

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP Reactant M2

C	41.039796	34.522844	44.558317
H	40.241400	33.843709	44.263674
H	41.752548	34.609686	43.744075
S	40.264258	36.123948	44.897058
N	40.785292	39.114206	44.623115
C	39.644682	39.636046	44.068535
C	40.891886	39.652014	45.871389
C	39.007012	40.548005	44.990431
C	39.792285	40.567175	46.119546
C	41.879150	39.334233	46.788684
H	41.867319	39.863396	47.730207
C	42.845741	38.363825	46.629268
N	43.012779	37.595969	45.504492
C	44.068279	36.756419	45.773364
C	44.564018	36.974611	47.118667
C	43.814388	37.990433	47.640534
C	44.607780	35.855779	44.887320
H	45.469278	35.287639	45.200462
C	44.181034	35.654525	43.584926
C	44.747636	34.661737	42.703010
C	43.127541	35.846795	41.675182
N	43.184159	36.348241	42.958596
C	44.130374	34.821711	41.493123
C	42.161936	36.166286	40.749663
H	42.198630	35.642995	39.806113
C	41.101432	37.038646	40.948870
C	40.018862	37.220938	40.018086
N	40.905104	37.789080	42.077009
C	39.724491	38.449157	41.900894
C	39.150459	39.309281	42.821853
H	38.231856	39.795487	42.534392
Fe	42.123705	37.895523	43.704541
C	39.141506	38.103104	40.614767
C	37.881904	38.633759	40.128562
H	37.492731	39.481755	40.683048
C	37.153863	38.214524	39.087435
H	37.431550	37.368768	38.477472
H	36.235599	38.723422	38.827408
C	39.575711	41.256887	47.380871
H	39.952958	40.748774	48.264010
C	38.950521	42.422935	47.556757
H	38.585678	43.015676	46.730475

H	38.799484	42.823873	48.549708
C	39.898694	36.550060	38.691842
H	39.130671	35.771593	38.711420
H	39.624305	37.273544	37.922233
H	40.825786	36.065137	38.393244
C	37.718188	41.255454	44.744188
H	37.047570	40.661850	44.122783
H	37.207006	41.468685	45.682978
H	37.868834	42.206164	44.226183
C	43.961015	38.666386	48.963306
H	44.827081	38.279898	49.496928
H	44.098928	39.742509	48.840514
H	43.085763	38.530174	49.603613
C	44.431119	34.097192	40.224016
H	43.548216	33.923439	39.607225
H	45.138944	34.669063	39.617921
H	44.906508	33.137965	40.426877
C	45.687041	33.569345	43.093851
H	45.704965	33.458099	44.177625
H	45.259151	32.644745	42.706758
C	45.713691	36.241117	47.731788
H	46.517487	36.157969	46.999433
H	46.111686	36.827536	48.560489
C	47.130183	33.662793	42.588322
H	47.168032	34.109669	41.590535
H	47.526185	32.654011	42.499766
C	45.401769	34.835043	48.259609
H	45.031915	34.191755	47.456177
H	44.614493	34.865515	49.016012
C	46.624640	34.134925	48.876450
C	48.076251	34.450016	43.492498
O	47.577070	35.347803	44.211854
O	46.403084	33.214853	49.697767
O	49.295987	34.131551	43.454273
O	47.769699	34.515552	48.520441
O	43.106400	39.077053	43.201825
O	48.079486	39.061600	43.259545
O	48.432619	41.529047	41.880566
O	49.992043	40.096125	41.032761
O	48.746395	40.244200	43.767087
O	51.662476	38.819696	40.422135
C	47.804148	39.163554	41.836775
C	46.278019	39.375650	41.703236
C	48.265179	37.825342	41.251237

C	45.758234	39.110747	40.274649
C	48.573452	40.324069	41.201675
C	47.779707	37.639707	39.814556
C	45.829080	40.756887	42.210852
C	46.267378	37.776604	39.732889
C	49.782909	37.681620	41.413974
C	48.095677	41.390127	43.273898
C	46.567599	41.300622	43.435412
C	44.232991	39.147925	40.225019
C	50.547512	38.874543	40.884006
C	50.338490	36.360752	40.899459
C	48.731954	42.539562	44.025647
H	45.840585	38.615840	42.359139
H	47.801492	37.052309	41.872275
H	46.144818	39.902690	39.620413
H	48.194271	40.485180	40.192608
H	48.260242	38.368864	39.152797
H	48.081148	36.653666	39.464983
H	45.935442	41.481848	41.398583
H	44.769285	40.698898	42.456697
H	45.799943	36.962996	40.298235
H	45.941892	37.670445	38.695014
H	49.961523	37.723777	42.491223
H	46.359157	40.696025	44.318838
H	46.193387	42.306318	43.638603
H	51.380595	36.240890	41.184994
H	49.777216	35.535814	41.336867
H	50.284552	36.286429	39.815666
H	43.809510	38.447980	40.940760
H	43.871269	38.883278	39.228392
H	43.845466	40.131899	40.479854
H	48.451290	42.488539	45.077752
H	49.814659	42.484354	43.930955
H	48.398761	43.491095	43.617774
H	41.543812	34.093727	45.424281

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP Reactant M4

C	41.059201	34.529065	44.567127
H	40.261421	33.850177	44.269625
H	41.773857	34.617087	43.754670
S	40.278903	36.126709	44.907077
N	40.786273	39.116646	44.618149
C	39.644139	39.640546	44.066229

C	40.897662	39.653970	45.866064
C	39.010811	40.553184	44.991113
C	39.799671	40.570715	46.118246
C	41.889028	39.335429	46.779226
H	41.883692	39.864846	47.720622
C	42.852782	38.363183	46.616164
N	43.015529	37.596895	45.489046
C	44.070143	36.752992	45.754698
C	44.568125	36.967321	47.099570
C	43.822688	37.985055	47.624362
C	44.609168	35.855381	44.866039
H	45.470512	35.285692	45.177466
C	44.183513	35.661065	43.561909
C	44.751003	34.672088	42.675802
C	43.124547	35.856711	41.655297
N	43.184207	36.354848	42.939935
C	44.129022	34.833634	41.468017
C	42.157011	36.178890	40.732636
H	42.192258	35.658407	39.787245
C	41.096836	37.051191	40.936452
C	40.015551	37.240201	40.005144
N	40.899062	37.795415	42.068690
C	39.719438	38.457734	41.895443
C	39.147349	39.316711	42.819816
H	38.229777	39.806430	42.533984
Fe	42.122070	37.901239	43.696036
C	39.137259	38.118676	40.606554
C	37.876873	38.649006	40.121033
H	37.487886	39.497769	40.675000
C	37.147950	38.228571	39.080786
H	37.424681	37.382076	38.471115
H	36.229240	38.736640	38.820383
C	39.586191	41.255632	47.382457
H	39.983992	40.751829	48.259106
C	38.941047	42.408732	47.573711
H	38.550487	42.999828	46.758149
H	38.797945	42.800386	48.571710
C	39.897933	36.578535	38.673711
H	39.140379	35.789799	38.688178
H	39.612540	37.303455	37.909919
H	40.830323	36.108289	38.367865
C	37.722454	41.264683	44.751262
H	37.060499	40.689182	44.104498
H	37.200223	41.448641	45.690438

H	37.876749	42.231386	44.264819
C	43.976129	38.661302	48.946311
H	44.848569	38.278463	49.472271
H	44.107375	39.737895	48.820599
H	43.105918	38.519890	49.592326
C	44.423757	34.109232	40.197313
H	43.540086	33.946939	39.578551
H	45.140047	34.673687	39.594335
H	44.887507	33.144240	40.399063
C	45.692376	33.578765	43.061260
H	45.697030	33.452365	44.143749
H	45.272393	32.658127	42.656853
C	45.719248	36.231658	47.708125
H	46.521215	36.153470	46.973081
H	46.118184	36.814911	48.538496
C	47.142184	33.679217	42.573676
H	47.191269	34.135461	41.580508
H	47.536421	32.670003	42.481720
C	45.408495	34.822810	48.231018
H	45.056313	34.177112	47.421431
H	44.610286	34.847412	48.976136
C	46.629019	34.131622	48.863796
C	48.082602	34.454665	43.494607
O	47.579986	35.347347	44.217956
O	46.404929	33.216228	49.689575
O	49.301708	34.132634	43.464148
O	47.774990	34.514289	48.513385
O	43.097954	39.083817	43.188385
O	48.086102	39.054432	43.289075
O	48.433712	41.514574	41.898970
O	49.985159	40.076675	41.044841
O	48.754875	40.239462	43.789539
O	51.649443	38.798152	40.422932
C	47.801604	39.149949	41.867311
C	46.274617	39.365699	41.739136
C	48.256550	37.805950	41.288777
C	45.753896	39.096642	40.311449
C	48.568563	40.307160	41.222372
C	47.752188	37.600188	39.860741
C	45.830272	40.749313	42.243747
C	46.239676	37.744811	39.794829
C	49.776969	37.662358	41.431892
C	48.101746	41.383037	43.293829
C	46.574195	41.293079	43.464771

C	44.230642	39.169503	40.247613
C	50.538128	38.854315	40.893424
C	50.323409	36.341738	40.906242
C	48.737654	42.538286	44.036949
H	45.836589	38.609016	42.398120
H	47.801892	37.040323	41.925483
H	46.162071	39.870623	39.649242
H	48.182880	40.465666	40.215396
H	48.228018	38.316625	39.181522
H	48.043984	36.607483	39.521722
H	45.935120	41.472323	41.429667
H	44.771166	40.693750	42.493093
H	45.772837	36.951264	40.388293
H	45.898717	37.614895	38.764760
H	49.970243	37.702971	42.506908
H	46.371993	40.687499	44.349082
H	46.200051	42.298121	43.671464
H	51.368430	36.219192	41.179230
H	49.765628	35.515999	41.346423
H	50.255763	36.272037	39.823036
H	43.781142	38.488678	40.965479
H	43.874386	38.903058	39.249639
H	43.865307	40.165953	40.487175
H	48.462202	42.490157	45.090504
H	49.819989	42.489257	43.936748
H	48.395548	43.485801	43.626798
H	41.560955	34.099349	45.434108

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP TS M2

C	41.078184	34.559527	44.563736
H	40.277227	33.886709	44.261312
H	41.795162	34.644545	43.752960
S	40.314023	36.167927	44.903620
N	40.853996	39.155600	44.501283
C	39.699252	39.654200	43.961438
C	40.975678	39.702499	45.742775
C	39.064778	40.569209	44.886841
C	39.869065	40.608826	46.002202
C	41.972815	39.388624	46.652978
H	41.970200	39.923475	47.591644
C	42.930496	38.406074	46.498978
N	43.092467	37.637554	45.376347
C	44.121450	36.771483	45.652414

C	44.611849	36.975351	47.003706
C	43.880799	38.007668	47.520139
C	44.636547	35.854309	44.767372
H	45.483600	35.268067	45.086062
C	44.207993	35.648333	43.464125
C	44.764984	34.638124	42.595816
C	43.137715	35.806111	41.557022
N	43.213170	36.337035	42.828739
C	44.139691	34.776508	41.386846
C	42.153244	36.108300	40.642455
H	42.169113	35.563645	39.709788
C	41.094089	36.986308	40.845069
C	40.003725	37.177117	39.925041
N	40.916083	37.745416	41.971028
C	39.740916	38.420087	41.806471
C	39.186276	39.296677	42.727552
H	38.260099	39.774442	42.448510
Fe	42.141630	37.864706	43.580269
C	39.142017	38.072790	40.526726
C	37.883001	38.613445	40.050635
H	37.502168	39.461210	40.611642
C	37.144292	38.202744	39.013534
H	37.413138	37.357247	38.399322
H	36.227652	38.718850	38.762171
C	39.658792	41.288483	47.269390
H	40.081495	40.792523	48.138876
C	38.988648	42.425110	47.472486
H	38.572189	43.006738	46.663070
H	38.850234	42.811889	48.472982
C	39.866036	36.504054	38.601234
H	39.091785	35.731924	38.628320
H	39.592275	37.227827	37.831535
H	40.787152	36.010274	38.298036
C	37.757763	41.250501	44.665687
H	37.098559	40.656493	44.033073
H	37.248105	41.426051	45.613584
H	37.880749	42.218218	44.172605
C	44.017047	38.664024	48.853979
H	44.869699	38.259368	49.396597
H	44.167762	39.740098	48.748827
H	43.129298	38.527641	49.477222
C	44.443624	34.041211	40.125070
H	43.563985	33.870630	39.503186
H	45.161332	34.605508	39.523223

H	44.912348	33.080368	40.335693
C	45.707794	33.555868	43.005407
H	45.689419	33.433458	44.088335
H	45.305160	32.630160	42.596637
C	45.745792	36.224369	47.626825
H	46.548623	36.122613	46.895732
H	46.151026	36.811725	48.451152
C	47.166406	33.662477	42.549253
H	47.231824	34.109097	41.552606
H	47.566644	32.654724	42.475081
C	45.415653	34.828498	48.172948
H	45.060918	34.171263	47.373908
H	44.612741	34.876584	48.912065
C	46.623810	34.136363	48.829829
C	48.094380	34.446254	43.474584
O	47.590620	35.351134	44.182205
O	46.386656	33.225705	49.657115
O	49.312781	34.120119	43.461615
O	47.776627	34.515302	48.496588
O	43.152635	39.148080	42.998048
O	48.182882	39.123690	43.401107
O	48.467516	41.559681	41.950835
O	49.932896	40.087804	41.019089
O	48.880675	40.315304	43.844191
O	51.567394	38.788709	40.367058
C	47.800000	39.202933	42.003084
C	46.271057	39.444260	41.994804
C	48.191224	37.840954	41.414524
C	45.618541	39.119401	40.632258
C	48.536819	40.338193	41.287400
C	47.556529	37.609963	40.042217
C	45.887702	40.855929	42.462810
C	46.041571	37.744474	40.122976
C	49.717729	37.676841	41.440918
C	48.218524	41.459852	43.364929
C	46.704026	41.407923	43.629014
C	44.116029	39.283327	40.664817
C	50.470138	38.858281	40.866522
C	50.208490	36.350752	40.872046
C	48.920612	42.612379	44.048496
H	45.879567	38.727770	42.722260
H	47.783163	37.093024	42.101705
H	45.995888	39.862399	39.911725
H	48.082674	40.486620	40.307014

H	47.956167	38.319654	39.308049
H	47.824281	36.615327	39.686079
H	45.982470	41.548219	41.621361
H	44.838563	40.842592	42.755376
H	45.638117	36.972475	40.784190
H	45.600044	37.582853	39.137048
H	49.988987	37.704568	42.499686
H	46.542359	40.822352	44.535051
H	46.362811	42.423873	43.837725
H	51.268535	36.213629	41.069075
H	49.674737	35.529168	41.347821
H	50.062488	36.286509	39.795978
H	43.596428	39.059639	41.937395
H	43.545976	38.582722	40.058470
H	43.772927	40.307652	40.567770
H	48.693326	42.598365	45.114483
H	49.994178	42.521743	43.899883
H	48.591842	43.560801	43.629914
H	41.577878	34.124446	45.429229

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP TS M4

C	41.079833	34.557656	44.561642
H	40.281372	33.883147	44.256315
H	41.798218	34.647368	43.752184
S	40.311346	36.161716	44.903680
N	40.858107	39.153294	44.506741
C	39.699314	39.652094	43.964172
C	40.973740	39.700408	45.750190
C	39.065429	40.566216	44.889212
C	39.867509	40.606386	46.005776
C	41.968668	39.389130	46.661824
H	41.967283	39.924332	47.599935
C	42.922291	38.404307	46.505028
N	43.081757	37.639844	45.377862
C	44.114398	36.769473	45.653791
C	44.605631	36.974093	47.002995
C	43.875077	38.005784	47.521871
C	44.633566	35.853796	44.773426
H	45.481279	35.270094	45.094691
C	44.207645	35.647945	43.468268
C	44.765777	34.639286	42.599508
C	43.137458	35.810699	41.565275
N	43.214003	36.337000	42.837147

C	44.138883	34.779869	41.391151
C	42.152970	36.113794	40.650857
H	42.170329	35.570918	39.717121
C	41.092791	36.990386	40.853071
C	40.004244	37.179184	39.930201
N	40.909535	37.748989	41.978307
C	39.737076	38.421078	41.810317
C	39.183753	39.298865	42.732989
H	38.258601	39.779439	42.455862
Fe	42.140045	37.881899	43.597537
C	39.139771	38.074394	40.530071
C	37.881295	38.614104	40.051661
H	37.498974	39.461378	40.612440
C	37.144060	38.203376	39.013341
H	37.413773	37.358405	38.398725
H	36.227264	38.718940	38.761264
C	39.656304	41.287722	47.271722
H	40.077776	40.792604	48.142234
C	38.987762	42.425759	47.472117
H	38.573296	43.006837	46.661299
H	38.848846	42.814333	48.471807
C	39.868229	36.505734	38.606368
H	39.093405	35.734120	38.632978
H	39.595219	37.229295	37.836124
H	40.789285	36.011356	38.304065
C	37.759476	41.248301	44.665895
H	37.100598	40.654154	44.033219
H	37.249316	41.425369	45.613094
H	37.884696	42.215170	44.171721
C	44.015520	38.662822	48.854735
H	44.869371	38.258123	49.395329
H	44.166713	39.738726	48.747950
H	43.129158	38.527818	49.480223
C	44.442438	34.045558	40.128681
H	43.563034	33.875670	39.506314
H	45.160901	34.609612	39.527475
H	44.910629	33.084283	40.338992
C	45.708585	33.556080	43.007030
H	45.691483	33.433022	44.089910
H	45.305202	32.630642	42.598144
C	45.741538	36.224555	47.624680
H	46.543739	36.123747	46.892764
H	46.146727	36.813069	48.448132
C	47.166899	33.662149	42.549772

H	47.232063	34.108586	41.553020
H	47.567234	32.654391	42.475587
C	45.413481	34.828678	48.172166
H	45.058760	34.170487	47.373944
H	44.611120	34.876508	48.911888
C	46.622748	34.137957	48.829022
C	48.094727	34.446314	43.474798
O	47.590473	35.351112	44.182082
O	46.386294	33.227060	49.656185
O	49.313166	34.120393	43.462136
O	47.775112	34.518119	48.495989
O	43.149749	39.142966	42.974114
O	48.180489	39.123789	43.400143
O	48.467872	41.559839	41.950499
O	49.934148	40.087915	41.020188
O	48.879501	40.314543	43.843646
O	51.568343	38.788659	40.368064
C	47.799793	39.203148	42.001376
C	46.270727	39.444945	41.989377
C	48.192223	37.840976	41.413847
C	45.624533	39.122544	40.622992
C	48.537779	40.338436	41.286980
C	47.560744	37.608502	40.040427
C	45.887369	40.856089	42.459757
C	46.046191	37.745855	40.117445
C	49.718558	37.677005	41.441939
C	48.218132	41.459571	43.364326
C	46.703306	41.407315	43.627210
C	44.122132	39.287098	40.644422
C	50.471134	38.858378	40.867606
C	50.209399	36.350945	40.873122
C	48.920812	42.611649	44.048240
H	45.876839	38.727397	42.714454
H	47.783154	37.093582	42.100971
H	46.009561	39.863655	39.904886
H	48.084817	40.487177	40.306159
H	47.962797	38.316945	39.306299
H	47.828154	36.613015	39.686485
H	45.982437	41.549876	41.619620
H	44.837914	40.842255	42.751490
H	45.639377	36.976533	40.779774
H	45.606049	37.583006	39.131040
H	49.989140	37.704778	42.500853
H	46.541450	40.821385	44.533003

