.20746300	N	0.35235000	-3.10174700	-0.77874600
H	-1.70946800	-3.07983400	0.13171000	N	-0.96603500	-1.32862000	-1.00022100
H	-3.14149300	-3.03396500	-0.89022500	C	3.39310500	-2.04129200	-0.73504600
C	-3.78235300	-4.65487900	1.14268600	C	4.68818500	-2.10597900	-0.23878200
H	-3.07537600	-2.89494500	2.16019600	C	4.89407600	-2.12616700	1.13846700
H	-4.53607400	-2.63051800	1.21167600	C	3.81193200	-2.07762400	2.01271200
C	-4.58512700	-5.19562600	2.32906600	C	2.51793100	-2.00837600	1.50828100
H	-4.29802200	-4.90888900	0.20548000	C	2.30017000	-1.98271900	0.13022300
H	-2.80712900	-5.16163400	1.10191000	C	0.20376500	-0.83763500	-0.55121600
H	-4.73334500	-6.27973300	2.25065000	C	-0.82190400	-2.68948400	-1.16156300
H	-4.07221700	-4.99940500	3.27955600	C	-2.00603900	-3.29825500	-1.82771800
H	-5.57705700	-4.72890600	2.38601700	H	-2.57290100	-3.92363400	-1.13126600
				H	-1.69996000	-3.93185700	-2.66433800

C	-2.79242100	-2.03751500	-2.29088300	H	-4.59648800	-3.68044800	2.01777000
H	-3.86857300	-2.16502700	-2.18144300	H	-4.16414000	-2.50669600	3.25287800
H	-2.58022100	-1.84855900	-3.34638100	H	-6.28278000	-3.68176800	3.86774600
C	-2.29389500	-0.81738200	-1.45311300	H	-6.61240200	-1.96331700	3.59755400
H	-2.10952900	0.04989800	-2.08715300	H	-7.04334700	-3.15263500	2.35839300
C	-3.28322600	-0.37792300	-0.30047700	C	0.59158100	0.60943900	-0.22274500
C	-4.01535200	1.46316900	-3.42743800	O	0.55371900	0.74360900	1.13011800
H	-3.10201600	1.96349100	-3.08355100	C	1.91444100	0.94260500	-0.91293900
H	-4.53250500	2.16529600	-4.09627800	C	2.94851500	1.47991600	-0.25039200
H	-3.72376000	0.59590100	-4.03222800	H	1.95453100	0.76696500	-1.98852600
C	-5.68748900	2.58069400	-1.11648800	H	2.80901600	1.67650800	0.81158100
H	-4.83120400	3.14113200	-0.72435300	C	4.25163900	1.86684200	-0.81520600
H	-6.37214300	2.38005300	-0.28352800	C	5.05240700	2.79260000	-0.12060000
H	-6.21390700	3.24090900	-1.81986100	C	4.74882700	1.33359400	-2.02094900
C	-6.71583800	0.15841500	-2.69578800	C	6.28953400	3.19564100	-0.62377000
H	-7.40362000	-0.13191700	-1.89139200	H	4.69222700	3.20305300	0.82011800
H	-7.26201300	0.83449400	-3.36668000	C	5.98597500	1.73486800	-2.52242200
H	-6.46933500	-0.74590800	-3.26620700	H	4.17486700	0.57947600	-2.55236700
F	1.48905500	-1.98517100	2.35455400	C	6.76046000	2.67147500	-1.82998600
F	4.02021400	-2.10559800	3.33295500	H	6.88698900	3.91732200	-0.07216600
F	6.13467100	-2.19115400	1.62279800	H	6.35282200	1.30739600	-3.45244800
F	5.73133600	-2.13727000	-1.07434100	H	7.72625200	2.98006300	-2.22178500
F	3.20070700	-1.99146100	-2.05663300	H	-0.17419500	1.20548600	-0.77023100
C	-2.76039200	0.90991000	0.37059000	C	0.82864200	5.56473400	1.79050200
C	-3.56581700	1.47036800	1.55421600	C	0.69888300	4.20055200	1.13028300
H	-2.67578800	1.68350700	-0.40590700	H	0.80818100	6.36236300	1.03808600
H	-1.74458700	0.72166600	0.73561700	H	0.00655300	5.73657000	2.49614100
C	-3.03935700	2.83832200	2.01149400	H	1.77292300	5.63852900	2.34389800
H	-4.62688700	1.56319500	1.29516500	H	-0.24778500	4.15304000	0.56624200
H	-3.50767200	0.77393500	2.40076900	H	1.51081300	4.06915500	0.39594100
C	-3.78428700	3.38501000	3.23297200	O	0.74868600	3.19087700	2.12998000
H	-1.96741100	2.76255400	2.23991200	H	0.66835800	2.28991800	1.68236300
H	-3.12658000	3.55610900	1.18262100				
H	-3.39509500	4.36606900	3.53241200	AcO-EtOH			
H	-4.85653500	3.50222300	3.02791300	C	2.02061800	-0.14249400	-0.02120100
H	-3.68349400	2.71217400	4.09437000	O	1.05967000	-0.93351300	0.26908000
C	-3.48509000	-1.52856900	0.72720000	O	3.19204400	-0.50717200	-0.28556300
C	-4.86254600	-1.62069200	1.40489600	C	1.69255500	1.35664800	-0.05681700
H	-2.70242900	-1.43727900	1.49091400	H	1.21683700	1.67076800	0.87951400
H	-3.31918600	-2.49418800	0.24028000	H	2.59159200	1.95759800	-0.22252100
C	-4.90396200	-2.72588000	2.46947000	H	0.97700000	1.56373300	-0.86270600
H	-5.14226300	-0.66851100	1.86717500	C	-2.13448200	-0.35276100	-0.35456600
H	-5.62310200	-1.82862300	0.64235100	C	-3.56151800	0.15180500	-0.21207500
C	-6.28586500	-2.89018000	3.10829900	H	-2.13282100	-1.45608300	-0.37000900