H	46.362095	42.423188	43.836471
H	51.269395	36.213764	41.070206
H	49.675414	35.529385	41.348703
H	50.063454	36.286820	39.797042
H	43.594209	39.051329	41.914152
H	43.557979	38.590431	40.027976
H	43.778555	40.311611	40.554596
H	48.693760	42.597922	45.114283
H	49.994347	42.520118	43.899562
H	48.593115	43.560446	43.629658
H	41.578330	34.122936	45.428006

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP Product M2

C	41.041192	34.515813	44.551021
H	40.263315	33.813405	44.258032
H	41.754748	34.616640	43.739026
S	40.225175	36.100874	44.882574
N	40.768448	39.139406	44.593083
C	39.631601	39.658875	44.033151
C	40.876090	39.674631	45.839994
C	38.995690	40.579586	44.953047
C	39.780104	40.599382	46.082938
C	41.866343	39.349313	46.756109
H	41.857034	39.879030	47.697699
C	42.837640	38.377942	46.598064
N	43.007662	37.619978	45.470548
C	44.064663	36.780433	45.727356
C	44.560800	36.987338	47.076689
C	43.810840	37.999960	47.606182
C	44.606598	35.891527	44.827532
H	45.468864	35.323706	45.140662
C	44.187812	35.687984	43.517866
C	44.756642	34.687775	42.641905
C	43.123600	35.855086	41.609548
N	43.192493	36.373098	42.885900
C	44.132604	34.832121	41.432794
C	42.137234	36.159966	40.696298
H	42.163392	35.624234	39.758599
C	41.067482	37.028351	40.896827
C	39.980852	37.215493	39.971391
N	40.877364	37.783827	42.022768
C	39.701604	38.452413	41.855942
C	39.139899	39.320995	42.784362

H	38.221404	39.808636	42.497010
Fe	42.058516	37.865705	43.681215
C	39.111505	38.106536	40.571143
C	37.854598	38.643901	40.086966
H	37.460053	39.478628	40.657794
C	37.133822	38.247808	39.031354
H	37.418507	37.419210	38.401557
H	36.215380	38.760170	38.779140
C	39.565064	41.293139	47.341772
H	39.942254	40.784853	48.224997
C	38.940932	42.459713	47.519128
H	38.575004	43.054025	46.694495
H	38.791277	42.858652	48.513086
C	39.848302	36.543803	38.645913
H	39.048856	35.797191	38.659333
H	39.611878	37.272543	37.868083
H	40.758385	36.019726	38.360589
C	37.709546	41.292663	44.707369
H	37.038757	40.704557	44.080690
H	37.196627	41.502834	45.646299
H	37.864054	42.246134	44.195131
C	43.962164	38.669910	48.931670
H	44.824599	38.274724	49.465422
H	44.109658	39.745248	48.810573
H	43.084531	38.539891	49.570242
C	44.431795	34.091948	40.172140
H	43.550302	33.925061	39.551430
H	45.153699	34.646466	39.565819
H	44.892237	33.127869	40.387068
C	45.697549	33.598204	43.040825
H	45.702098	33.485387	44.125128
H	45.276261	32.672558	42.648593
C	45.709542	36.248577	47.688083
H	46.515060	36.169846	46.956463
H	46.106936	36.830933	48.520283
C	47.147618	33.687086	42.553119
H	47.198920	34.132495	41.554787
H	47.536807	32.675152	42.472004
C	45.400342	34.838910	48.210547
H	45.047871	34.193511	47.400447
H	44.601103	34.861375	48.954935
C	46.621029	34.145676	48.842604
C	48.093017	34.466463	43.464563
O	47.602516	35.382850	44.166680

O	46.397373	33.228035	49.665866
O	49.306922	34.123508	43.448849
O	47.768291	34.528499	48.495142
O	43.118895	39.199470	43.102995
O	48.152632	39.090777	43.302806
O	48.521340	41.538724	41.894667
O	50.041101	40.073144	41.037077
O	48.837257	40.271049	43.791735
O	51.681262	38.769418	40.406359
C	47.856097	39.182174	41.885282
C	46.330158	39.422538	41.783803
C	48.280611	37.825717	41.310321
C	45.779400	39.129610	40.359202
C	48.632179	40.324977	41.225023
C	47.746416	37.609402	39.894602
C	45.915459	40.822926	42.262875
C	46.233769	37.760941	39.857170
C	49.801479	37.661046	41.430354
C	48.200146	41.422170	43.293594
C	46.673591	41.362474	43.475537
C	44.302541	39.271338	40.293902
C	50.574652	38.841733	40.883720
C	50.324202	36.334736	40.894708
C	48.863651	42.566634	44.027856
H	45.894788	38.684095	42.463064
H	47.827362	37.073569	41.964002
H	46.215855	39.891665	39.692750
H	48.238526	40.483134	40.220220
H	48.210963	38.316325	39.197415
H	48.025339	36.612049	39.558341
H	46.037894	41.531346	41.438263
H	44.856798	40.799856	42.519022
H	45.771483	36.984405	40.475321
H	45.869140	37.619591	38.837180
H	50.009394	37.697669	42.502906
H	46.463485	40.766009	44.364224
H	46.318165	42.375014	43.676671
H	51.369473	36.196567	41.159037
H	49.759309	35.513572	41.334198
H	50.248761	36.272641	39.811298
H	43.476390	38.965337	42.229305
H	43.682719	38.487234	39.881814
H	43.835224	40.216642	40.522750
H	48.583868	42.534650	45.080917

H	49.944166	42.483064	43.932209
H	48.552853	43.520895	43.609135
H	41.554254	34.100723	45.418508

QM atoms (linking H atom included): 121

XE12 Cluster0 def2TZVP Product M4

C	41.041859	34.516340	44.550305
H	40.263434	33.813807	44.257755
H	41.755974	34.617048	43.738494
S	40.227269	36.100265	44.883979
N	40.769177	39.139974	44.593337
C	39.631477	39.659173	44.032351
C	40.876100	39.674885	45.839895
C	38.995669	40.579495	44.952750
C	39.779725	40.599397	46.082969
C	41.866103	39.349846	46.757009
H	41.856778	39.879250	47.698786
C	42.836583	38.378834	46.598848
N	43.007320	37.620168	45.470352
C	44.065134	36.779946	45.727323
C	44.560579	36.987368	47.076633
C	43.810059	38.000153	47.606229
C	44.607135	35.891287	44.827528
H	45.469267	35.323242	45.140313
C	44.188477	35.687780	43.517717
C	44.756787	34.687644	42.641641
C	43.123786	35.855356	41.610221
N	43.193059	36.372974	42.885875
C	44.132617	34.832056	41.432606
C	42.137528	36.159851	40.696009
H	42.163144	35.624387	39.757957
C	41.067588	37.028420	40.896898
C	39.981192	37.215367	39.971683
N	40.877237	37.784101	42.022624
C	39.702159	38.452178	41.855850
C	39.139464	39.321590	42.784431
H	38.220666	39.809053	42.497133
Fe	42.059124	37.866648	43.681316
C	39.111432	38.106762	40.571505
C	37.854505	38.644026	40.087188
H	37.459835	39.478603	40.658081
C	37.133733	38.247988	39.031448
H	37.418295	37.419428	38.401428
H	36.215199	38.760201	38.779012

C	39.564932	41.292800	47.342242
H	39.942285	40.784697	48.225598
C	38.940859	42.459574	47.519255
H	38.575163	43.053681	46.694285
H	38.790909	42.859242	48.512947
C	39.848657	36.543430	38.646301
H	39.049324	35.797194	38.659994
H	39.612154	37.272277	37.868795
H	40.758501	36.019439	38.360943
C	37.709701	41.292394	44.707108
H	37.039075	40.704409	44.080565
H	37.196908	41.502638	45.645935
H	37.864202	42.245493	44.194941
C	43.961831	38.669943	48.931852
H	44.824210	38.274621	49.465385
H	44.109340	39.745078	48.811172
H	43.084699	38.540146	49.570578
C	44.431848	34.091839	40.172094
H	43.550605	33.924822	39.551474
H	45.153544	34.646247	39.566022
H	44.892441	33.127939	40.387037
C	45.697086	33.598621	43.040915
H	45.701886	33.486022	44.124746
H	45.275792	32.672947	42.649027
C	45.709740	36.249239	47.688094
H	46.514904	36.170367	46.956762
H	46.106972	36.831069	48.520318
C	47.147235	33.687017	42.553335
H	47.198668	34.131961	41.555213
H	47.537228	32.675417	42.472408
C	45.400591	34.839014	48.210416
H	45.047989	34.194039	47.400540
H	44.601854	34.861719	48.954965
C	46.620998	34.145424	48.842755
C	48.092781	34.466385	43.464616
O	47.602246	35.383005	44.166286
O	46.397175	33.227538	49.665763
O	49.306754	34.123576	43.448804
O	47.768182	34.528227	48.495233
O	43.115857	39.195700	43.103600
O	48.152271	39.090710	43.302489
O	48.521606	41.539159	41.894540
O	50.041069	40.073322	41.037223
O	48.836773	40.271130	43.791431

O	51.681257	38.769793	40.406609
C	47.855819	39.182176	41.885092
C	46.330330	39.422430	41.783704
C	48.280564	37.825758	41.310249
C	45.779635	39.129601	40.359316
C	48.632070	40.324896	41.225044
C	47.746386	37.609593	39.894401
C	45.915610	40.822952	42.262886
C	46.233996	37.761179	39.856971
C	49.801102	37.661442	41.430184
C	48.200004	41.422223	43.293488
C	46.673647	41.362498	43.475297
C	44.302629	39.270794	40.293637
C	50.574532	38.841731	40.883787
C	50.324380	36.334794	40.894692
C	48.864028	42.566611	44.027737
H	45.895079	38.683946	42.463240
H	47.827446	37.073526	41.963645
H	46.215657	39.892099	39.692668
H	48.238853	40.483146	40.220467
H	48.210918	38.316238	39.197587
H	48.025430	36.612129	39.558332
H	46.037976	41.531238	41.438750
H	44.856841	40.800069	42.519001
H	45.771882	36.984630	40.474918
H	45.869376	37.619824	38.837152
H	50.009309	37.697658	42.502521
H	46.463697	40.766394	44.363892
H	46.318337	42.375143	43.676374
H	51.369638	36.196560	41.159021
H	49.759478	35.514111	41.334927
H	50.248847	36.272486	39.811550
H	43.477046	38.965490	42.229969
H	43.682619	38.486772	39.881278
H	43.834871	40.216115	40.522757
H	48.584394	42.534848	45.080797
H	49.944371	42.482613	43.931995
H	48.553522	43.520941	43.608962
H	41.554154	34.100917	45.418086

QM atoms (linking H atom included): 121

XE12 Cluster0 Reactant M2

C	41.102081	34.563088	44.567986
H	40.296976	33.884654	44.249378

H	41.834333	34.648079	43.756377
S	40.326756	36.168440	44.906892
N	40.794420	39.129681	44.610624
C	39.650593	39.654440	44.058004
C	40.903552	39.661813	45.864041
C	39.007969	40.566352	44.987545
C	39.799501	40.579600	46.123321
C	41.898427	39.338373	46.784051
H	41.892931	39.869941	47.735316
C	42.869565	38.363790	46.611757
N	43.028475	37.595561	45.480318
C	44.097649	36.764064	45.735298
C	44.606626	36.974081	47.082391
C	43.850213	37.989412	47.619633
C	44.647719	35.872658	44.834906
H	45.535868	35.317236	45.129760
C	44.211206	35.677314	43.527556
C	44.775882	34.676064	42.645346
C	43.145352	35.866035	41.618525
N	43.206037	36.368337	42.904772
C	44.151137	34.835330	41.429631
C	42.172796	36.190741	40.690235
H	42.203752	35.667334	39.735707
C	41.107611	37.066213	40.902352
C	40.015902	37.249562	39.971403
N	40.913026	37.810128	42.038923
C	39.724826	38.466460	41.874193
C	39.147515	39.325649	42.806483
H	38.214564	39.809168	42.524411
Fe	42.137226	37.912880	43.672372
C	39.131146	38.126319	40.584075
C	37.860773	38.655471	40.106864
H	37.462745	39.498226	40.683129
C	37.130014	38.247601	39.052589
H	37.417879	37.406672	38.421740
H	36.199017	38.760498	38.799838
C	39.585931	41.262584	47.394596
H	40.007165	40.759263	48.273293
C	38.916272	42.409629	47.599553
H	38.499461	43.000615	46.782816
H	38.777804	42.797893	48.611528
C	39.891037	36.582197	38.639331
H	39.154352	35.760242	38.669155
H	39.561132	37.300720	37.873869

H	40.840485	36.140104	38.308699
C	37.720716	41.284726	44.742406
H	37.055076	40.714250	44.078551
H	37.182990	41.467988	45.684699
H	37.882660	42.263770	44.259924
C	44.000843	38.654144	48.951356
H	44.887697	38.271744	49.474472
H	44.119837	39.744089	48.842481
H	43.129676	38.496190	49.609364
C	44.448617	34.101844	40.160959
H	43.559914	33.930623	39.534220
H	45.172241	34.670673	39.552456
H	44.921994	33.131291	40.368350
C	45.709717	33.575476	43.040569
H	45.692320	33.443100	44.131846
H	45.285511	32.652732	42.620354
C	45.744656	36.216811	47.696130
H	46.567322	36.121125	46.971389
H	46.145756	36.792000	48.544202
C	47.167598	33.672709	42.581174
H	47.234279	34.105665	41.567232
H	47.579600	32.658081	42.517316
C	45.418504	34.804786	48.206341
H	45.072025	34.162443	47.377229
H	44.599503	34.820150	48.944343
C	46.638194	34.107302	48.856642
C	48.093231	34.478652	43.500465
O	47.569904	35.367351	44.218015
O	46.400783	33.189737	49.673578
O	49.317849	34.181526	43.465131
O	47.781968	34.503515	48.512135
O	43.111416	39.102186	43.199438
O	48.072414	39.043514	43.315236
O	48.405897	41.496417	41.914842
O	49.957798	40.059063	41.065166
O	48.757707	40.219610	43.794671
O	51.631145	38.783502	40.436897
C	47.783126	39.128711	41.896717
C	46.253165	39.350883	41.774117
C	48.238041	37.776092	41.326031
C	45.726036	39.071222	40.346724
C	48.550572	40.289996	41.242233
C	47.715919	37.546694	39.906044
C	45.816115	40.738134	42.284737

C	46.201344	37.703299	39.850205
C	49.763868	37.643585	41.462262
C	48.103859	41.367349	43.312762
C	46.573555	41.280529	43.503168
C	44.203156	39.172789	40.270819
C	50.520899	38.840354	40.912284
C	50.329849	36.326104	40.944801
C	48.767954	42.517890	44.044815
H	45.812031	38.593680	42.444860
H	47.789095	37.016553	41.988779
H	46.155996	39.836083	39.670779
H	48.151313	40.441955	40.228058
H	48.195955	38.250808	39.200941
H	47.999548	36.536535	39.578721
H	45.915495	41.470251	41.465119
H	44.750043	40.681358	42.545289
H	45.730487	36.917216	40.466463
H	45.847726	37.553881	38.817064
H	49.953751	37.696933	42.546490
H	46.377478	40.667733	44.395840
H	46.198587	42.293827	43.718295
H	51.400215	36.249548	41.175233
H	49.818319	35.484918	41.431819
H	50.224348	36.230636	39.855748
H	43.730667	38.512346	41.006649
H	43.840939	38.894897	39.267323
H	43.855732	40.190470	40.491569
H	48.518407	42.473235	45.114833
H	49.856207	42.447564	43.915332
H	48.430653	43.478853	43.635845
H	41.591509	34.120744	45.435661

QM atoms (linking H atom included): 121

XE12 Cluster0 TS M2

C	41.127244	34.579662	44.550973
H	40.330505	33.894464	44.226494
H	41.867016	34.668262	43.746473
S	40.342792	36.186031	44.875183
N	40.848818	39.154550	44.501058
C	39.701486	39.664999	43.948504
C	40.961370	39.694477	45.749578
C	39.057664	40.584333	44.872664
C	39.855198	40.613977	46.003932
C	41.953877	39.368315	46.673568

H	41.947745	39.902276	47.623599
C	42.920461	38.384316	46.511498
N	43.081066	37.617425	45.382406
C	44.134736	36.772840	45.640387
C	44.639109	36.973164	46.992968
C	43.889985	37.995252	47.528025
C	44.671083	35.872332	44.738278
H	45.550790	35.307201	45.038707
C	44.236410	35.665373	43.429785
C	44.793816	34.643788	42.565075
C	43.156871	35.811638	41.520977
N	43.233891	36.347389	42.793321
C	44.161195	34.775399	41.349621
C	42.169131	36.116616	40.598712
H	42.182325	35.566193	39.658338
C	41.109102	37.004255	40.803897
C	40.006202	37.184641	39.885710
N	40.938473	37.774404	41.926978
C	39.754264	38.440733	41.771390
C	39.191689	39.313635	42.703359
H	38.255418	39.793222	42.424865
Fe	42.141837	37.868319	43.563061
C	39.141589	38.086136	40.493469
C	37.869988	38.620053	40.026829
H	37.468865	39.448883	40.621073
C	37.136483	38.232767	38.966557
H	37.426408	37.408458	38.315336
H	36.202039	38.747284	38.730425
C	39.645269	41.313505	47.266420
H	40.079711	40.830324	48.150318
C	38.966788	42.457988	47.456303
H	38.540419	43.028983	46.630424
H	38.831187	42.865850	48.460768
C	39.852500	36.491865	38.570074
H	39.073148	35.711165	38.618167
H	39.562244	37.206706	37.784658
H	40.777945	35.990489	38.256205
C	37.760904	41.285999	44.629445
H	37.093808	40.692834	43.986880
H	37.233967	41.483341	45.574864
H	37.905778	42.255013	44.122149
C	44.034903	38.648027	48.866848
H	44.903339	38.241287	49.403237
H	44.180426	39.735769	48.767021

H	43.148364	38.506709	49.508305
C	44.462514	34.025348	40.091497
H	43.575227	33.842947	39.465895
H	45.186249	34.586934	39.476006
H	44.939397	33.059517	40.311939
C	45.733768	33.556043	42.979536
H	45.695282	33.423827	44.070939
H	45.329268	32.628086	42.552869
C	45.767327	36.204349	47.612137
H	46.582842	36.085178	46.882509
H	46.184394	36.784552	48.448737
C	47.199545	33.661381	42.547520
H	47.281284	34.086623	41.531316
H	47.615019	32.647654	42.500596
C	45.424799	34.804806	48.147331
H	45.075757	34.149859	47.329000
H	44.602705	34.841904	48.881364
C	46.635136	34.109465	48.818753
C	48.115125	34.473138	43.469701
O	47.592614	35.380739	44.165214
O	46.387737	33.196178	49.637428
O	49.337033	34.163975	43.457445
O	47.783856	34.504399	48.488342
O	43.178053	39.140537	43.021574
O	48.183607	39.110555	43.422093
O	48.444963	41.536042	41.958648
O	49.914897	40.064426	41.034319
O	48.894454	40.294770	43.840352
O	51.562809	38.770690	40.381338
C	47.793775	39.174912	42.027919
C	46.262994	39.416521	42.024718
C	48.190312	37.803118	41.453148
C	45.609136	39.081545	40.660524
C	48.527954	40.314517	41.300759
C	47.540432	37.543262	40.091957
C	45.879122	40.827892	42.504760
C	46.024915	37.689997	40.180114
C	49.721083	37.654260	41.473285
C	48.228021	41.441456	43.374108
C	46.712552	41.390715	43.659719
C	44.107147	39.264101	40.682299
C	50.465971	38.839724	40.884379
C	50.237893	36.329332	40.920745
C	48.951163	42.593038	44.044701

H	45.870323	38.692259	42.757171
H	47.792284	37.065287	42.170571
H	46.008344	39.811374	39.924815
H	48.060373	40.454868	40.313500
H	47.944348	38.237375	39.330745
H	47.802398	36.530250	39.753265
H	45.950415	41.531235	41.657435
H	44.826916	40.801538	42.820389
H	45.620232	36.929768	40.867660
H	45.569108	37.502029	39.195053
H	49.988882	37.701464	42.541333
H	46.559279	40.811463	44.582892
H	46.371401	42.418096	43.863193
H	51.322712	36.250439	41.065795
H	49.767154	35.493435	41.455087
H	50.044440	36.222997	39.844496
H	43.598554	39.046052	41.958149
H	43.523117	38.559008	40.076882
H	43.766169	40.299616	40.579559
H	48.745765	42.581956	45.124924
H	50.029756	42.486364	43.871850
H	48.622008	43.552520	43.625596
H	41.614771	34.140888	45.421526

QM atoms (linking H atom included): 121

XE12 Cluster0 Product M2

C	41.099594	34.558853	44.560082
H	40.311913	33.862879	44.236887
H	41.835076	34.662573	43.753056
S	40.293015	36.150819	44.904376
N	40.793241	39.155948	44.578750
C	39.650726	39.672260	44.019830
C	40.895677	39.683862	45.832545
C	39.003720	40.589072	44.945346
C	39.790087	40.605553	46.084415
C	41.887615	39.352584	46.757112
H	41.872917	39.876625	47.712680
C	42.865819	38.379510	46.589406
N	43.035486	37.626859	45.452506
C	44.100626	36.790832	45.700221
C	44.605368	36.987331	47.053506
C	43.845665	37.997180	47.598078
C	44.648132	35.902682	44.791043
H	45.530101	35.340703	45.092170

C	44.221964	35.700593	43.476777
C	44.788349	34.689058	42.603352
C	43.150794	35.863104	41.566229
N	43.222641	36.385706	42.843222
C	44.160522	34.832034	41.386737
C	42.156231	36.166851	40.649370
H	42.176731	35.627797	39.702247
C	41.081292	37.036979	40.861782
C	39.985844	37.222743	39.936073
N	40.893073	37.789938	41.993405
C	39.711314	38.455993	41.834320
C	39.147489	39.328239	42.769278
H	38.214179	39.811912	42.486525
Fe	42.085464	37.881132	43.648994
C	39.110880	38.112818	40.547129
C	37.844001	38.648967	40.070985
H	37.440599	39.478572	40.662354
C	37.120225	38.264298	39.002977
H	37.414364	37.439765	38.353928
H	36.189640	38.780838	38.756474
C	39.576744	41.303662	47.347089
H	39.988813	40.807644	48.234557
C	38.920519	42.461770	47.532136
H	38.518386	43.045174	46.702691
H	38.779437	42.868131	48.536403
C	39.846057	36.544333	38.611215
H	39.072410	35.757333	38.644857
H	39.555417	37.265708	37.832158
H	40.777440	36.054423	38.296936
C	37.718371	41.307519	44.690946
H	37.046772	40.723583	44.044598
H	37.187167	41.515669	45.631555
H	37.881752	42.273000	44.182456
C	43.996617	38.653500	48.934235
H	44.876496	38.259040	49.460570
H	44.128080	39.742628	48.830205
H	43.120287	38.504134	49.587329
C	44.456042	34.079797	40.128401
H	43.566885	33.905235	39.503199
H	45.185835	34.632384	39.511957
H	44.922661	33.109098	40.350545
C	45.718961	33.589829	43.010581
H	45.693884	33.463126	44.102740
H	45.296289	32.664928	42.593018

C	45.742672	36.225284	47.665276
H	46.562468	36.124124	46.937647
H	46.150942	36.801000	48.509681
C	47.180467	33.677013	42.560002
H	47.254870	34.098002	41.541329
H	47.587823	32.659665	42.510553
C	45.415374	34.814901	48.180966
H	45.067771	34.170711	47.353605
H	44.596329	34.833408	48.918924
C	46.633502	34.116127	48.834413
C	48.107063	34.487391	43.473427
O	47.591082	35.396432	44.170748
O	46.393905	33.197044	49.649034
O	49.328338	34.173838	43.453454
O	47.779075	34.512310	48.494924
O	43.133870	39.198502	43.051598
O	48.125070	39.069840	43.332355
O	48.471486	41.511109	41.913902
O	49.996337	40.049906	41.060449
O	48.822561	40.243580	43.799539
O	51.650210	38.755464	40.421643
C	47.823299	39.148472	41.918439
C	46.294053	39.387575	41.820878
C	48.254253	37.786302	41.349958
C	45.744847	39.091614	40.393449
C	48.595806	40.298304	41.248466
C	47.709073	37.549754	39.939268
C	45.878044	40.787725	42.311639
C	46.195629	37.713939	39.900962
C	49.780442	37.636844	41.465732
C	48.179580	41.396401	43.315268
C	46.650760	41.335741	43.516388
C	44.265336	39.253964	40.305788
C	50.545156	38.823985	40.905940
C	50.324583	36.312749	40.940451
C	48.865770	42.539648	44.038214
H	45.852830	38.642848	42.503555
H	47.805003	37.037820	42.025068
H	46.197313	39.853914	39.720513
H	48.186947	40.448808	40.237376
H	48.184964	38.241865	39.220126
H	47.980187	36.534427	39.617954
H	45.982755	41.505645	41.480445
H	44.814989	40.749300	42.587839

H	45.725730	36.938256	40.529817
H	45.826544	37.563343	38.873737
H	49.984021	37.687655	42.547634
H	46.448991	40.741930	44.420609
H	46.290350	42.357577	43.714106
H	51.398876	36.230230	41.149464
H	49.817276	35.477964	41.442404
H	50.194844	36.215192	39.854085
H	43.474250	38.949031	42.169196
H	43.643418	38.508042	39.805159
H	43.807171	40.208215	40.563959
H	48.614636	42.506907	45.108281
H	49.951872	42.442405	43.910779
H	48.551821	43.506503	43.624495
H	41.594358	34.123363	45.428198

QM atoms (linking H atom included): 121

XE12 Cluster0 Reactant M4

C	41.102081	34.563088	44.567986
H	40.296976	33.884654	44.249378
H	41.834333	34.648079	43.756377
S	40.326756	36.168440	44.906892
N	40.794420	39.129681	44.610624
C	39.650593	39.654440	44.058004
C	40.903552	39.661813	45.864041
C	39.007969	40.566352	44.987545
C	39.799501	40.579600	46.123321
C	41.898427	39.338373	46.784051
H	41.892931	39.869941	47.735316
C	42.869565	38.363790	46.611757
N	43.028475	37.595561	45.480318
C	44.097649	36.764064	45.735298
C	44.606626	36.974081	47.082391
C	43.850213	37.989412	47.619633
C	44.647719	35.872658	44.834906
H	45.535868	35.317236	45.129760
C	44.211206	35.677314	43.527556
C	44.775882	34.676064	42.645346
C	43.145352	35.866035	41.618525
N	43.206037	36.368337	42.904772
C	44.151137	34.835330	41.429631
C	42.172796	36.190741	40.690235
H	42.203752	35.667334	39.735707
C	41.107611	37.066213	40.902352

C	40.015902	37.249562	39.971403
N	40.913026	37.810128	42.038923
C	39.724826	38.466460	41.874193
C	39.147515	39.325649	42.806483
H	38.214564	39.809168	42.524411
Fe	42.137226	37.912880	43.672372
C	39.131146	38.126319	40.584075
C	37.860773	38.655471	40.106864
H	37.462745	39.498226	40.683129
C	37.130014	38.247601	39.052589
H	37.417879	37.406672	38.421740
H	36.199017	38.760498	38.799838
C	39.585931	41.262584	47.394596
H	40.007165	40.759263	48.273293
C	38.916272	42.409629	47.599553
H	38.499461	43.000615	46.782816
H	38.777804	42.797893	48.611528
C	39.891037	36.582197	38.639331
H	39.154352	35.760242	38.669155
H	39.561132	37.300720	37.873869
H	40.840485	36.140104	38.308699
C	37.720716	41.284726	44.742406
H	37.055076	40.714250	44.078551
H	37.182990	41.467988	45.684699
H	37.882660	42.263770	44.259924
C	44.000843	38.654144	48.951356
H	44.887697	38.271744	49.474472
H	44.119837	39.744089	48.842481
H	43.129676	38.496190	49.609364
C	44.448617	34.101844	40.160959
H	43.559914	33.930623	39.534220
H	45.172241	34.670673	39.552456
H	44.921994	33.131291	40.368350
C	45.709717	33.575476	43.040569
H	45.692320	33.443100	44.131846
H	45.285511	32.652732	42.620354
C	45.744656	36.216811	47.696130
H	46.567322	36.121125	46.971389
H	46.145756	36.792000	48.544202
C	47.167598	33.672709	42.581174
H	47.234279	34.105665	41.567232
H	47.579600	32.658081	42.517316
C	45.418504	34.804786	48.206341
H	45.072025	34.162443	47.377229

H	44.599503	34.820150	48.944343
C	46.638194	34.107302	48.856642
C	48.093231	34.478652	43.500465
O	47.569904	35.367351	44.218015
O	46.400783	33.189737	49.673578
O	49.317849	34.181526	43.465131
O	47.781968	34.503515	48.512135
O	43.111416	39.102186	43.199438
O	48.072414	39.043514	43.315236
O	48.405897	41.496417	41.914842
O	49.957798	40.059063	41.065166
O	48.757707	40.219610	43.794671
O	51.631145	38.783502	40.436897
C	47.783126	39.128711	41.896717
C	46.253165	39.350883	41.774117
C	48.238041	37.776092	41.326031
C	45.726036	39.071222	40.346724
C	48.550572	40.289996	41.242233
C	47.715919	37.546694	39.906044
C	45.816115	40.738134	42.284737
C	46.201344	37.703299	39.850205
C	49.763868	37.643585	41.462262
C	48.103859	41.367349	43.312762
C	46.573555	41.280529	43.503168
C	44.203156	39.172789	40.270819
C	50.520899	38.840354	40.912284
C	50.329849	36.326104	40.944801
C	48.767954	42.517890	44.044815
H	45.812031	38.593680	42.444860
H	47.789095	37.016553	41.988779
H	46.155996	39.836083	39.670779
H	48.151313	40.441955	40.228058
H	48.195955	38.250808	39.200941
H	47.999548	36.536535	39.578721
H	45.915495	41.470251	41.465119
H	44.750043	40.681358	42.545289
H	45.730487	36.917216	40.466463
H	45.847726	37.553881	38.817064
H	49.953751	37.696933	42.546490
H	46.377478	40.667733	44.395840
H	46.198587	42.293827	43.718295
H	51.400215	36.249548	41.175233
H	49.818319	35.484918	41.431819
H	50.224348	36.230636	39.855748

H	43.730667	38.512346	41.006649
H	43.840939	38.894897	39.267323
H	43.855732	40.190470	40.491569
H	48.518407	42.473235	45.114833
H	49.856207	42.447564	43.915332
H	48.430653	43.478853	43.635845
H	41.591509	34.120744	45.435661

QM atoms (linking H atom included): 121

XE12 Cluster0 TS M4

C	41.121813	34.591548	44.573860
H	40.306825	33.928944	44.246403
H	41.855890	34.675553	43.763322
S	40.380254	36.210437	44.931281
N	40.873333	39.181645	44.505299
C	39.709411	39.676158	43.964992
C	40.980815	39.716470	45.757498
C	39.061209	40.584027	44.897172
C	39.863481	40.616766	46.024089
C	41.975775	39.397424	46.679464
H	41.966882	39.927964	47.631223
C	42.936805	38.410820	46.515220
N	43.096537	37.648463	45.380847
C	44.136682	36.781981	45.650809
C	44.635385	36.978835	47.004438
C	43.894372	38.009594	47.534745
C	44.660351	35.864479	44.761959
H	45.529475	35.288101	45.071426
C	44.225701	35.658145	43.452760
C	44.784927	34.640631	42.585722
C	43.153768	35.818187	41.544014
N	43.226547	36.344332	42.819310
C	44.158800	34.782676	41.367993
C	42.166841	36.125969	40.622041
H	42.184473	35.584173	39.676886
C	41.102469	37.006939	40.832953
C	40.005990	37.194446	39.908825
N	40.921159	37.763051	41.963461
C	39.742641	38.433293	41.802847
C	39.185213	39.314390	42.731315
H	38.245208	39.789413	42.457922
Fe	42.161216	37.897570	43.581294
C	39.135638	38.088347	40.520213
C	37.867328	38.627294	40.050765

H	37.473690	39.464511	40.637932
C	37.130424	38.234417	38.995083
H	37.413711	37.400413	38.353324
H	36.200075	38.753441	38.753127
C	39.644540	41.288372	47.300335
H	40.075944	40.784135	48.173771
C	38.960391	42.424715	47.516236
H	38.534585	43.016015	46.704285
H	38.819763	42.803939	48.531347
C	39.864592	36.518619	38.583108
H	39.106321	35.716973	38.620434
H	39.553556	37.238876	37.811033
H	40.802005	36.047552	38.258147
C	37.754516	41.271461	44.670057
H	37.089590	40.680465	44.023726
H	37.232270	41.449236	45.622077
H	37.884847	42.249947	44.177224
C	44.027256	38.654097	48.878099
H	44.892551	38.248044	49.419678
H	44.166688	39.743145	48.787542
H	43.135212	38.503197	49.509574
C	44.464457	34.042255	40.105628
H	43.578987	33.862590	39.476871
H	45.188058	34.610949	39.496458
H	44.943166	33.076007	40.320303
C	45.724491	33.552299	42.998289
H	45.688854	33.419937	44.089572
H	45.319980	32.624058	42.572219
C	45.757505	36.206930	47.631586
H	46.578371	36.088711	46.908104
H	46.168008	36.788353	48.470895
C	47.188643	33.663746	42.562519
H	47.265669	34.097182	41.549391
H	47.607356	32.651895	42.505885
C	45.417350	34.806589	48.165673
H	45.066423	34.152390	47.347744
H	44.598165	34.840964	48.903142
C	46.631307	34.110945	48.831732
C	48.103062	34.473142	43.488862
O	47.576568	35.366838	44.198277
O	46.387030	33.196275	49.649931
O	49.327803	34.175141	43.465177
O	47.778894	34.506423	48.498438
O	43.175729	39.138563	42.944562

O	48.151559	39.093742	43.390460
O	48.437499	41.530477	41.951453
O	49.926977	40.067812	41.040405
O	48.852982	40.275178	43.831773
O	51.574900	38.775092	40.382679
C	47.789543	39.168987	41.989274
C	46.258670	39.407453	41.957642
C	48.195531	37.803921	41.408730
C	45.624026	39.080558	40.583018
C	48.534275	40.315227	41.284250
C	47.576260	37.560862	40.029599
C	45.863211	40.815185	42.438584
C	46.058600	37.701055	40.085228
C	49.725926	37.654729	41.459908
C	48.191899	41.423177	43.361855
C	46.670919	41.363220	43.617736
C	44.117593	39.245112	40.599283
C	50.476541	38.842793	40.882535
C	50.251572	36.330349	40.915404
C	48.896527	42.572469	44.055437
H	45.854827	38.678951	42.679629
H	47.781139	37.057014	42.107390
H	46.012186	39.827671	39.857524
H	48.084174	40.462443	40.289976
H	47.994978	38.265522	39.286618
H	47.846479	36.552536	39.684117
H	45.954435	41.524570	41.598230
H	44.804482	40.785775	42.730528
H	45.640364	36.926448	40.748891
H	45.627767	37.531254	39.085364
H	49.972283	37.702603	42.533210
H	46.502427	40.764275	44.525558
H	46.319269	42.384401	43.833745
H	51.332106	36.245760	41.087781
H	49.762462	35.494452	41.433511
H	50.085169	36.230879	39.834138
H	43.591495	39.016415	41.878456
H	43.545590	38.554008	39.965289
H	43.774752	40.280883	40.512697
H	48.674725	42.548019	45.132211
H	49.978613	42.477069	43.898238
H	48.566187	43.533747	43.641425
H	41.605872	34.136926	45.438193

QM atoms (linking H atom included): 121

XE12 Cluster0 Product M4

C	41.102383	34.555907	44.562447
H	40.312732	33.861688	44.239804
H	41.837497	34.660633	43.755329
S	40.302447	36.149416	44.912263
N	40.791218	39.156149	44.575311
C	39.650246	39.674649	44.014000
C	40.891454	39.682507	45.829693
C	39.004394	40.594426	44.937715
C	39.788910	40.609504	46.077786
C	41.879326	39.347105	46.757603
H	41.864947	39.870697	47.713783
C	42.855999	38.372920	46.589567
N	43.026612	37.620058	45.451560
C	44.094118	36.784948	45.699122
C	44.599067	36.983331	47.051428
C	43.837700	37.991963	47.596583
C	44.645148	35.899016	44.790254
H	45.527557	35.338205	45.092134
C	44.221142	35.697225	43.475255
C	44.788675	34.686485	42.601620
C	43.153147	35.863541	41.563988
N	43.222114	36.382354	42.841847
C	44.162334	34.831476	41.384253
C	42.160742	36.170485	40.645814
H	42.184107	35.635420	39.697000
C	41.083099	37.037194	40.859656
C	39.988923	37.222096	39.932563
N	40.891335	37.788241	41.991861
C	39.711057	38.455319	41.830434
C	39.147005	39.329267	42.764470
H	38.214302	39.813411	42.480972
Fe	42.084045	37.883982	43.648934
C	39.112613	38.112312	40.542529
C	37.845774	38.647950	40.065740
H	37.437272	39.471020	40.662672
C	37.126489	38.269116	38.992600
H	37.426034	37.451980	38.336790
H	36.193837	38.783150	38.748984
C	39.577759	41.313102	47.337660
H	39.984683	40.818180	48.227882
C	38.929437	42.476763	47.515057
H	38.534273	43.058400	46.681127

H	38.788547	42.889647	48.516492
C	39.850129	36.543350	38.607671
H	39.069181	35.763524	38.638107
H	39.570117	37.265640	37.825529
H	40.778402	36.044057	38.298843
C	37.722533	41.317245	44.679605
H	37.049258	40.733389	44.035181
H	37.191841	41.532180	45.618902
H	37.890505	42.279418	44.166508
C	43.992083	38.650762	48.930987
H	44.871289	38.254232	49.456893
H	44.127713	39.739099	48.823530
H	43.115569	38.506152	49.584856
C	44.458897	34.080941	40.124899
H	43.570549	33.908938	39.497746
H	45.190875	34.633013	39.510390
H	44.923019	33.108760	40.345558
C	45.719751	33.587152	43.008076
H	45.692822	33.457798	44.099986
H	45.299097	32.662358	42.588326
C	45.738595	36.224426	47.662967
H	46.558148	36.124664	46.934810
H	46.146408	36.800686	48.507213
C	47.181818	33.676427	42.559870
H	47.256829	34.099021	41.541947
H	47.590454	32.659675	42.509555
C	45.413995	34.813087	48.178771
H	45.068398	34.167856	47.351346
H	44.594275	34.829791	48.916124
C	46.633191	34.116468	48.833278
C	48.106995	34.486478	43.474731
O	47.590461	35.395664	44.171456
O	46.394588	33.196461	49.647149
O	49.328350	34.172856	43.456130
O	47.778269	34.514737	48.494698
O	43.126072	39.197912	43.042905
O	48.130314	39.073920	43.342301
O	48.476880	41.512973	41.920712
O	49.999048	40.049248	41.067699
O	48.831216	40.246198	43.806642
O	51.648844	38.752129	40.424598
C	47.825056	39.151963	41.928434
C	46.297519	39.396315	41.832262
C	48.252038	37.787196	41.363640