H	-1.72148200	-0.02498800	-1.32400500
H	-4.18801200	-0.21511800	-1.03380700
H	-3.99978100	-0.19019500	0.73356700
H	-3.58805800	1.24837500	-0.22237000
O	-1.35459900	0.14075300	0.72670700
H	-0.43523300	-0.23382300	0.60850200

TS7-EtOH

Si	-5.28706500	-0.72776100	-1.46424100
O	-4.37808700	-0.82611200	-0.04358800
N	1.31826500	-1.47168400	0.73726600
N	0.80881300	-2.60582300	1.38212800
N	-0.71774000	-1.64379400	0.08135000
C	3.55359500	-2.15438100	0.06749700
C	4.93405100	-2.00877700	0.09661800
C	5.49893900	-0.98439900	0.85109300
C	4.68816900	-0.10468200	1.56168000
C	3.30780500	-0.26817500	1.53500400
C	2.72029300	-1.27624600	0.76838200
C	0.40676300	-0.90436100	-0.12029100
C	-0.41022400	-2.67246200	0.94464300
C	-1.54750900	-3.62476500	1.09561600
H	-1.94494700	-3.61345600	2.11466200
H	-1.22523300	-4.64808100	0.88280400
C	-2.55941500	-3.09054400	0.03955500
H	-3.58574800	-3.12397200	0.40408300
H	-2.50224800	-3.70798600	-0.86061100
C	-2.14681300	-1.63053300	-0.32817000
H	-2.17932100	-1.46546100	-1.40266600
C	-3.03788100	-0.51765600	0.36043000
C	-4.34879900	-1.29694600	-2.99925000
H	-3.49669200	-0.64841200	-3.23726200
H	-5.02764900	-1.26443100	-3.86307300
H	-3.98131500	-2.32678100	-2.91564400
C	-5.93615100	1.01729000	-1.76882900
H	-5.14115600	1.72533600	-2.03031100
H	-6.47269000	1.41510900	-0.89878900
H	-6.64635400	0.99994000	-2.60737900
C	-6.73579800	-1.87789100	-1.11717000
H	-7.27484600	-1.57606300	-0.21011500
H	-7.45528600	-1.86622300	-1.94642400
H	-6.40686300	-2.91545300	-0.97854100
F	2.54397900	0.58842700	2.22424500
F	5.23655400	0.88070400	2.28036600
F	6.82469900	-0.82602000	0.86768300
F	5.71591300	-2.84612500	-0.58926500
F	3.01847000	-3.13529800	-0.66504700
C	-2.60853300	0.88133200	-0.13394800
C	-3.29463300	2.10450100	0.49342900
H	-2.74173200	0.91365800	-1.22168300
H	-1.53185700	0.98337400	0.03931600
C	-2.87272700	3.41051700	-0.19576200
H	-4.38537700	2.00642800	0.44002500
H	-3.03665000	2.17189000	1.55819300
C	-3.46173700	4.65792600	0.46822400
H	-1.77576400	3.48225400	-0.19855700
H	-3.17710700	3.38016800	-1.25190500
H	-3.14761600	5.57187100	-0.05092400
H	-4.55931500	4.63424400	0.46251700
H	-3.13817500	4.74314000	1.51366600
C	-2.97249900	-0.62376100	1.91168600
C	-4.23841900	-0.22373800	2.68898700
H	-2.12457600	-0.01710600	2.25471900
H	-2.74492300	-1.65170300	2.20736700
C	-4.00819000	-0.24520500	4.20675800
H	-4.58715600	0.77175500	2.39514200
H	-5.04838100	-0.91952400	2.43750100
C	-5.26181700	0.11913400	5.00686200
H	-3.65826200	-1.24261800	4.51099300
H	-3.19834400	0.45351300	4.46202300
H	-5.06670100	0.10103300	6.08624600
H	-5.61811800	1.12546300	4.75137200
H	-6.08194300	-0.58239500	4.80604800
C	0.67208800	0.06012100	-1.16961800
O	-0.34222800	0.09391100	-2.15571000
C	1.24124200	1.36333700	-0.81322900
C	1.21648700	2.45999600	-1.60380500
H	1.73675800	1.41416300	0.15135200
H	0.70449600	2.39579300	-2.56179500
C	1.82481900	3.76004300	-1.30056000
C	1.70515600	4.80254600	-2.24263100
C	2.53880100	4.03416900	-0.11310900
C	2.27212900	6.05669500	-2.01660800
H	1.15908300	4.61785200	-3.16538500
C	3.10389000	5.28710400	0.11147100
H	2.65527700	3.26219800	0.64304100
C	2.97649300	6.30823200	-0.83711000
H	2.16334500	6.83848900	-2.76470300