C	45.746831	39.103176	40.406071
C	48.599047	40.299582	41.256483
C	47.700518	37.544982	39.956194
C	45.882444	40.794007	42.331843
C	46.187523	37.720519	39.918524
C	49.778654	37.636502	41.471304
C	48.189868	41.400467	43.323373
C	46.662530	41.340402	43.532788
C	44.268960	39.276954	40.316644
C	50.544498	38.822517	40.910280
C	50.319486	36.311885	40.944175
C	48.880262	42.543139	44.041969
H	45.855829	38.648826	42.511242
H	47.808221	37.041765	42.045604
H	46.206506	39.857950	39.730014
H	48.190966	40.449595	40.244867
H	48.180049	38.229315	39.231344
H	47.962209	36.525647	39.639361
H	45.977809	41.516787	41.503497
H	44.821737	40.751490	42.616010
H	45.711539	36.950426	40.548910
H	45.817600	37.569083	38.891394
H	49.989012	37.687253	42.552006
H	46.466295	40.745011	44.437170
H	46.305039	42.362294	43.735672
H	51.394885	36.227946	41.146412
H	49.815727	35.476861	41.449246
H	50.183773	36.212254	39.858815
H	43.481626	38.941370	42.167713
H	43.650229	38.556667	39.776272
H	43.816011	40.231778	40.582909
H	48.632783	42.512150	45.112859
H	49.965773	42.445006	43.910905
H	48.565114	43.509232	43.627398
H	41.597214	34.119402	45.430014

QM atoms (linking H atom included): 121

XE12 Cluster1 Reactant

C	34.529582	40.283718	34.548992
H	35.073820	40.123752	33.605690
H	34.533069	39.354396	35.130673
S	35.400049	41.611074	35.439129
N	36.433984	42.573216	38.241253
C	37.770407	42.896645	38.234442

C	35.763183	43.719033	38.559388
C	37.959990	44.299804	38.544278
C	36.696713	44.824289	38.763125
C	34.379364	43.819490	38.673522
H	33.965906	44.785615	38.958650
C	33.472082	42.795287	38.462701
N	33.782374	41.509124	38.073328
C	32.580865	40.832849	38.009148
C	31.475780	41.720779	38.348646
C	32.039516	42.939900	38.637847
C	32.441339	39.485459	37.714031
H	31.429465	39.080778	37.694255
C	33.485443	38.600363	37.449503
C	33.300164	37.203734	37.087995
C	35.495197	37.773879	37.114796
N	34.819206	38.926516	37.459342
C	34.559888	36.680269	36.909388
C	36.863386	37.688346	36.915781
H	37.248170	36.734010	36.558692
C	37.789296	38.712210	37.121111
C	39.212218	38.580387	36.893869
N	37.482813	39.977360	37.558149
C	38.662115	40.666001	37.614834
C	38.798170	42.008884	37.953580
H	39.807737	42.412156	37.986364
Fe	35.645802	40.678208	38.063018
C	39.770624	39.810136	37.209774
C	41.152972	40.255330	37.156433
H	41.300416	41.320065	37.361677
C	42.267717	39.536510	36.924438
H	42.255254	38.463211	36.736870
H	43.241257	40.031257	36.939607
C	36.291887	46.165518	39.162352
H	35.245290	46.256344	39.471292
C	37.039114	47.283845	39.218881
H	38.084371	47.325613	38.913218
H	36.599913	48.219446	39.575551
C	39.910134	37.359497	36.394839
H	40.513047	37.602318	35.504661
H	40.599486	36.962938	37.159444
H	39.213204	36.563169	36.106995
C	39.273509	45.009006	38.597689
H	40.121626	44.312408	38.646344
H	39.416487	45.652384	37.711146

H	39.332115	45.673520	39.473393
C	31.363550	44.178646	39.134335
H	30.289561	44.005839	39.288562
H	31.796992	44.496093	40.096612
H	31.472698	45.028461	38.440402
C	34.893266	35.249673	36.630010
H	35.842513	35.120476	36.090981
H	34.964123	34.671447	37.567170
H	34.091526	34.768402	36.051405
C	32.002958	36.465822	36.964137
H	31.169753	37.154897	36.771825
H	32.042670	35.800700	36.087601
C	30.025887	41.357457	38.376474
H	29.884653	40.308557	38.669411
H	29.521683	41.951004	39.155207
C	31.687399	35.615363	38.197719
H	31.566063	36.267346	39.080120
H	32.534383	34.951092	38.436091
C	29.281820	41.582741	37.051094
H	29.754986	40.989056	36.246832
H	29.329963	42.637307	36.735749
C	27.799411	41.158293	37.145692
C	30.431162	34.724986	38.090678
O	30.167083	34.017432	39.098945
O	26.963550	41.785474	36.457869
O	29.756801	34.774906	37.039518
O	27.542776	40.185121	37.906205
O	35.694458	40.335521	39.632869
O	32.467526	37.702234	41.862053
O	33.744167	37.917544	44.387035
O	32.757887	35.873648	44.323652
O	31.974424	38.413995	43.021406
O	31.306081	34.235994	44.386875
C	33.602614	36.861763	42.190434
C	34.837582	37.572126	41.574596
C	33.298947	35.496334	41.556130
C	36.062962	36.645989	41.445439
C	33.752231	36.709816	43.707242
C	34.542954	34.608516	41.552637
C	35.202315	38.872790	42.316303
C	35.671810	35.311159	40.810006
C	32.046433	34.862838	42.188308
C	33.057852	38.981084	43.727916
C	34.026872	39.725287	42.790080

C	37.197459	37.325491	40.672649
C	32.012369	34.940782	43.702247
C	31.762460	33.435589	41.715218
C	32.443525	39.852774	44.802258
H	34.511944	37.844883	40.555362
H	33.054794	35.699282	40.504546
H	36.418443	36.425464	42.469274
H	34.717987	36.231491	43.922443
H	34.859144	34.359661	42.582584
H	34.302393	33.660389	41.056852
H	35.829165	38.624362	43.189013
H	35.806124	39.489662	41.639496
H	35.365394	35.480276	39.762458
H	36.544995	34.648617	40.779520
H	31.195118	35.495231	41.881993
H	33.456126	40.121647	41.937483
H	34.427327	40.587604	43.344613
H	30.797393	33.096362	42.110441
H	31.689734	33.415806	40.622018
H	32.535619	32.733247	42.059946
H	38.063354	36.653252	40.563696
H	37.547739	38.237441	41.173867
H	36.859494	37.621417	39.668911
H	33.236106	40.150861	45.500917
H	31.998903	40.755537	44.362978
H	31.680506	39.289298	45.353507
H	33.498366	40.545786	34.312388

QM atoms (linking H atom included): 121

XE12 Cluster1 TS

C	34.564743	40.221362	34.495119
H	35.083747	40.070568	33.536534
H	34.580147	39.285164	35.065950
S	35.458667	41.541977	35.375707
N	36.458373	42.461209	38.221356
C	37.795463	42.767308	38.244904
C	35.791018	43.602767	38.554803
C	37.994476	44.162552	38.593824
C	36.732775	44.694992	38.794106
C	34.405376	43.708582	38.665368
H	33.998308	44.680119	38.944240
C	33.489931	42.686190	38.462654
N	33.797175	41.397351	38.089726
C	32.599522	40.724323	38.012022

C	31.490252	41.616374	38.338757
C	32.054069	42.835057	38.627607
C	32.466158	39.379125	37.693067
H	31.453571	38.975670	37.658894
C	33.507364	38.492719	37.407725
C	33.311883	37.100950	37.033320
C	35.513094	37.653422	37.051039
N	34.845303	38.806571	37.412848
C	34.567550	36.568491	36.847279
C	36.882590	37.567635	36.844145
H	37.262463	36.617343	36.470518
C	37.815383	38.585520	37.061111
C	39.241195	38.455901	36.850143
N	37.507057	39.845772	37.510603
C	38.684051	40.535803	37.588374
C	38.818795	41.874270	37.956109
H	39.830411	42.272710	38.009542
Fe	35.667249	40.564131	37.979726
C	39.795631	39.683484	37.183454
C	41.176393	40.133119	37.138085
H	41.316888	41.203170	37.322355
C	42.296801	39.417163	36.925307
H	42.290625	38.341035	36.753132
H	43.266031	39.920179	36.941045
C	36.341414	46.029801	39.230997
H	35.362999	46.088730	39.721257
C	37.043501	47.171615	39.121793
H	38.007797	47.231196	38.614425
H	36.648741	48.104736	39.532425
C	39.947716	37.243050	36.343984
H	40.535426	37.495466	35.446331
H	40.651176	36.854482	37.099697
H	39.255612	36.439854	36.065622
C	39.319775	44.839115	38.728496
H	40.111718	44.133448	39.020856
H	39.634221	45.317717	37.783677
H	39.274610	45.640453	39.480982
C	31.373825	44.076645	39.109608
H	30.289301	43.922620	39.195940
H	31.755670	44.368941	40.101913
H	31.540575	44.936746	38.440283
C	34.882849	35.130713	36.583686
H	35.831540	34.980198	36.049727
H	34.941188	34.566155	37.530262

H	34.074962	34.654152	36.009813
C	32.008305	36.373214	36.913296
H	31.183783	37.068210	36.703974
H	32.048953	35.694672	36.047944
C	30.038759	41.257956	38.358503
H	29.895750	40.207500	38.643829
H	29.536050	41.847691	39.141161
C	31.672108	35.546105	38.156452
H	31.550284	36.213224	39.026345
H	32.507480	34.873791	38.414476
C	29.293464	41.494337	37.034267
H	29.758737	40.896849	36.228207
H	29.350325	42.548824	36.720232
C	27.807467	41.082955	37.132874
C	30.397260	34.681706	38.062429
O	30.128830	33.988139	39.078216
O	26.970737	41.725720	36.460401
O	29.714432	34.740089	37.017218
O	27.546268	40.104157	37.885380
O	35.763658	40.213923	39.667538
O	32.332933	37.939124	42.102366
O	33.790030	38.033269	44.525828
O	32.953726	35.933463	44.321137
O	31.863594	38.471541	43.363722
O	31.496506	34.304100	44.314474
C	33.558193	37.182592	42.255061
C	34.659135	38.074798	41.636564
C	33.319846	35.875855	41.485601
C	35.951399	37.297653	41.299066
C	33.837444	36.895980	43.732429
C	34.630838	35.120827	41.249225
C	34.963641	39.325614	42.479409
C	35.631664	36.016903	40.523815
C	32.181257	35.061116	42.138092
C	32.944553	39.076820	44.042779
C	33.754613	40.007556	43.118983
C	36.960998	38.175045	40.583472
C	32.185956	35.050937	43.657703
C	32.025854	33.634116	41.601586
C	32.336413	39.770984	45.243669
H	34.227403	38.411304	40.679594
H	32.957882	36.184638	40.494401
H	36.404114	36.993695	42.264355
H	34.850468	36.479464	43.831888

H	35.059311	34.763996	42.205013
H	34.427554	34.226289	40.644018
H	35.676778	39.062940	43.278391
H	35.455212	40.054509	41.823195
H	35.234094	36.284488	39.529942
H	36.566693	35.466904	40.352452
H	31.247457	35.602056	41.907094
H	33.077248	40.420366	42.356477
H	34.115961	40.851284	43.725632
H	31.151619	33.160317	42.065810
H	31.843417	33.650195	40.520607
H	32.908390	33.017267	41.826801
H	37.506180	37.708204	39.753616
H	37.606455	38.769941	41.238423
H	36.306912	39.236999	39.962199
H	33.148450	40.165195	45.868751
H	31.691271	40.598946	44.918163
H	31.754955	39.053732	45.835048
H	33.528895	40.487961	34.285327

QM atoms (linking H atom included): 121

XE12 Cluster1 intermediate

C	34.654094	40.172387	34.446331
H	35.127404	39.983727	33.472773
H	34.663721	39.242267	35.029162
S	35.645960	41.446131	35.288812
N	36.389518	42.572741	38.150725
C	37.730382	42.869483	38.184239
C	35.718644	43.714009	38.486403
C	37.926730	44.261920	38.538459
C	36.664801	44.798995	38.732701
C	34.336596	43.819414	38.606343
H	33.927182	44.790911	38.878625
C	33.428356	42.782485	38.438868
N	33.726027	41.490623	38.078588
C	32.529893	40.813415	38.009121
C	31.429144	41.706814	38.344592
C	31.996363	42.927901	38.624249
C	32.380226	39.470753	37.685055
H	31.367418	39.069180	37.664042
C	33.419443	38.591576	37.393211
C	33.241554	37.193275	37.046056
C	35.442149	37.761481	37.055303
N	34.758679	38.914545	37.384722

C	34.503901	36.668835	36.870291
C	36.814310	37.661547	36.866020
H	37.192793	36.697906	36.527339
C	37.746600	38.680641	37.061300
C	39.172515	38.545478	36.856779
N	37.448744	39.951406	37.491892
C	38.626601	40.642748	37.559852
C	38.762472	41.981242	37.914954
H	39.772404	42.380241	37.979179
Fe	35.575718	40.684176	37.953632
C	39.732315	39.776200	37.172617
C	41.116797	40.216390	37.130663
H	41.262463	41.284688	37.318117
C	42.231166	39.489981	36.920933
H	42.214681	38.414054	36.748919
H	43.206804	39.980860	36.938812
C	36.280470	46.132130	39.178411
H	35.283879	46.200914	39.627877
C	37.008082	47.262243	39.124066
H	37.993780	47.316653	38.660348
H	36.612052	48.193274	39.537462
C	39.873136	37.316536	36.382384
H	40.490069	37.545494	35.498288
H	40.549310	36.925639	37.161870
H	39.175542	36.521145	36.094460
C	39.251730	44.936346	38.682847
H	40.050429	44.223322	38.934029
H	39.549308	45.454999	37.754042
H	39.216364	45.704186	39.469990
C	31.320603	44.168607	39.114050
H	30.238826	44.009852	39.220375
H	31.719268	44.461585	40.098851
H	31.473179	45.028581	38.441917
C	34.836221	35.233568	36.611932
H	35.777492	35.095396	36.060783
H	34.925039	34.674177	37.559113
H	34.026021	34.741856	36.054452
C	31.947608	36.448396	36.931644
H	31.111923	37.134731	36.740737
H	31.988897	35.783745	36.055535
C	29.978631	41.349661	38.365378
H	29.832645	40.302167	38.659879
H	29.471348	41.949262	39.137138
C	31.636870	35.597858	38.166256

H	31.518358	36.250109	39.048199
H	32.483125	34.931826	38.404463
C	29.244174	41.569739	37.032960
H	29.726323	40.974867	36.234825
H	29.288909	42.622769	36.712943
C	27.765969	41.134837	37.122278
C	30.377074	34.711242	38.063766
O	30.114655	34.008147	39.074741
O	26.923727	41.760096	36.440495
O	29.701103	34.758623	37.013922
O	27.516065	40.155375	37.877776
O	35.716715	40.272157	39.729360
O	32.436618	37.835249	41.978675
O	33.707979	37.957272	44.509605
O	32.789476	35.891505	44.348192
O	31.931189	38.490032	43.166430
O	31.339036	34.254525	44.344181
C	33.587793	37.003947	42.262562
C	34.797047	37.777901	41.673631
C	33.305657	35.667584	41.559398
C	36.049100	36.879634	41.453195
C	33.750919	36.783991	43.770768
C	34.568471	34.809567	41.489452
C	35.153826	39.027311	42.496957
C	35.668866	35.566931	40.760698
C	32.073011	34.974658	42.171154
C	33.005308	39.038581	43.900822
C	33.965670	39.842927	43.004040
C	37.123188	37.607084	40.710531
C	32.040244	34.989308	43.687593
C	31.820918	33.557613	41.647902
C	32.371463	39.853483	45.008884
H	34.448244	38.114179	40.683416
H	33.044597	35.924946	40.522343
H	36.431538	36.630906	42.461668
H	34.733138	36.325095	43.958478
H	34.910800	34.514946	42.498679
H	34.343664	33.880915	40.950262
H	35.772149	38.733034	43.361058
H	35.758750	39.692630	41.869342
H	35.343747	35.783276	39.728019
H	36.558747	34.931951	40.685651
H	31.204391	35.597965	41.897107
H	33.393762	40.271756	42.167825

H	34.354305	40.682962	43.599328
H	30.868768	33.178521	42.039909
H	31.734548	33.567088	40.555344
H	32.616184	32.865494	41.962621
H	37.236636	37.485966	39.630605
H	37.796767	38.295097	41.223344
H	36.308485	39.508096	39.861007
H	33.161562	40.158031	45.707959
H	31.887688	40.749159	44.596063
H	31.634882	39.248332	45.551223
H	33.616769	40.463556	34.281271

QM atoms (linking H atom included): 121

XE12 Cluster1 TS2

C	34.641957	40.177715	34.479769
H	35.125658	39.977262	33.514224
H	34.644567	39.255544	35.075233
S	35.616714	41.462134	35.331008
N	36.442680	42.467977	38.219073
C	37.781077	42.778739	38.203210
C	35.768973	43.606870	38.560070
C	37.974330	44.172145	38.555236
C	36.712669	44.699473	38.779535
C	34.386103	43.707257	38.687075
H	33.976833	44.678728	38.961158
C	33.473092	42.675906	38.506060
N	33.766514	41.381991	38.147408
C	32.568264	40.716398	38.053860
C	31.466430	41.616835	38.375477
C	32.037828	42.833300	38.664216
C	32.418438	39.376658	37.714972
H	31.404537	38.978176	37.679794
C	33.458380	38.500438	37.413577
C	33.276509	37.109035	37.039706
C	35.477864	37.674888	37.041482
N	34.798204	38.820945	37.408738
C	34.536530	36.585086	36.849400
C	36.845840	37.586042	36.815395
H	37.219647	36.627123	36.459186
C	37.783358	38.604882	37.000578
C	39.210055	38.467225	36.796799
N	37.490340	39.873748	37.431486
C	38.666930	40.562665	37.508236
C	38.807139	41.895668	37.888814

H	39.817334	42.296510	37.935941
Fe	35.623570	40.579542	37.941443
C	39.771829	39.694928	37.119334
C	41.156953	40.131473	37.093891
H	41.302310	41.201581	37.272799
C	42.274464	39.404372	36.906066
H	42.262128	38.327054	36.741568
H	43.247006	39.900189	36.934938
C	36.327149	46.034614	39.221310
H	35.349094	46.096567	39.711433
C	37.032951	47.174471	39.112553
H	37.997686	47.233548	38.606282
H	36.639868	48.108325	39.522990
C	39.913614	37.242200	36.318514
H	40.513598	37.476820	35.424346
H	40.605208	36.860747	37.089109
H	39.218340	36.440313	36.045302
C	39.297846	44.854874	38.671751
H	40.100220	44.148500	38.931011
H	39.586575	45.353796	37.729478
H	39.267233	45.640130	39.441719
C	31.358096	44.083648	39.124955
H	30.270096	43.940462	39.182988
H	31.716558	44.376525	40.125404
H	31.550747	44.938784	38.456421
C	34.856880	35.149290	36.581392
H	35.800909	35.005333	36.037878
H	34.929285	34.583304	37.526165
H	34.045755	34.669233	36.015102
C	31.978988	36.371761	36.919172
H	31.150269	37.059611	36.703609
H	32.028397	35.688979	36.057632
C	30.012264	41.269181	38.381012
H	29.860633	40.216855	38.653390
H	29.507180	41.853912	39.165723
C	31.642630	35.547956	38.164261
H	31.515528	36.218691	39.030824
H	32.478724	34.878667	38.427683
C	29.278528	41.523312	37.053992
H	29.753036	40.938996	36.243890
H	29.335397	42.582271	36.755273
C	27.793867	41.105539	37.134243
C	30.370602	34.679687	38.066736
O	30.102403	33.984129	39.081319

O	26.960437	41.746124	36.455847
O	29.689109	34.738018	37.020889
O	27.530174	40.121996	37.880196
O	35.920433	40.126269	39.737218
O	32.310175	37.926608	42.074281
O	33.728731	38.030925	44.522484
O	32.883933	35.935217	44.329203
O	31.831353	38.483218	43.322307
O	31.442046	34.290821	44.329871
C	33.522946	37.155649	42.253782
C	34.641334	38.030287	41.633558
C	33.281667	35.836869	41.506264
C	35.932376	37.228059	41.320445
C	33.780125	36.886527	43.740002
C	34.588341	35.062033	41.316558
C	34.955276	39.274998	42.478571
C	35.606222	35.926630	40.578730
C	32.124131	35.045579	42.150572
C	32.909445	39.081353	44.010931
C	33.749164	39.986609	43.089819
C	36.939637	38.046978	40.582576
C	32.125381	35.040114	43.670105
C	31.953275	33.618887	41.617905
C	32.297645	39.804587	45.191798
H	34.228531	38.366486	40.668973
H	32.946092	36.126900	40.500115
H	36.369993	36.955248	42.302009
H	34.789551	36.465595	43.857798
H	34.997880	34.730220	42.289078
H	34.385194	34.152485	40.735138
H	35.645510	39.001038	43.293952
H	35.473942	39.982545	41.822615
H	35.220741	36.172070	39.574520
H	36.535777	35.361316	40.432715
H	31.201593	35.602430	41.912210
H	33.091002	40.403659	42.312885
H	34.117343	40.829803	43.693478
H	31.061593	33.162915	42.066443
H	31.793394	33.634299	40.533301
H	32.820621	32.988827	41.865089
H	37.151059	37.854958	39.531607
H	37.615713	38.700650	41.131880
H	36.742403	40.554384	40.024464
H	33.108752	40.158362	45.841799

H	31.705201	40.663750	44.848616
H	31.663123	39.120401	45.766417
H	33.605554	40.464382	34.301559

QM atoms (linking H atom included): 121

XE12 Cluster1 Product

C	34.678453	40.139540	34.386460
H	35.174143	40.058377	33.410850
H	34.680582	39.156665	34.868259
S	35.634883	41.351735	35.378868
N	36.425770	42.459320	38.006795
C	37.764283	42.769563	38.055702
C	35.758282	43.598448	38.357603
C	37.960790	44.152727	38.447943
C	36.698830	44.683920	38.636925
C	34.378676	43.700033	38.488575
H	33.969150	44.666043	38.779828
C	33.474072	42.662696	38.316425
N	33.775203	41.379479	37.924224
C	32.569185	40.711399	37.861301
C	31.475140	41.591568	38.253567
C	32.046841	42.805511	38.543993
C	32.400574	39.379509	37.505448
H	31.383555	38.988328	37.491038
C	33.431135	38.501731	37.182322
C	33.256046	37.099018	36.861096
C	35.452168	37.678723	36.849622
N	34.770023	38.836874	37.177052
C	34.519529	36.577268	36.689152
C	36.827932	37.586768	36.695980
H	37.219210	36.619873	36.383103
C	37.756289	38.606239	36.909979
C	39.188434	38.441188	36.772951
N	37.456665	39.889898	37.309518
C	38.647704	40.553120	37.417662
C	38.795694	41.885453	37.785405
H	39.807298	42.275535	37.872495
Fe	35.605410	40.686221	37.470908
C	39.755320	39.666557	37.091537
C	41.145173	40.088888	37.108594
H	41.295529	41.153839	37.311978
C	42.261721	39.358658	36.925887
H	42.245300	38.286317	36.733363
H	43.236757	39.847256	36.982566

C	36.310305	46.007578	39.108473
H	35.321397	46.063299	39.576507
C	37.028283	47.143839	39.051323
H	38.004108	47.208456	38.567808
H	36.635183	48.068503	39.482142
C	39.895656	37.195369	36.356972
H	40.488361	37.383417	35.446920
H	40.595127	36.862450	37.141995
H	39.205928	36.374817	36.130037
C	39.286067	44.813834	38.644204
H	40.065031	44.090502	38.927124
H	39.628102	45.329524	37.729018
H	39.226381	45.582014	39.429860
C	31.378066	44.030986	39.083590
H	30.288924	43.893069	39.137145
H	31.740574	44.259430	40.100056
H	31.574898	44.925127	38.469607
C	34.852483	35.131184	36.499568
H	35.806546	34.965109	35.980764
H	34.909486	34.614616	37.473022
H	34.054734	34.615253	35.945921
C	31.965714	36.342136	36.813538
H	31.118332	37.012500	36.615947
H	31.988992	35.636189	35.970433
C	30.025075	41.233331	38.309608
H	29.886812	40.177668	38.576029
H	29.542003	41.807051	39.116568
C	31.695214	35.547239	38.093309
H	31.603814	36.237855	38.949553
H	32.545892	34.887919	38.335218
C	29.256068	41.498822	37.005772
H	29.712379	40.925250	36.177673
H	29.304333	42.560871	36.716438
C	27.776157	41.078597	37.115416
C	30.422816	34.674130	38.076391
O	30.211390	33.990301	39.112020
O	26.929804	41.720174	36.453502
O	29.683673	34.723422	37.068200
O	27.527164	40.092910	37.863791
O	35.590761	39.728022	39.584706
O	32.199063	38.026870	42.396111
O	33.899308	38.151521	44.637080
O	33.193926	35.999256	44.374042
O	31.811118	38.436826	43.729154

O	31.802697	34.309033	44.365573
C	33.510153	37.410864	42.364946
C	34.430327	38.463645	41.714321
C	33.350370	36.141512	41.518958
C	35.766760	37.900431	41.195008
C	33.953474	37.059250	43.783264
C	34.725181	35.566746	41.149248
C	34.663311	39.710909	42.580434
C	35.554597	36.609983	40.393628
C	32.346739	35.177366	42.190182
C	32.888105	39.116270	44.333272
C	33.470998	40.195078	43.400472
C	36.505628	38.986319	40.383114
C	32.427793	35.110613	43.710123
C	32.310870	33.765765	41.592980
C	32.337244	39.644198	45.642395
H	33.843708	38.777119	40.837710
H	32.886843	36.463573	40.573030
H	36.410176	37.658185	42.062100
H	35.000664	36.722918	43.770211
H	35.268786	35.231711	42.052086
H	34.585835	34.674959	40.521209
H	35.503884	39.521705	43.267640
H	34.965018	40.522693	41.904945
H	35.050983	36.839592	39.438667
H	36.538410	36.193271	40.132414
H	31.349518	35.621428	42.029845
H	32.667522	40.562278	42.747913
H	33.803351	41.042407	44.013945
H	31.555089	33.168511	42.118893
H	32.011438	33.802678	40.537177
H	33.279888	33.255115	41.691660
H	37.291481	38.529482	39.755147
H	36.989706	39.714272	41.047872
H	35.059763	39.092621	39.069253
H	33.138198	40.153165	46.194338
H	31.520128	40.353604	45.448593
H	31.970804	38.805645	46.247596
H	33.642423	40.437532	34.225493

QM atoms (linking H atom included): 121

XE12 Cluster2 Reactant

C	39.456300	33.315256	43.692699
H	39.237697	32.537555	42.946341

H	40.482436	33.674627	43.547019
S	38.263839	34.657408	43.427170
N	37.906577	37.629979	43.628640
C	37.402896	38.075572	42.431857
C	36.901438	37.771289	44.544084
C	36.031618	38.514313	42.580991
C	35.701066	38.303575	43.906611
C	37.002874	37.439624	45.891184
H	36.140596	37.643647	46.524615
C	38.116482	36.888943	46.505887
N	39.274182	36.511552	45.856684
C	40.120482	36.044318	46.836505
C	39.492261	36.136060	48.144360
C	38.233602	36.645443	47.932209
C	41.387159	35.519564	46.617156
H	41.933197	35.156054	47.487160
C	42.003015	35.381620	45.376693
C	43.288749	34.733136	45.173636
C	42.386622	35.440463	43.217771
N	41.470921	35.803868	44.183840
C	43.524461	34.765881	43.819448
C	42.246617	35.693192	41.863097
H	43.023133	35.303256	41.206186
C	41.214368	36.416624	41.269360
C	41.115250	36.671146	39.847644
N	40.139683	36.945847	41.938525
C	39.334787	37.504477	40.987915
C	38.074753	38.042429	41.220187
H	37.541903	38.447692	40.363275
Fe	39.808541	36.945238	43.946884
C	39.927537	37.361533	39.663109
C	39.307076	37.859331	38.446255
H	38.388824	38.437383	38.593563
C	39.728957	37.718337	37.177157
H	40.645283	37.190197	36.920969
H	39.164995	38.178042	36.363184
C	34.437821	38.521841	44.598648
H	34.520189	38.612490	45.687477
C	33.207079	38.592481	44.058828
H	33.021600	38.464342	42.990896
H	32.329269	38.766435	44.686577
C	42.107148	36.251142	38.813717
H	42.443274	37.126159	38.232560
H	42.987842	35.760836	39.245546

H	41.660891	35.534195	38.104644
C	35.188622	39.090612	41.491244
H	34.625426	38.311431	40.947542
H	34.445219	39.788228	41.903157
H	35.798591	39.635810	40.755971
C	37.201417	36.943701	48.976492
H	37.193474	36.165814	49.754861
H	37.410573	37.901745	49.482798
H	36.184277	37.012798	48.562448
C	44.755128	34.285337	43.119150
H	45.583779	35.005352	43.233925
H	45.106315	33.341483	43.560887
H	44.602662	34.122741	42.041208
C	44.223270	34.287066	46.253755
H	43.672136	33.812329	47.082773
H	44.928337	33.531462	45.878498
C	40.103816	35.713320	49.439269
H	41.193616	35.847050	49.429643
H	39.731304	36.361099	50.248498
C	45.029268	35.488145	46.771910
H	44.352681	36.274881	47.140184
H	45.584999	35.924161	45.923497
C	39.835109	34.249650	49.807651
H	40.128440	33.595939	48.965731
H	38.764629	34.067108	49.993741
C	40.638015	33.794455	51.045875
C	46.080519	35.191971	47.868977
O	46.753409	34.137947	47.736001
O	41.796458	34.277127	51.183315
O	46.193848	36.069128	48.755176
O	40.085136	32.956478	51.789948
O	40.494955	38.358092	44.295482
O	44.549719	39.798366	47.778411
O	44.707904	42.384134	46.613431
O	46.852196	41.714956	47.034867
O	44.335549	41.049637	48.459249
O	48.912409	41.184505	47.610323
C	45.147196	39.978404	46.466783
C	44.031803	39.670171	45.436974
C	46.307791	38.972951	46.422918
C	44.598315	39.479473	44.012529
C	45.664317	41.418722	46.294931
C	46.855737	38.820008	45.002665
C	42.886238	40.703599	45.463432

C	45.742471	38.459450	44.023291
C	47.355833	39.353810	47.479161
C	43.726721	41.954999	47.567707
C	42.534944	41.312608	46.827002
C	43.510101	39.100024	43.007924
C	47.802145	40.794549	47.356010
C	48.532178	38.387369	47.593990
C	43.371325	43.145137	48.429356
H	43.621411	38.695815	45.757483
H	45.890046	38.007462	46.742387
H	45.023900	40.450564	43.699969
H	45.923281	41.577505	45.237882
H	47.356249	39.751915	44.679885
H	47.626135	38.037448	44.991726
H	43.143347	41.530265	44.780600
H	41.983376	40.226106	45.054803
H	45.334961	37.465712	44.279791
H	46.169219	38.364580	43.015081
H	46.811549	39.332367	48.436210
H	42.081267	40.569743	47.501279
H	41.778275	42.097242	46.668572
H	49.124941	38.348348	46.667373
H	49.206291	38.709380	48.400334
H	48.143394	37.386559	47.833964
H	43.921399	39.055916	41.988323
H	42.685712	39.823743	42.993623
H	43.068873	38.122871	43.252739
H	43.061763	43.986487	47.796042
H	42.559301	42.891938	49.124470
H	44.255203	43.447116	49.003095
H	39.380870	32.860476	44.680399

QM atoms (linking H atom included): 121

XE12 Cluster2 TS

C	39.463855	33.263779	43.662528
H	39.221293	32.469432	42.941658
H	40.494817	33.598365	43.493062
S	38.294359	34.626283	43.383403
N	38.030117	37.639786	43.615180
C	37.539251	38.080862	42.414900
C	37.023658	37.797173	44.525673
C	36.171625	38.544455	42.555416
C	35.835253	38.352207	43.882311
C	37.114547	37.451160	45.871073

H	36.254031	37.665939	46.504505
C	38.217326	36.875466	46.488318
N	39.368791	36.478139	45.847582
C	40.202346	35.990830	46.824696
C	39.570241	36.093721	48.132991
C	38.321753	36.624919	47.915428
C	41.457560	35.436265	46.596913
H	41.993817	35.055162	47.465975
C	42.075852	35.277550	45.357066
C	43.352040	34.606198	45.160457
C	42.475692	35.324244	43.196224
N	41.563435	35.707323	44.157809
C	43.600167	34.638216	43.808336
C	42.344443	35.579189	41.838890
H	43.115170	35.172973	41.183704
C	41.330965	36.329506	41.239866
C	41.233607	36.595480	39.820171
N	40.273202	36.886808	41.915350
C	39.470606	37.461094	40.969139
C	38.219201	38.023074	41.205170
H	37.690967	38.425753	40.343515
Fe	39.916022	36.842280	43.921882
C	40.057337	37.307205	39.641435
C	39.442245	37.808096	38.423647
H	38.506510	38.358851	38.564707
C	39.881038	37.694488	37.157039
H	40.812897	37.194029	36.900571
H	39.310956	38.149419	36.344984
C	34.574641	38.599812	44.570622
H	34.658408	38.730951	45.655678
C	33.344668	38.657895	44.028011
H	33.161441	38.491826	42.964842
H	32.466065	38.858252	44.646689
C	42.219692	36.176145	38.781022
H	42.583430	37.056775	38.224373
H	43.083884	35.652633	39.205676
H	41.759329	35.491271	38.050035
C	35.340051	39.120417	41.456490
H	34.781758	38.340692	40.908556
H	34.590629	39.818599	41.857234
H	35.958619	39.663835	40.727459
C	37.281554	36.951773	48.941255
H	37.422385	36.347480	49.848287
H	37.326808	38.013366	49.239545

H	36.258754	36.769062	48.575119
C	44.839301	34.169865	43.117593
H	45.648122	34.915534	43.210892
H	45.215161	33.248173	43.583741
H	44.688145	33.975857	42.044937
C	44.277821	34.167907	46.250454
H	43.721607	33.698205	47.078310
H	44.992150	33.414872	45.887989
C	40.169034	35.656862	49.428399
H	41.262587	35.750084	49.412469
H	39.827249	36.322889	50.236274
C	45.067369	35.379982	46.766571
H	44.373975	36.168452	47.098538
H	45.647791	35.798961	45.927212
C	39.849847	34.207064	49.807789
H	40.129818	33.534275	48.976490
H	38.772372	34.059642	49.984892
C	40.628495	33.747362	51.058122
C	46.087490	35.108110	47.895193
O	46.775515	34.061202	47.787651
O	41.789376	34.222367	51.209314
O	46.167090	35.994735	48.775563
O	40.060770	32.916867	51.798465
O	40.712473	38.317421	44.371147
O	44.429480	39.911044	47.833013
O	44.572308	42.381729	46.443143
O	46.717327	41.653437	46.714913
O	44.325993	41.220105	48.423380
O	48.785415	41.106576	47.234543
C	44.902253	39.956108	46.461698
C	43.672689	39.622390	45.579599
C	46.004808	38.889699	46.402181
C	44.077708	39.255765	44.131989
C	45.457071	41.350925	46.118496
C	46.375244	38.543788	44.957910
C	42.594870	40.721289	45.605832
C	45.142626	38.157095	44.143070
C	47.182025	39.309508	47.300464
C	43.670319	42.078477	47.518840
C	42.388546	41.440147	46.943438
C	42.896636	38.928794	43.236777
C	47.656831	40.728608	47.053892
C	48.337616	38.310862	47.341807
C	43.452364	43.352957	48.299280

H	43.247333	38.706831	46.026447
H	45.579163	37.989087	46.869139
H	44.548941	40.161585	43.701186
H	45.613626	41.410864	45.031036
H	46.888860	39.399357	44.480070
H	47.097093	37.716072	44.955365
H	42.847400	41.481003	44.848465
H	41.646390	40.263117	45.292509
H	44.699181	37.229757	44.539242
H	45.444674	37.938307	43.110840
H	46.758658	39.365077	48.316567
H	41.970703	40.768899	47.710025
H	41.652696	42.245311	46.792543
H	48.827302	38.208013	46.361509
H	49.097476	38.651754	48.058854
H	47.950789	37.335423	47.671350
H	43.047240	38.093543	42.544026
H	42.449400	39.795261	42.740180
H	41.758701	38.497824	43.905786
H	43.129987	44.151867	47.619357
H	42.697301	43.215509	49.084959
H	44.400626	43.647737	48.763189
H	39.396798	32.835669	44.662674

QM atoms (linking H atom included): 121

XE12 Cluster2 intermediate

C	39.470419	33.256776	43.619510
H	39.261642	32.448830	42.904859
H	40.495856	33.613644	43.458175
S	38.285150	34.588119	43.284291
N	37.852475	37.561490	43.642982
C	37.370450	38.018050	42.440839
C	36.844845	37.691380	44.556828
C	36.002743	38.465964	42.588719
C	35.658576	38.241977	43.912085
C	36.941444	37.356412	45.904696
H	36.073573	37.548621	46.533731
C	38.066808	36.838708	46.532410
N	39.239103	36.471561	45.910917
C	40.083243	36.015679	46.894081
C	39.441056	36.123962	48.192985
C	38.177007	36.616523	47.962316
C	41.349091	35.477650	46.690459
H	41.886980	35.117927	47.566570