H	3.64927300	5.46920800	1.03465600
H	3.42026700	7.28396800	-0.65721800
H	1.77303800	-0.53136300	-1.92419200
H	-0.10674400	-0.61621400	-2.80269600
C	2.03944600	-1.79693000	-3.53013200
O	0.81440000	-1.92119500	-3.67200000
O	2.58054400	-0.95886900	-2.67512700
C	3.03115200	-2.62200200	-4.31023700
H	3.82482400	-1.98529000	-4.71375600
H	3.50355700	-3.33910700	-3.62784900
H	2.53388900	-3.16362500	-5.11717000
C	5.67182700	0.88063800	-2.59699500
C	7.14789800	1.07824700	-2.29744200
H	5.06104100	1.35349700	-1.81274400
H	5.40909300	1.37160500	-3.54797200
H	7.76633600	0.61703400	-3.07699700
H	7.39260500	2.14581400	-2.25195600
H	7.40861200	0.61981000	-1.33638800
O	5.40486300	-0.52191900	-2.66562800
H	4.43322500	-0.63978700	-2.68396400

H-TS9-ReSi-EtOH

Si	-5.59085500	-0.00435800	-1.81119900
O	-4.64055400	-0.55312100	-0.52698800
N	0.97420800	-2.11831600	-0.12729000
N	0.24735100	-3.30725300	-0.08286400
N	-1.02752100	-1.60225900	-0.74452800
C	3.25203300	-2.42695200	-0.95281900
C	4.61318800	-2.58235300	-0.72214800
C	5.09601600	-2.55284400	0.58384400
C	4.22559500	-2.35708600	1.65247100
C	2.86557100	-2.19416700	1.41190000
C	2.36641100	-2.21456100	0.10736100
C	0.22158000	-1.05839700	-0.58241100
C	-0.93497500	-2.95001000	-0.47352100
C	-2.19294900	-3.67774300	-0.78975300
H	-2.70262800	-4.00692100	0.12080800
H	-1.98959200	-4.56660300	-1.39297200
C	-2.98529100	-2.59546700	-1.56738500
H	-4.05216300	-2.64999600	-1.36204300
H	-2.83540000	-2.74154500	-2.64086300
C	-2.40661200	-1.19969800	-1.17302800
H	-2.30657300	-0.55820600	-2.04575600
C	-3.28174700	-0.42689900	-0.08834200