C	41.959806	35.316086	45.451746
C	43.246729	34.673402	45.246582
C	42.351067	35.372874	43.281333
N	41.431998	35.725793	44.249701
C	43.488315	34.707789	43.891449
C	42.223942	35.622811	41.924091
H	43.009853	35.235838	41.277337
C	41.197047	36.341712	41.315409
C	41.108921	36.602226	39.894777
N	40.115550	36.883148	41.967403
C	39.314787	37.449813	41.013802
C	38.058372	38.000923	41.235033
H	37.539736	38.418977	40.376146
Fe	39.750165	36.836159	43.993052
C	39.927968	37.304503	39.699363
C	39.330804	37.808882	38.473894
H	38.408211	38.382994	38.607353
C	39.776262	37.673177	37.211930
H	40.697476	37.147524	36.968378
H	39.224111	38.133320	36.390355
C	34.393441	38.467387	44.598846
H	34.470085	38.536102	45.689739
C	33.168691	38.572025	44.051246
H	32.989163	38.470955	42.979609
H	32.289571	38.748398	44.676327
C	42.107949	36.184269	38.866254
H	42.475532	37.065109	38.312622
H	42.967876	35.660111	39.299074
H	41.655709	35.498037	38.131347
C	35.170539	39.058607	41.499238
H	34.586730	38.290266	40.961818
H	34.445997	39.777785	41.907659
H	35.790997	39.582072	40.757837
C	37.133875	36.939837	48.986387
H	37.246010	36.302642	49.874663
H	37.213073	37.988137	49.320721
H	36.110537	36.803342	48.604116
C	44.725275	34.235696	43.197569
H	45.539887	34.974739	43.290317
H	45.095625	33.309781	43.661179
H	44.572124	34.045851	42.124549
C	44.183550	34.234964	46.326948
H	43.634475	33.779874	47.167047
H	44.882671	33.469808	45.959183

C	40.045176	35.710880	49.493460
H	41.132629	35.864158	49.493962
H	39.653751	36.347164	50.302439
C	45.002805	35.437157	46.819082
H	44.334634	36.228096	47.193279
H	45.543043	35.864794	45.956921
C	39.796965	34.239087	49.843438
H	40.095778	33.601332	48.991246
H	38.729580	34.040363	50.029673
C	40.612421	33.777718	51.069353
C	46.075393	35.144065	47.895034
O	46.751549	34.094555	47.745393
O	41.770818	34.263724	51.197690
O	46.201070	36.020290	48.780464
O	40.071079	32.931414	51.812315
O	40.508381	38.481004	44.352305
O	44.561173	39.807141	47.729969
O	44.808871	42.350993	46.490155
O	46.930397	41.638605	46.941072
O	44.369618	41.084082	48.368593
O	48.961095	41.076585	47.584549
C	45.182140	39.929439	46.421118
C	44.069828	39.613316	45.391294
C	46.314640	38.893590	46.426645
C	44.633692	39.340144	43.977071
C	45.738134	41.349939	46.206311
C	46.871270	38.673550	45.018926
C	42.966524	40.690242	45.355248
C	45.761772	38.282364	44.045122
C	47.361875	39.282284	47.481111
C	43.800816	41.977055	47.439254
C	42.605376	41.346262	46.693968
C	43.554318	38.963557	43.014041
C	47.846870	40.706392	47.317998
C	48.514002	38.291461	47.634567
C	43.461351	43.205754	48.252328
H	43.622840	38.668761	45.749274
H	45.866810	37.951529	46.773791
H	45.108683	40.273869	43.619098
H	46.004533	41.468657	45.145464
H	47.388662	39.583105	44.660925
H	47.629667	37.880150	45.046515
H	43.275773	41.484103	44.656384
H	42.059022	40.232031	44.937057

H	45.326033	37.315451	44.344898
H	46.194322	38.131571	43.047393
H	46.809840	39.302667	48.434072
H	42.115532	40.635536	47.377634
H	41.878060	42.150005	46.498106
H	49.115949	38.217545	46.716016
H	49.185275	38.620265	48.440565
H	48.098964	37.306156	47.893757
H	42.643035	38.462753	43.353242
H	43.675490	39.161124	41.945215
H	40.250929	39.125442	43.673495
H	43.192223	44.031588	47.580719
H	42.625455	43.003169	48.935216
H	44.339377	43.502759	48.837801
H	39.399110	32.848414	44.627588

QM atoms (linking H atom included): 121

XE12 Cluster2 TS2

C	39.461140	33.253006	43.614459
H	39.236080	32.449335	42.900517
H	40.491651	33.591693	43.448483
S	38.303312	34.618477	43.304727
N	38.004449	37.637494	43.615849
C	37.508254	38.059705	42.407687
C	36.999743	37.773007	44.531562
C	36.139004	38.508540	42.556894
C	35.806052	38.309748	43.886340
C	37.096180	37.433396	45.879211
H	36.230112	37.630361	46.509986
C	38.213011	36.890873	46.502398
N	39.376171	36.505468	45.877518
C	40.206910	36.014444	46.851956
C	39.567391	36.123707	48.155433
C	38.316264	36.648458	47.930531
C	41.457038	35.443472	46.632211
H	41.994499	35.069290	47.502837
C	42.051869	35.254924	45.387205
C	43.329712	34.593516	45.180353
C	42.421052	35.263952	43.209297
N	41.520630	35.652609	44.182892
C	43.558886	34.601348	43.823175
C	42.290639	35.512981	41.849705
H	43.069251	35.114895	41.199874
C	41.280030	36.262315	41.243803

C	41.195161	36.543683	39.825690
N	40.215429	36.822903	41.903135
C	39.422724	37.416051	40.960170
C	38.181468	37.999674	41.193685
H	37.656765	38.408745	40.333694
Fe	39.868883	36.792738	43.936338
C	40.026431	37.268581	39.640536
C	39.431534	37.792698	38.422696
H	38.507578	38.363118	38.563245
C	39.875860	37.678047	37.158155
H	40.797038	37.156845	36.904995
H	39.322171	38.150707	36.344872
C	34.541971	38.539042	44.574266
H	34.622417	38.644109	45.662194
C	33.312424	38.606230	44.030949
H	33.129262	38.465412	42.964249
H	32.432605	38.787659	44.653851
C	42.186860	36.127997	38.790816
H	42.547591	37.008268	38.231654
H	43.051718	35.610578	39.220431
H	41.733136	35.438045	38.060314
C	35.292470	39.071265	41.462399
H	34.709307	38.287255	40.947586
H	34.564100	39.792971	41.861204
H	35.903116	39.583334	40.704895
C	37.273921	36.976590	48.953419
H	37.407905	36.368455	49.858841
H	37.325505	38.036505	49.255579
H	36.251787	36.801555	48.582654
C	44.794582	34.128716	43.128615
H	45.604430	34.874320	43.211291
H	45.174317	33.211962	43.601315
H	44.638246	33.926102	42.058627
C	44.271419	34.176657	46.265064
H	43.724720	33.724250	47.108421
H	44.978917	33.414969	45.907277
C	40.159808	35.687725	49.453695
H	41.252328	35.791151	49.446161
H	39.804275	36.345639	50.262375
C	45.071868	35.394847	46.750811
H	44.386114	36.193238	47.074334
H	45.648430	35.793859	45.898709
C	39.851071	34.232165	49.820293
H	40.134288	33.570283	48.981433

H	38.774971	34.075999	49.997633
C	40.635384	33.764471	51.063421
C	46.093473	35.137243	47.882461
O	46.775757	34.085155	47.793526
O	41.797552	34.237633	51.211727
O	46.176172	36.037336	48.749692
O	40.071448	32.929197	51.801482
O	40.793418	38.411713	44.261461
O	44.515185	39.891271	47.874459
O	44.615364	42.368128	46.489759
O	46.776147	41.686034	46.782008
O	44.390001	41.197328	48.467462
O	48.842452	41.176761	47.348700
C	45.001095	39.951051	46.509569
C	43.783531	39.581634	45.625370
C	46.137519	38.923750	46.445695
C	44.190904	39.251809	44.162453
C	45.525954	41.359327	46.173262
C	46.561290	38.678756	44.996492
C	42.672780	40.648034	45.657612
C	45.370594	38.258417	44.137564
C	47.269072	39.354832	47.391830
C	43.718922	42.044138	47.563856
C	42.452906	41.377389	46.988342
C	43.060343	38.722546	43.335955
C	47.723989	40.779328	47.150688
C	48.437000	38.373988	47.478197
C	43.472694	43.311782	48.346956
H	43.393484	38.647522	46.064273
H	45.735885	37.986864	46.859350
H	44.526277	40.204093	43.713289
H	45.693357	41.426694	45.087962
H	47.040252	39.581783	44.574817
H	47.322535	37.887087	44.964796
H	42.896502	41.407030	44.889999
H	41.741569	40.148732	45.356190
H	45.004671	37.275429	44.474052
H	45.705169	38.125580	43.101515
H	46.803354	39.402649	48.389229
H	42.042036	40.709858	47.761524
H	41.707720	42.171905	46.826966
H	48.966946	38.279174	46.518098
H	49.165218	38.721737	48.224538
H	48.049915	37.392339	47.789745

H	42.916270	37.648675	43.270371
H	42.602984	39.331832	42.556792
H	40.408583	39.112390	43.709599
H	43.141853	44.107485	47.667392
H	42.714226	43.159224	49.126492
H	44.413122	43.621670	48.817100
H	39.394357	32.844020	44.622595

QM atoms (linking H atom included): 121

XE12 Cluster2 Product

C	39.522717	33.324359	43.628504
H	39.189663	32.571909	42.901544
H	40.571788	33.567255	43.431518
S	38.473496	34.807020	43.417623
N	37.990015	37.605098	43.573853
C	37.487517	38.040784	42.370018
C	36.990206	37.781146	44.490048
C	36.129934	38.523761	42.521333
C	35.803188	38.344965	43.852479
C	37.091052	37.471265	45.842386
H	36.231855	37.686549	46.476505
C	38.219018	36.952529	46.462112
N	39.376872	36.565586	45.825361
C	40.212618	36.095089	46.811591
C	39.590780	36.231892	48.120311
C	38.339583	36.753920	47.895863
C	41.461941	35.525342	46.607058
H	42.006748	35.181526	47.485965
C	42.044723	35.303675	45.364749
C	43.348182	34.683865	45.174270
C	42.392097	35.254716	43.199234
N	41.481840	35.645003	44.160376
C	43.559999	34.644577	43.818321
C	42.265896	35.507043	41.843158
H	43.052337	35.126834	41.192282
C	41.250503	36.251131	41.243108
C	41.193198	36.550945	39.829366
N	40.174396	36.802946	41.901035
C	39.400435	37.401462	40.941033
C	38.159311	37.985890	41.158941
H	37.644250	38.404526	40.297751
Fe	39.714748	36.574843	43.857726
C	40.024438	37.272912	39.632046
C	39.450505	37.812121	38.410713

H	38.541385	38.407481	38.544526
C	39.898166	37.680523	37.149016
H	40.802446	37.126990	36.903787
H	39.363022	38.166322	36.331190
C	34.552422	38.619327	44.548066
H	34.646553	38.756554	45.631357
C	33.319594	38.693696	44.013278
H	33.126290	38.520798	42.953004
H	32.447887	38.912133	44.635505
C	42.213766	36.160384	38.811999
H	42.535169	37.044936	38.236778
H	43.100590	35.697311	39.260161
H	41.804692	35.429678	38.094462
C	35.293018	39.097816	41.425493
H	34.711080	38.319805	40.899970
H	34.564245	39.819655	41.823207
H	35.911926	39.611993	40.676093
C	37.318405	37.137302	48.919828
H	37.474644	36.586269	49.857502
H	37.376640	38.214089	49.152242
H	36.287419	36.942377	48.585209
C	44.798416	34.172765	43.126067
H	45.614525	34.909194	43.223063
H	45.166689	33.247470	43.592589
H	44.646634	33.980514	42.053520
C	44.309757	34.332129	46.262770
H	43.777420	33.898347	47.126070
H	45.023102	33.566101	45.925757
C	40.195269	35.814921	49.422830
H	41.290387	35.892775	49.397149
H	39.868421	36.501846	50.219380
C	45.119752	35.559863	46.719632
H	44.445438	36.377689	47.022677
H	45.718897	35.930052	45.867760
C	39.851849	34.376088	49.830535
H	40.102350	33.689011	49.001250
H	38.773306	34.256280	50.021957
C	40.634900	33.895848	51.072594
C	46.079551	35.257743	47.900197
O	46.820866	34.248833	47.755816
O	41.803409	34.350697	51.218882
O	46.028544	36.043680	48.866794
O	40.063775	33.063151	51.809793
O	40.878059	38.586527	44.149483

O	44.657631	40.011595	47.503861
O	43.981764	42.584249	46.468473
O	46.212527	42.214884	46.180317
O	44.548269	41.239236	48.258361
O	48.377610	41.978912	46.489205
C	44.681484	40.268240	46.077283
C	43.315844	39.756275	45.556899
C	45.865701	39.487456	45.497902
C	43.241830	39.592172	44.024951
C	44.907878	41.768558	45.817220
C	45.857574	39.619656	43.970403
C	42.146474	40.621859	46.057453
C	44.552799	39.068707	43.396205
C	47.164970	39.926556	46.188451
C	43.517236	42.032491	47.721693
C	42.239644	41.213796	47.466323
C	42.182944	38.575618	43.559075
C	47.324615	41.436803	46.276007
C	48.427623	39.269200	45.623604
C	43.365118	43.174092	48.700900
H	43.236040	38.748126	46.001212
H	45.707730	38.424513	45.746428
H	43.019783	40.585989	43.596701
H	44.790017	41.969728	44.743017
H	46.036405	40.665026	43.666952
H	46.696054	39.037383	43.562389
H	42.040829	41.462558	45.353088
H	41.235515	40.015956	45.982633
H	44.578652	37.973497	43.529924
H	44.496302	39.253176	42.313067
H	47.061818	39.619537	47.244163
H	42.170427	40.437712	48.241637
H	41.377547	41.884534	47.607853
H	48.672147	39.639657	44.617904
H	49.292423	39.491517	46.261914
H	48.297636	38.177355	45.571858
H	42.567447	37.584667	43.809186
H	42.096259	38.618912	42.461712
H	40.309458	39.257258	43.743826
H	42.789899	43.987302	48.240759
H	42.856794	42.842403	49.616576
H	44.360424	43.557059	48.956813
H	39.450396	32.895253	44.627856

QM atoms (linking H atom included): 121

XE12 Cluster3 Reactant

C	32.792648	38.659064	39.949467
H	32.699315	38.476573	38.867647
H	33.343583	37.828813	40.410184
S	33.722108	40.207215	40.123787
N	36.109255	41.582900	41.530746
C	37.054945	42.075518	40.662345
C	35.570519	42.660878	42.166675
C	37.148453	43.518592	40.772472
C	36.206265	43.896335	41.716609
C	34.517360	42.594300	43.076303
H	34.170791	43.529703	43.512903
C	33.852598	41.445190	43.462398
N	34.163927	40.158013	43.059826
C	33.291790	39.328250	43.731636
C	32.376211	40.110300	44.549575
C	32.727379	41.427832	44.374894
C	33.302819	37.941529	43.680199
H	32.571907	37.414307	44.292324
C	34.161423	37.165706	42.904553
C	34.125638	35.710921	42.842440
C	35.674878	36.576844	41.423971
N	35.109489	37.668998	42.047040
C	35.084552	35.346027	41.923751
C	36.618424	36.642124	40.409803
H	36.916177	35.697976	39.954983
C	37.193777	37.806354	39.898517
C	38.112459	37.844235	38.779541
N	36.947731	39.074518	40.365801
C	37.682051	39.925920	39.588890
C	37.761879	41.306596	39.750418
H	38.455673	41.838411	39.103677
Fe	35.759091	39.593416	41.933585
C	38.407747	39.182355	38.565713
C	39.218554	39.812639	37.534470
H	39.159683	40.905653	37.507967
C	40.037030	39.240410	36.632145
H	40.204380	38.164994	36.580214
H	40.592345	39.869663	35.933210
C	35.830188	45.222554	42.185903
H	34.936964	45.253773	42.819184
C	36.427961	46.402048	41.931963
H	37.332379	46.498924	41.332103

H	36.015807	47.324336	42.348935
C	38.611013	36.666560	38.009120
H	39.703184	36.562249	38.131573
H	38.136793	35.728745	38.322888
H	38.411880	36.793379	36.931839
C	38.083037	44.393805	40.003721
H	38.669951	43.827175	39.271150
H	37.541235	45.192914	39.470032
H	38.802735	44.891801	40.675329
C	32.123183	42.636864	45.018912
H	32.021567	43.472243	44.306672
H	31.120020	42.412622	45.406384
H	32.736621	43.005176	45.860644
C	35.466303	33.957516	41.519545
H	36.242377	33.544637	42.187199
H	34.598815	33.285611	41.590617
H	35.862162	33.903202	40.494442
C	33.236675	34.792115	43.631718
H	32.391303	35.338276	44.070341
H	32.788473	34.053476	42.946152
C	31.292675	39.545965	45.407210
H	31.612164	38.589306	45.839440
H	31.124147	40.221662	46.260259
C	33.992542	34.057178	44.750677
H	34.485011	34.804038	45.396992
H	34.798687	33.433554	44.336668
C	29.950016	39.287183	44.701383
H	30.120993	38.657253	43.809922
H	29.476799	40.228948	44.379182
C	28.994342	38.520088	45.647151
C	33.153162	33.163656	45.687007
O	33.756503	32.190539	46.195283
O	27.857525	38.987457	45.844861
O	31.951616	33.483062	45.920746
O	29.480413	37.465564	46.154018
O	36.848494	39.474139	43.108199
O	36.512637	36.321815	47.307863
O	39.023809	37.262916	48.246537
O	38.985979	35.026430	48.671666
O	36.758723	37.009672	48.555059
O	38.773719	32.973167	49.413445
C	37.746191	35.885181	46.673645
C	37.936535	36.802106	45.439010
C	37.528876	34.409824	46.304929

C	38.988415	36.251979	44.446804
C	38.936037	36.020305	47.636268
C	38.639569	33.902040	45.380798
C	38.244071	38.261338	45.830331
C	38.734117	34.773407	44.130967
C	37.320286	33.582957	47.584870
C	37.779087	37.963714	48.356063
C	37.540301	38.800130	47.081421
C	39.051336	37.090273	43.167421
C	38.423341	33.799168	48.604556
C	37.024090	32.102687	47.347911
C	37.818425	38.767468	49.641497
H	36.955377	36.783239	44.932406
H	36.586634	34.369328	45.737754
H	39.972822	36.308607	44.946770
H	39.859763	35.884609	47.054722
H	39.611506	33.886813	45.906591
H	38.422384	32.864007	45.095387
H	39.331460	38.364437	45.981765
H	37.970882	38.904285	44.982529
H	37.797669	34.684007	43.551909
H	39.543751	34.402185	43.483308
H	36.431632	34.015993	48.072632
H	36.453725	38.883490	46.927544
H	37.912698	39.819227	47.269611
H	36.131982	32.005364	46.710728
H	37.873124	31.580809	46.880808
H	36.817308	31.611799	48.308847
H	38.056469	37.191549	42.714175
H	39.721349	36.626259	42.425563
H	39.413070	38.110326	43.355627
H	37.854582	38.082078	50.499870
H	38.727576	39.384124	49.650190
H	36.931683	39.412910	49.719297
H	31.787345	38.688153	40.369688

QM atoms (linking H atom included): 121

XE12 Cluster3 TS

C	32.818139	38.619809	39.936585
H	32.705519	38.443643	38.855761
H	33.363652	37.778562	40.384075
S	33.772012	40.156011	40.106580
N	36.151424	41.476509	41.550875
C	37.074122	41.963796	40.659221

C	35.624024	42.554335	42.194775
C	37.159762	43.410436	40.752974
C	36.246458	43.788559	41.724049
C	34.590969	42.490400	43.128749
H	34.257559	43.428694	43.569895
C	33.921478	41.344684	43.524799
N	34.220641	40.060763	43.118147
C	33.337128	39.233989	43.770907
C	32.424741	40.018261	44.594830
C	32.792056	41.332261	44.435729
C	33.326660	37.846705	43.684716
H	32.583074	37.318928	44.282127
C	34.173301	37.065740	42.896502
C	34.114230	35.612552	42.821295
C	35.693857	36.460165	41.424826
N	35.136882	37.557372	42.048231
C	35.080825	35.236706	41.914390
C	36.647998	36.519145	40.417732
H	36.932024	35.572840	39.957863
C	37.239481	37.679448	39.910956
C	38.153465	37.720855	38.787514
N	36.997222	38.946543	40.383770
C	37.717254	39.802663	39.598446
C	37.777521	41.187698	39.747932
H	38.457057	41.722832	39.088158
Fe	35.769742	39.474187	41.922645
C	38.441314	39.060718	38.571774
C	39.238568	39.694805	37.532799
H	39.160786	40.786793	37.497682
C	40.059372	39.128866	36.628462
H	40.241017	38.055537	36.579709
H	40.603008	39.761282	35.923492
C	35.876392	45.117801	42.191480
H	34.912643	45.178119	42.710059
C	36.566333	46.264776	42.053587
H	37.552733	46.313485	41.592575
H	36.152567	47.202776	42.431846
C	38.648356	36.546728	38.008860
H	39.742670	36.447848	38.115507
H	38.182064	35.606659	38.327090
H	38.433919	36.674117	36.934469
C	38.045794	44.285493	39.929832
H	38.421384	43.763267	39.040721
H	37.512484	45.190806	39.598870

H	38.928761	44.622322	40.499709
C	32.191087	42.540833	45.082045
H	32.128519	43.391174	44.383498
H	31.172853	42.329140	45.435877
H	32.784006	42.882054	45.949476
C	35.457317	33.844557	41.518941
H	36.228822	33.428704	42.190700
H	34.585052	33.179126	41.586753
H	35.855683	33.784500	40.495199
C	33.212611	34.705703	43.608914
H	32.345133	35.248681	44.007951
H	32.799680	33.936654	42.935435
C	31.326176	39.460991	45.437464
H	31.636755	38.504122	45.874804
H	31.147201	40.138322	46.287413
C	33.956437	34.024870	44.767839
H	34.387340	34.807940	45.414697
H	34.805912	33.435357	44.392793
C	29.990683	39.208030	44.715593
H	30.167767	38.572622	43.829464
H	29.529671	40.152614	44.383855
C	29.021178	38.456774	45.658802
C	33.122106	33.120007	45.694380
O	33.730950	32.152988	46.207468
O	27.896874	38.948266	45.868789
O	31.917056	33.431317	45.921424
O	29.486435	37.387277	46.155267
O	36.923428	39.385829	43.203598
O	36.483155	36.553305	47.437500
O	39.038648	37.428090	48.319669
O	39.016651	35.164250	48.525574
O	36.794760	37.117743	48.732813
O	38.800471	33.065895	49.117186
C	37.680435	36.208816	46.688759
C	37.795134	37.265568	45.559974
C	37.439385	34.782121	46.167850
C	38.793003	36.829517	44.455092
C	38.920204	36.250314	47.595997
C	38.460520	34.390855	45.092895
C	38.122714	38.676769	46.087597
C	38.478284	35.415025	43.958379
C	37.327735	33.804002	47.354167
C	37.798866	38.097609	48.580887
C	37.486105	39.069649	47.424344

C	38.908188	37.833124	43.326715
C	38.448762	33.947158	48.371011
C	37.089698	32.344071	46.966624
C	37.910294	38.755623	49.942749
H	36.793523	37.295520	45.098336
H	36.453612	34.805315	45.678989
H	39.791025	36.787967	44.936144
H	39.815620	36.178424	46.960449
H	39.470767	34.295972	45.531855
H	38.199905	33.398351	44.697311
H	39.215767	38.776860	46.190167
H	37.799944	39.400702	45.326609
H	37.501996	35.419565	43.442134
H	39.231740	35.127031	43.208627
H	36.442418	34.131265	47.923772
H	36.393174	39.157797	47.338758
H	37.866950	40.064757	47.702995
H	36.144727	32.253762	46.411196
H	37.914385	31.934904	46.364504
H	37.005418	31.735351	47.877271
H	37.738586	38.571630	43.169658
H	39.054849	37.412171	42.323286
H	39.567943	38.685832	43.526185
H	37.985064	37.980356	50.718006
H	38.822535	39.367046	49.971236
H	37.033660	39.391364	50.133197
H	31.820017	38.659024	40.372799

QM atoms (linking H atom included): 121

XE12 Cluster3 Product

C	32.858057	38.592319	39.827462
H	32.694583	38.379036	38.761705
H	33.411700	37.755485	40.276315
S	33.863036	40.103201	39.903172
N	36.047932	41.575254	41.514224
C	36.995608	42.058316	40.643281
C	35.491817	42.652309	42.141523
C	37.072473	43.503204	40.741723
C	36.123423	43.882635	41.679574
C	34.454076	42.588851	43.066441
H	34.096421	43.528210	43.484571
C	33.830406	41.429903	43.505691
N	34.153615	40.146963	43.135402
C	33.292658	39.309528	43.800789

C	32.378529	40.089986	44.622525
C	32.715694	41.409670	44.435242
C	33.281489	37.921063	43.724628
H	32.550429	37.392744	44.335191
C	34.115583	37.152029	42.920106
C	34.082031	35.700543	42.843484
C	35.630369	36.567794	41.418069
N	35.059857	37.654868	42.049359
C	35.040303	35.339604	41.919740
C	36.578623	36.624317	40.404842
H	36.870352	35.676747	39.953414
C	37.161809	37.784353	39.893002
C	38.085134	37.825093	38.777166
N	36.929418	39.053538	40.361925
C	37.659622	39.911987	39.587057
C	37.726789	41.292316	39.744777
H	38.422385	41.829850	39.104956
Fe	35.675469	39.591893	41.926606
C	38.385311	39.163687	38.567192
C	39.201049	39.791946	37.538405
H	39.132660	40.884402	37.504383
C	40.028773	39.217149	36.645885
H	40.202410	38.142213	36.601613
H	40.587203	39.842789	35.946187
C	35.741341	45.213584	42.132967
H	34.761553	45.276631	42.620037
C	36.437938	46.359050	42.016159
H	37.437863	46.406319	41.584949
H	36.014782	47.298193	42.381271
C	38.582308	36.647467	38.005301
H	39.673388	36.536113	38.133088
H	38.099722	35.711377	38.312000
H	38.390600	36.780685	36.927432
C	37.992829	44.380017	39.958414
H	38.426278	43.853842	39.098663
H	37.469836	45.275816	39.587629
H	38.836596	44.734234	40.575079
C	32.100845	42.613346	45.077429
H	32.027185	43.461799	44.378248
H	31.085772	42.388935	45.432010
H	32.689271	42.962513	45.944616
C	35.423561	33.951701	41.515011
H	36.220941	33.547635	42.162869
H	34.563889	33.273520	41.611249

H	35.792757	33.895449	40.480111
C	33.200643	34.775936	43.634313
H	32.349828	35.313926	44.072179
H	32.761768	34.030893	42.949681
C	31.289630	39.520902	45.469845
H	31.601816	38.557795	45.892465
H	31.116750	40.186769	46.329656
C	33.967131	34.051274	44.751699
H	34.445828	34.806101	45.399166
H	34.784191	33.442612	44.336919
C	29.952923	39.278106	44.747710
H	30.133427	38.668512	43.843996
H	29.483724	40.226509	44.440634
C	28.987611	38.493395	45.666243
C	33.139049	33.145766	45.686074
O	33.751718	32.173804	46.186908
O	27.846826	38.953843	45.857714
O	31.937025	33.455975	45.926567
O	29.468083	37.429406	46.159585
O	36.950497	39.440421	43.214601
O	36.516301	36.375334	47.360479
O	39.043605	37.252394	48.324565
O	38.986466	35.006258	48.665914
O	36.774413	37.023519	48.627264
O	38.732983	32.943495	49.364256
C	37.740303	35.944628	46.708240
C	37.930254	36.908254	45.506957
C	37.503093	34.484922	46.290638
C	38.965686	36.364010	44.473790
C	38.939379	36.034530	47.668123
C	38.594237	33.994053	45.333913
C	38.288373	38.339832	45.951966
C	38.679605	34.901534	44.109997
C	37.298562	33.613993	47.542687
C	37.809582	37.967352	48.459803
C	37.588574	38.851320	47.215316
C	39.064636	37.226496	43.257636
C	38.401372	33.790680	48.570672
C	37.000234	32.142661	47.256808
C	37.858730	38.727687	49.771135
H	36.945766	36.933021	45.008955
H	36.553503	34.475214	45.733798
H	39.947260	36.395136	44.985587
H	39.858929	35.912330	47.075610

H	39.574009	33.947965	45.843343
H	38.358470	32.969266	45.017238
H	39.376944	38.401103	46.116002
H	38.043417	39.029721	45.133255
H	37.729700	34.850691	43.548591
H	39.469982	34.543907	43.432883
H	36.410906	34.029749	48.046384
H	36.505001	38.960034	47.058239
H	37.983200	39.855004	47.436825
H	36.096381	32.064747	46.633995
H	37.841459	31.638632	46.757373
H	36.810531	31.617780	48.203046
H	37.506877	38.646680	43.087641
H	38.686404	36.880549	42.292002
H	39.609127	38.172247	43.283648
H	37.876263	38.014956	50.607449
H	38.778376	39.327834	49.802459
H	36.983583	39.386957	49.863593
H	31.883126	38.655025	40.310831

QM atoms (linking H atom included): 121

IVH4 Cluster1 Reactant

C	38.337713	37.890100	33.886112
H	37.910531	38.756443	33.358737
H	39.428898	38.003613	33.920657
S	37.652510	37.893617	35.563603
N	38.416460	37.438650	38.403575
C	37.977471	38.472732	39.194972
C	37.705913	36.333483	38.775543
C	36.963822	38.013419	40.121859
C	36.767336	36.671601	39.841605
C	37.823410	35.078236	38.182705
H	37.197499	34.277957	38.575656
C	38.635918	34.760710	37.105746
N	39.498273	35.633225	36.472063
C	40.094800	34.907406	35.460367
C	39.578677	33.544560	35.431840
C	38.675003	33.457065	36.465735
C	41.075310	35.388856	34.605285
H	41.466517	34.697849	33.858044
C	41.612317	36.675197	34.630754
C	42.647250	37.141933	33.722633
C	42.004994	38.769923	35.161765
N	41.230396	37.676041	35.490686

C	42.913559	38.444596	34.074461
C	41.868265	40.031812	35.717805
H	42.503992	40.822503	35.321941
C	40.945925	40.391424	36.698207
C	40.764955	41.744908	37.184977
N	40.076100	39.530207	37.318362
C	39.362168	40.279041	38.211573
C	38.397371	39.790412	39.084088
H	37.946262	40.505472	39.768641
Fe	39.976082	37.522870	37.092425
C	39.759938	41.678081	38.132405
C	39.186560	42.740019	38.949351
H	38.809878	42.421488	39.925769
C	39.090827	44.041910	38.630505
H	39.413069	44.431034	37.662464
H	38.658755	44.753342	39.338349
C	35.809909	35.734680	40.412060
H	36.041713	34.675361	40.261222
C	34.670346	36.029352	41.063296
H	34.337581	37.054424	41.233631
H	34.020779	35.232792	41.432892
C	41.535707	42.945586	36.743506
H	42.532695	42.681299	36.366532
H	41.020853	43.471896	35.921598
H	41.653242	43.655460	37.576759
C	36.320090	38.844754	41.184242
H	36.131341	38.241890	42.085820
H	36.952988	39.693723	41.479528
H	35.345730	39.252001	40.860046
C	37.902869	32.257067	36.920147
H	37.952611	31.445272	36.181271
H	38.298692	31.859464	37.871028
H	36.838643	32.489827	37.093226
C	43.948335	39.342323	33.472998
H	43.734302	40.409135	33.626045
H	44.947196	39.134738	33.894049
H	44.037704	39.164981	32.391089
C	43.317638	36.339944	32.651173
H	42.597822	35.680724	32.148882
H	43.690691	37.020632	31.870024
C	39.973909	32.479496	34.454006
H	41.052487	32.532843	34.249017
H	39.814851	31.491806	34.907962
C	44.487549	35.497552	33.178705

H	44.113550	34.779346	33.929314
H	45.225605	36.136509	33.688699
C	39.212121	32.519504	33.121092
H	39.397444	33.465103	32.584245
H	38.120996	32.479951	33.292441
C	39.560348	31.359077	32.158482
C	45.229861	34.666202	32.109975
O	46.452713	34.454670	32.327561
O	38.940482	31.327507	31.072170
O	44.565541	34.242657	31.133821
O	40.427801	30.530297	32.531291
O	41.078805	37.165619	38.205300
O	46.470253	33.321384	38.445571
O	47.283807	34.069837	35.834816
O	45.200747	33.139427	35.674483
O	47.350585	32.568457	37.574498
O	43.436943	31.828633	35.573196
C	45.812787	34.402656	37.741491
C	46.458681	35.720707	38.241297
C	44.328016	34.304900	38.108704
C	45.631883	36.983343	37.894296
C	45.986950	34.248647	36.230957
C	43.559802	35.515783	37.576127
C	47.924658	35.863311	37.786384
C	44.133293	36.800473	38.164628
C	43.780047	32.939354	37.673112
C	48.140581	33.475193	36.831692
C	48.750043	34.574183	37.724296
C	46.156047	38.206525	38.653561
C	44.097401	32.605333	36.229190
C	42.297888	32.737350	37.988953
C	49.158880	32.640539	36.091779
H	46.437538	35.604896	39.339612
H	44.278664	34.335295	39.210886
H	45.754491	37.174545	36.810635
H	45.599685	35.139059	35.720909
H	43.594583	35.546663	36.472466
H	42.496887	35.449442	37.838967
H	47.939855	36.319613	36.783028
H	48.442941	36.567956	38.452577
H	43.961248	36.789591	39.256434
H	43.569633	37.664746	37.781864
H	44.366490	32.190125	38.234583
H	48.906580	34.141395	38.723766

H	49.741149	34.828639	37.322554
H	49.729878	33.290240	35.415895
H	48.645358	31.877346	35.496112
H	49.848475	32.161686	36.797892
H	47.188563	38.468881	38.383591
H	45.509715	39.077764	38.465398
H	46.141892	38.019078	39.740524
H	42.005071	31.691188	37.836628
H	42.099352	33.003003	39.038645
H	41.653511	33.358877	37.351937
H	38.099055	37.001580	33.301611

QM atoms (linking H atom included): 121

IVH4 Cluster1 TS

C	38.429225	37.976051	33.915058
H	38.010619	38.821474	33.351182
H	39.521948	38.089377	33.945517
S	37.773087	38.040799	35.606690
N	38.572224	37.444814	38.404174
C	38.119643	38.486336	39.178523
C	37.870901	36.333712	38.775096
C	37.116798	38.019838	40.111885
C	36.929757	36.674046	39.837610
C	37.994646	35.075043	38.190524
H	37.362707	34.278174	38.580130
C	38.831995	34.745580	37.133637
N	39.711322	35.597865	36.508437
C	40.302769	34.879010	35.498414
C	39.781964	33.517217	35.470939
C	38.867146	33.438094	36.496473
C	41.263621	35.366757	34.620865
H	41.657133	34.676695	33.875133
C	41.755298	36.668728	34.614421
C	42.768901	37.152805	33.694861
C	42.083283	38.798884	35.098225
N	41.346381	37.683880	35.453389
C	42.996079	38.472090	34.017026
C	41.925301	40.069814	35.630779
H	42.547578	40.861903	35.218461
C	41.003032	40.432713	36.609382
C	40.806560	41.788141	37.089455
N	40.150493	39.570838	37.248474
C	39.435462	40.310765	38.147389
C	38.499795	39.814173	39.043990

H	38.037377	40.525877	39.724152
Fe	40.103255	37.533507	37.049792
C	39.812151	41.715298	38.047914
C	39.225633	42.774050	38.859532
H	38.845570	42.456317	39.835716
C	39.112223	44.073195	38.534180
H	39.430689	44.461462	37.564586
H	38.666280	44.781725	39.236468
C	35.980185	35.735013	40.416145
H	36.216470	34.676644	40.265841
C	34.844060	36.029259	41.073675
H	34.513036	37.054916	41.243583
H	34.195985	35.233966	41.447954
C	41.560285	42.994379	36.634801
H	42.560921	42.738403	36.261425
H	41.039396	43.504267	35.806168
H	41.666793	43.716154	37.459314
C	36.477091	38.849851	41.178197
H	36.299630	38.247949	42.082673
H	37.109676	39.701961	41.464430
H	35.497688	39.252275	40.863713
C	38.052914	32.253256	36.916979
H	38.079243	31.460811	36.155958
H	38.424604	31.815370	37.859630
H	36.996472	32.518690	37.087985
C	44.004057	39.385138	33.393302
H	43.768948	40.448018	33.538799
H	45.012279	39.204429	33.803824
H	44.084349	39.199563	32.312282
C	43.453799	36.348311	32.634799
H	42.732243	35.720778	32.094639
H	43.876698	37.030933	31.881647
C	40.147265	32.461076	34.471594
H	41.212110	32.534673	34.211654
H	40.029144	31.467941	34.925585
C	44.574405	35.454457	33.183529
H	44.142398	34.717801	33.883252
H	45.307781	36.046868	33.751689
C	39.317491	32.502496	33.178816
H	39.462828	33.456335	32.644678
H	38.237998	32.449579	33.410357
C	39.622135	31.353896	32.188876
C	45.330031	34.645859	32.109388
O	46.551262	34.430911	32.335188

O	38.982783	31.349021	31.113860
O	44.675968	34.241926	31.118672
O	40.478637	30.501478	32.535345
O	41.265606	37.301103	38.305464
O	46.405336	33.362797	38.532548
O	46.826452	34.132915	35.827761
O	44.919160	32.906701	35.820297
O	47.331429	32.759229	37.602719
O	43.363405	31.360098	35.802792
C	45.477850	34.247615	37.866695
C	45.872330	35.688955	38.284389
C	44.094843	33.824188	38.381692
C	44.739455	36.730737	38.012298
C	45.553445	34.108773	36.341841
C	43.019183	34.851045	38.016433
C	47.223538	36.112149	37.667916
C	43.434529	36.192112	38.559001
C	43.791515	32.388103	37.937924
C	47.863798	33.765019	36.764830
C	48.297602	35.018103	37.552119
C	45.064477	38.106640	38.599356
C	43.974039	32.182952	36.446894
C	42.444144	31.864205	38.434078
C	48.970497	33.086379	35.987357
H	45.991479	35.617824	39.379697
H	44.183328	33.807741	39.481148
H	44.635010	36.839355	36.915814
H	44.992777	34.933844	35.882966
H	42.881350	34.910757	36.922552
H	42.046757	34.559285	38.434990
H	47.040534	36.517664	36.659172
H	47.646376	36.934252	38.264755
H	43.388811	36.235113	39.659526
H	42.409210	36.944038	38.283914
H	44.595006	31.780065	38.386853
H	48.649201	34.689434	38.541697
H	49.163035	35.456933	37.034601
H	49.242195	33.714426	35.130767
H	48.618547	32.114653	35.616661
H	49.851819	32.936740	36.625369
H	45.970676	38.541429	38.153419
H	44.226580	38.798045	38.422336
H	45.222981	38.039792	39.688793
H	42.399431	30.770956	38.355970