C	-4.61494400	0.29182200	-3.39896100
H	-3.88051400	1.10071400	-3.30578500
H	-5.31309600	0.57878500	-4.19773400
H	-4.08853200	-0.60795800	-3.73853800
C	-6.52284300	1.56758000	-1.34607400
H	-5.86601200	2.43575700	-1.22082900
H	-7.09460000	1.44009200	-0.41827000
H	-7.24195300	1.81353200	-2.13983600
C	-6.84096800	-1.38935100	-2.07400000
H	-7.39194300	-1.61000300	-1.15076000
H	-7.57851900	-1.10876900	-2.83744500
H	-6.36030600	-2.31868200	-2.40401100
F	2.03728900	-2.01582100	2.44145200
F	4.69918400	-2.33428600	2.90264400
F	6.40087200	-2.70947800	0.81098500
F	5.45668900	-2.77190300	-1.74227000
F	2.79115800	-2.45995400	-2.20569900
C	-2.86665700	1.06134800	-0.05421400
C	-3.65867800	2.00329200	0.87076600
H	-2.93164800	1.43858100	-1.08336800
H	-1.81191100	1.11041900	0.22863700
C	-3.52743400	3.47667700	0.45710300
H	-4.72025800	1.73352600	0.87426700
H	-3.29990800	1.89419800	1.90130400
C	-4.25990300	4.43039400	1.40467100
H	-2.46551900	3.75681900	0.40987500
H	-3.91805100	3.60289700	-0.56299500
H	-4.15982400	5.47327100	1.07920400
H	-5.33194600	4.19884700	1.45033200
H	-3.86285700	4.36117700	2.42555500
C	-3.16165700	-1.12753100	1.29112100
C	-4.27721600	-0.89433000	2.32303500
H	-2.19915300	-0.83886400	1.72957900
H	-3.11534600	-2.20959900	1.13103400
C	-4.05650300	-1.73747500	3.58835200
H	-4.33626300	0.15986100	2.61017300
H	-5.24662100	-1.15468200	1.88026900
C	-5.13134100	-1.50794400	4.65362300
H	-4.03457100	-2.80318200	3.31683500
H	-3.06753500	-1.50940900	4.00981600
H	-4.95207000	-2.12661300	5.54179200
H	-5.15234000	-0.45981500	4.97916800
H	-6.13097000	-1.75635400	4.27343500
C	0.65812700	0.24953500	-0.93515900

O	-0.24099800	0.94351300	-1.73867400
C	1.91851200	0.75875100	-0.66907300
C	2.36125900	2.04129200	-1.04704700
H	2.58786700	0.15316100	-0.07396300
H	1.76477800	2.55237600	-1.79980500
C	3.79392800	2.38753600	-1.05832400
C	4.28979400	3.26380300	-2.04478100
C	4.70601600	1.89590000	-0.10015400
C	5.63910200	3.61724700	-2.08684200
H	3.60737400	3.65538100	-2.79589500
C	6.05422700	2.24701400	-0.14638000
H	4.35403500	1.24574600	0.69701100
C	6.53138600	3.10777200	-1.14031100
H	5.99362100	4.28919100	-2.86485300
H	6.73566200	1.85224100	0.60355000
H	7.58286400	3.38087600	-1.17198700
H	-0.42335700	1.80977600	-1.33621000
C	1.65634700	3.29792800	0.68780900
C	0.51361200	2.76733100	1.28803300
H	2.60220200	3.06556400	1.16711300
H	-0.48789500	3.12890300	1.10152900
N	0.57496800	1.71763500	2.16110400
O	-0.51127100	1.32666600	2.72500600
O	1.67367400	1.15219800	2.43483200
C	1.55575300	4.65018300	0.02231300
C	1.63273100	5.79288500	1.05174100
H	0.61439000	4.72442100	-0.53618700
H	2.37151800	4.77316200	-0.69738100
H	1.57967400	6.76359700	0.54422700
H	0.80927900	5.74043200	1.77303500
H	2.57460900	5.75752700	1.61229200
C	0.61000200	-0.88357800	5.22288200
C	0.84898500	-2.22185100	5.90012100
H	0.19030800	-0.16703000	5.94901300
H	1.56413900	-0.46300700	4.87269700
H	1.52043200	-2.10406200	6.75889800
H	-0.09475000	-2.65036400	6.25893600
H	1.30434300	-2.93273400	5.20029000
O	-0.28231800	-1.07102100	4.12586600
H	-0.28817700	-0.23213800	3.60927500