H	42.306431	32.129571	39.493842
H	41.603913	32.283586	37.859946
H	38.195560	37.061860	33.369419

QM atoms (linking H atom included): 121

IVH4 Cluster1 Product

C	38.338977	38.007334	33.867344
H	37.927578	38.847549	33.291096
H	39.430700	38.124184	33.918419
S	37.651564	38.073967	35.545133
N	38.397056	37.419065	38.388604
C	37.975560	38.456804	39.186589
C	37.678041	36.313756	38.744102
C	36.970366	37.991800	40.117165
C	36.752401	36.654365	39.818890
C	37.789668	35.057328	38.149884
H	37.145886	34.265114	38.529065
C	38.642192	34.721392	37.106213
N	39.534412	35.567821	36.494234
C	40.143971	34.849451	35.494608
C	39.622907	33.487484	35.464222
C	38.693163	33.410495	36.476924
C	41.118704	35.334861	34.629857
H	41.523720	34.641566	33.892959
C	41.614900	36.635058	34.626157
C	42.641518	37.115276	33.720620
C	41.944208	38.769646	35.110640
N	41.199314	37.656015	35.458160
C	42.868983	38.435298	34.044068
C	41.786039	40.042942	35.639153
H	42.414067	40.832715	35.230504
C	40.865591	40.407203	36.619255
C	40.683243	41.759493	37.112365
N	40.017531	39.546731	37.266226
C	39.317433	40.282117	38.180872
C	38.385996	39.779726	39.079512
H	37.943457	40.485479	39.778423
Fe	39.919483	37.501677	37.038394
C	39.704080	41.684490	38.087125
C	39.143700	42.742202	38.918042
H	38.783264	42.418552	39.899102
C	39.036608	44.045230	38.605893
H	39.339345	44.440201	37.633856
H	38.613655	44.752548	39.323500

C	35.786667	35.723780	40.385346
H	35.995223	34.664516	40.205060
C	34.663728	36.024407	41.062664
H	34.354456	37.050945	41.264590
H	34.004471	35.231346	41.422829
C	41.437241	42.964421	36.654187
H	42.431403	42.705479	36.265482
H	40.906925	43.482630	35.836537
H	41.559372	43.680606	37.481465
C	36.349288	38.814859	41.199527
H	36.170224	38.203375	42.097303
H	36.992750	39.656299	41.492874
H	35.373106	39.233042	40.895627
C	37.901701	32.216238	36.913774
H	37.931079	31.418375	36.158629
H	38.296526	31.791385	37.853167
H	36.843742	32.464920	37.099693
C	43.893161	39.339586	33.434400
H	43.668655	40.405082	33.578218
H	44.893895	39.147345	33.858458
H	43.986627	39.153361	32.354457
C	43.336729	36.314936	32.663773
H	42.628863	35.644608	32.159779
H	43.708184	36.995357	31.881785
C	40.013046	32.424534	34.482010
H	41.090421	32.474724	34.271316
H	39.850946	31.434770	34.929708
C	44.511478	35.486974	33.202803
H	44.139519	34.771925	33.957749
H	45.245908	36.133823	33.708635
C	39.242504	32.480132	33.154068
H	39.422216	33.434174	32.630447
H	38.152955	32.438221	33.334244
C	39.582848	31.333797	32.173610
C	45.258412	34.653553	32.138067
O	46.481507	34.444519	32.358087
O	38.956808	31.315038	31.090468
O	44.597266	34.226418	31.161721
O	40.452518	30.499908	32.530787
O	41.188235	37.193713	38.310330
O	46.564135	33.228548	38.436321
O	47.190207	34.067183	35.800287
O	45.147436	33.052520	35.726987
O	47.431349	32.538669	37.501432

O	43.422763	31.689414	35.665702
C	45.818020	34.288686	37.793972
C	46.436627	35.626675	38.283715
C	44.365557	34.101365	38.251250
C	45.522626	36.862685	38.005461
C	45.911567	34.177829	36.272435
C	43.494514	35.299558	37.826348
C	47.862336	35.853123	37.746215
C	44.102319	36.555070	38.353225
C	43.840605	32.734732	37.787788
C	48.132479	33.496324	36.734192
C	48.742256	34.607568	37.610544
C	46.025226	38.115872	38.729303
C	44.090415	32.463128	36.316295
C	42.383957	32.471227	38.173473
C	49.144664	32.724982	35.922816
H	46.485538	35.495316	39.378186
H	44.388396	34.081105	39.353581
H	45.576359	37.049083	36.911559
H	45.459596	35.064116	35.808219
H	43.410392	35.327592	36.721647
H	42.469518	35.189253	38.198988
H	47.795413	36.326612	36.753185
H	48.382471	36.569936	38.397829
H	43.658634	37.021360	39.239399
H	42.073772	37.464353	38.008163
H	44.480558	31.990112	38.293393
H	48.979453	34.166521	38.590220
H	49.694002	34.916252	37.155165
H	49.567480	33.396061	35.164447
H	48.650199	31.887816	35.417645
H	49.950800	32.347699	36.563764
H	47.031211	38.414155	38.403008
H	45.335605	38.956588	38.554399
H	46.069137	37.941783	39.817064
H	42.127641	31.415259	38.026063
H	42.226215	32.716145	39.235071
H	41.683759	33.070863	37.573404
H	38.120713	37.088164	33.323694

QM atoms (linking H atom included): 121

IVH4 Cluster1 UTS

C	38.270592	37.955169	33.887138
H	37.789375	38.807543	33.383759

H	39.356729	38.112517	33.879675
S	37.665610	37.914111	35.596853
N	38.667704	37.483735	38.412240
C	38.198156	38.519097	39.181025
C	37.980551	36.371575	38.800142
C	37.209434	38.048910	40.133086
C	37.044865	36.699938	39.874880
C	38.096392	35.120468	38.198115
H	37.508138	34.306278	38.620248
C	38.841944	34.823291	37.066430
N	39.631795	35.713522	36.367310
C	40.169957	35.000265	35.314503
C	39.704044	33.620898	35.339581
C	38.872259	33.517883	36.431427
C	41.075351	35.510675	34.394721
H	41.434151	34.829688	33.622906
C	41.603618	36.802099	34.403275
C	42.650996	37.259297	33.505749
C	42.048838	38.876928	34.976630
N	41.259087	37.791030	35.291344
C	42.949115	38.549283	33.882226
C	41.949502	40.125525	35.575145
H	42.602292	40.909369	35.196186
C	41.043030	40.484927	36.572370
C	40.869739	41.832251	37.081038
N	40.179858	39.617947	37.193707
C	39.481156	40.353039	38.108887
C	38.556407	39.849633	39.018474
H	38.093660	40.563865	39.696379
Fe	40.109699	37.615228	36.949575
C	39.870660	41.753913	38.035389
C	39.291206	42.804859	38.863150
H	38.920980	42.480201	39.841049
C	39.170258	44.105227	38.548001
H	39.477336	44.500734	37.577640
H	38.728735	44.806022	39.260492
C	36.111830	35.749881	40.463262
H	36.377839	34.694207	40.343170
C	34.959072	36.032547	41.095713
H	34.600487	37.054021	41.233155
H	34.324113	35.232247	41.480909
C	41.635698	43.040810	36.653396
H	42.634849	42.784273	36.276472
H	41.121324	43.572145	35.834414

H	41.745811	43.743376	37.493882
C	36.563009	38.880381	41.193988
H	36.377960	38.278124	42.096759
H	37.195087	39.731482	41.485006
H	35.586238	39.284850	40.873971
C	38.153690	32.304423	36.933183
H	38.176671	31.491469	36.194339
H	38.607250	31.919136	37.862999
H	37.095788	32.517882	37.160985
C	44.027379	39.423577	33.326859
H	43.812340	40.494568	33.444904
H	44.995546	39.220973	33.816466
H	44.182581	39.222747	32.257196
C	43.347388	36.425509	32.475795
H	42.641592	35.760380	31.960482
H	43.765547	37.077866	31.694474
C	40.085561	32.544872	34.369459
H	41.154023	32.622497	34.122153
H	39.971857	31.562571	34.848947
C	44.480521	35.581448	33.081097
H	44.057532	34.890567	33.832696
H	45.200978	36.223358	33.612526
C	39.274946	32.537705	33.066801
H	39.428932	33.467937	32.495019
H	38.191954	32.495599	33.282451
C	39.593708	31.351189	32.129623
C	45.260539	34.707074	32.075570
O	46.461049	34.464438	32.371405
O	38.944481	31.293471	31.062012
O	44.643765	34.285155	31.068708
O	40.466482	30.527238	32.502112
O	41.422256	37.294675	38.027240
O	46.207291	33.580962	38.698804
O	47.245112	34.015325	36.092759
O	45.276736	32.870059	35.828246
O	47.278393	32.841202	38.066211
O	43.629332	31.414308	35.704611
C	45.514135	34.438114	37.761162
C	45.902837	35.879858	38.144597
C	44.022304	34.182865	37.959702
C	44.942338	36.993449	37.619964
C	45.897911	34.109566	36.315511
C	43.206130	35.063848	37.017671
C	47.368204	36.181812	37.771574

C	43.611499	36.524838	37.011671
C	43.739149	32.693192	37.738899
C	48.031785	33.728401	37.264751
C	48.368885	35.042521	38.005798
C	44.714554	38.049817	38.714562
C	44.183909	32.275788	36.349946
C	42.294799	32.289305	38.030993
C	49.247483	32.949575	36.814339
H	45.826233	35.857177	39.244805
H	43.781894	34.434712	39.006315
H	45.477572	37.500891	36.797680
H	45.504072	34.885246	35.644795
H	43.262726	34.661255	35.991288
H	42.142144	34.994288	37.285732
H	47.416930	36.454171	36.704678
H	47.708489	37.065910	38.334123
H	42.509005	37.069811	37.595617
H	43.462519	36.975815	36.029270
H	44.412683	32.148444	38.422576
H	48.470975	34.804227	39.074897
H	49.353628	35.385341	37.657187
H	49.788571	33.533820	36.058361
H	48.943945	31.993118	36.370603
H	49.908860	32.768556	37.671793
H	45.672707	38.446842	39.088559
H	44.107855	38.883529	38.331354
H	44.164167	37.611869	39.562286
H	42.203908	31.198475	38.106739
H	41.974562	32.721993	38.991666
H	41.601392	32.637507	37.251586
H	38.046867	37.061085	33.305222

QM atoms (linking H atom included): 121

IVH4 Cluster1 UPr

C	38.302606	37.943582	33.867877
H	37.871966	38.796115	33.322216
H	39.392729	38.064454	33.907778
S	37.603631	37.953288	35.543735
N	38.388496	37.407099	38.420633
C	37.971342	38.441990	39.219970
C	37.658959	36.312160	38.778489
C	36.951685	37.990099	40.147412
C	36.727831	36.655378	39.852309
C	37.767707	35.059913	38.172105

H	37.130699	34.263203	38.555163
C	38.588366	34.735701	37.098915
N	39.462550	35.600913	36.479944
C	40.060474	34.884490	35.464565
C	39.541329	33.520390	35.429281
C	38.628564	33.432119	36.454876
C	41.038350	35.376012	34.607495
H	41.421278	34.686971	33.853635
C	41.580402	36.666159	34.620747
C	42.605499	37.133846	33.699300
C	41.967905	38.769094	35.132156
N	41.213310	37.666690	35.482858
C	42.867303	38.441184	34.038581
C	41.823364	40.033389	35.685552
H	42.443189	40.829004	35.272986
C	40.915932	40.393137	36.685306
C	40.725354	41.745249	37.170205
N	40.074394	39.522777	37.330140
C	39.360742	40.262736	38.229995
C	38.405314	39.758802	39.110120
H	37.955321	40.471734	39.798182
Fe	39.903271	37.514423	37.057428
C	39.737009	41.668365	38.136583
C	39.158917	42.728861	38.951368
H	38.782058	42.410226	39.927662
C	39.055203	44.030574	38.632259
H	39.374938	44.423755	37.665227
H	38.616596	44.738921	39.339108
C	35.753412	35.730422	40.412868
H	35.957004	34.669733	40.232868
C	34.628797	36.035186	41.085767
H	34.322605	37.062799	41.287677
H	33.965280	35.244253	41.443067
C	41.468750	42.955069	36.706930
H	42.460044	42.703017	36.306855
H	40.927313	43.472174	35.896022
H	41.596518	43.670264	37.534354
C	36.328884	38.822039	41.221825
H	36.135308	38.214892	42.119504
H	36.978044	39.657760	41.520152
H	35.359848	39.249461	40.908119
C	37.853283	32.231733	36.903105
H	37.894751	31.425599	36.157647
H	38.252205	31.823789	37.848380

H	36.791454	32.468455	37.084890
C	43.900149	39.337051	33.432044
H	43.678137	40.404336	33.570051
H	44.896575	39.142565	33.864791
H	44.000511	39.146190	32.353668
C	43.281800	36.329037	32.633939
H	42.573495	35.642142	32.154354
H	43.629704	37.002364	31.835167
C	39.946237	32.453683	34.457861
H	41.027947	32.501887	34.266711
H	39.776218	31.466924	34.909828
C	44.477792	35.529629	33.168865
H	44.127895	34.826386	33.944882
H	45.204090	36.200979	33.653947
C	39.204012	32.497118	33.114938
H	39.396129	33.444726	32.583722
H	38.110866	32.457818	33.270141
C	39.567119	31.340244	32.155455
C	45.230742	34.678479	32.124190
O	46.452598	34.475125	32.359287
O	38.947221	31.300103	31.069267
O	44.577598	34.229918	31.152668
O	40.445467	30.523136	32.528775
O	41.130265	37.102224	38.309344
O	46.451660	33.453933	38.460443
O	47.392594	33.995970	35.845309
O	45.296008	33.094540	35.663325
O	47.359048	32.626425	37.690502
O	43.538646	31.773063	35.607968
C	45.846079	34.491134	37.650402
C	46.494040	35.820881	38.098909
C	44.345590	34.446725	37.949425
C	45.719997	37.097540	37.671783
C	46.083858	34.227549	36.165967
C	43.612483	35.568436	37.207760
C	47.974405	35.918123	37.683888
C	44.271296	36.891260	37.357394
C	43.806266	33.047021	37.627373
C	48.194522	33.467793	36.919728
C	48.784113	34.620853	37.760734
C	45.897868	38.206712	38.728461
C	44.176290	32.598443	36.224778
C	42.310908	32.881309	37.897634
C	49.229361	32.572357	36.280383

H	46.442997	35.752296	39.198612
H	44.232926	34.610505	39.033870
H	46.201076	37.469558	36.739553
H	45.739088	35.084546	35.573743
H	43.512918	35.307959	36.130342
H	42.571112	35.648824	37.558351
H	48.029515	36.280576	36.645212
H	48.470621	36.679214	38.304287
H	41.919639	37.654899	38.192151
H	43.708609	37.777655	37.047107
H	44.362742	32.348094	38.276305
H	48.888688	34.262394	38.795627
H	49.794169	34.835335	37.384776
H	49.892161	33.180777	35.651352
H	48.729870	31.833344	35.643946
H	49.823754	32.065682	37.050232
H	46.959697	38.445706	38.893457
H	45.373100	39.126232	38.426355
H	45.464970	37.886863	39.690300
H	42.010723	31.831507	37.787203
H	42.077538	33.206531	38.923020
H	41.702020	33.479044	37.206248
H	38.076982	37.044893	33.293838

QM atoms (linking H atom included): 121

IVH4 Cluster2 Reactant

C	34.954065	41.651690	35.131040
H	34.488086	42.647521	35.204612
H	35.980637	41.757967	34.753314
S	34.961495	40.942578	36.803374
N	36.408357	39.059583	38.572778
C	36.526270	39.706655	39.778176
C	35.675509	37.929637	38.804109
C	35.847919	38.967576	40.823626
C	35.290051	37.855151	40.212219
C	35.348615	36.992512	37.826856
H	34.782354	36.116208	38.140112
C	35.662750	37.072334	36.476915
N	36.352923	38.102988	35.878087
C	36.413727	37.787925	34.537189
C	35.734248	36.525100	34.272072
C	35.280161	36.076143	35.489469
C	37.078881	38.533838	33.573615
H	37.041934	38.166567	32.548102

C	37.838755	39.676250	33.816833
C	38.591642	40.387115	32.795470
C	38.881760	41.314794	34.841859
N	38.019608	40.257814	35.049984
C	39.274281	41.387308	33.447003
C	39.271323	42.228833	35.808393
H	39.918256	43.043036	35.483988
C	38.872604	42.221667	37.143416
C	39.229283	43.240789	38.108834
N	38.073151	41.265550	37.716380
C	37.904494	41.632700	39.020599
C	37.191456	40.910059	39.970574
H	37.206858	41.294627	40.987418
Fe	37.398684	39.549692	36.861590
C	38.622551	42.873219	39.297320
C	38.682318	43.501166	40.607512
H	37.988211	43.091034	41.342818
C	39.520149	44.462409	41.036914
H	40.297724	44.901022	40.411523
H	39.474124	44.800606	42.074005
C	34.465093	36.794612	40.771177
H	34.266178	35.958802	40.093338
C	33.905916	36.725899	41.993897
H	34.017507	37.505217	42.748336
H	33.303969	35.857207	42.271970
C	40.080976	44.439432	37.845764
H	40.207354	44.634300	36.773215
H	39.630548	45.338540	38.296478
H	41.083343	44.319830	38.295364
C	35.815682	39.343636	42.269517
H	34.827576	39.735749	42.569069
H	36.015977	38.467482	42.905717
H	36.569468	40.102478	42.520381
C	34.591315	34.783127	35.792006
H	35.264102	34.085730	36.315774
H	33.713190	34.918175	36.442929
H	34.254030	34.280880	34.875418
C	40.263869	42.339718	32.855731
H	40.060047	42.501484	31.787180
H	40.269349	43.318352	33.355173
H	41.288067	41.932092	32.924269
C	38.621663	40.087878	31.328794
H	37.643507	39.721222	30.992382
H	38.780521	41.032100	30.783686

C	35.593046	35.853380	32.939373
H	36.461943	36.068515	32.304249
H	35.611591	34.763807	33.086143
C	39.708164	39.090139	30.893937
H	39.522529	38.106079	31.359661
H	40.705235	39.418470	31.228538
C	34.315510	36.211767	32.164393
H	34.292720	37.290571	31.928841
H	33.413626	36.017012	32.771185
C	34.167203	35.442862	30.829966
C	39.768677	38.869773	29.364399
O	40.873177	38.563465	28.870916
O	33.062863	35.548033	30.229953
O	38.682954	39.007454	28.727594
O	35.158344	34.782028	30.437596
O	38.669564	38.644382	37.256239
O	43.339026	35.440254	34.254344
O	43.131103	36.666626	31.706342
O	41.037230	35.881815	32.168415
O	43.804568	34.893779	32.997227
O	39.088111	34.920513	32.493945
C	42.506202	36.609353	34.067219
C	43.333955	37.840133	34.515873
C	41.275597	36.372528	34.950782
C	42.458517	39.092934	34.748525
C	42.085260	36.779991	32.604717
C	40.427166	37.634205	35.081979
C	44.497116	38.131405	33.554776
C	41.261632	38.775224	35.643894
C	40.491388	35.155243	34.441313
C	44.290819	35.943938	32.198925
C	45.207350	36.909994	32.968425
C	43.273360	40.251986	35.316732
C	40.124525	35.317124	32.981115
C	39.282136	34.815077	35.312786
C	44.965360	35.304216	31.007766
H	43.747240	37.538962	35.494582
H	41.664698	36.119034	35.951447
H	42.060279	39.415415	33.766683
H	41.658990	37.783295	32.476068
H	40.006745	37.923353	34.102022
H	39.571506	37.451730	35.741458
H	44.118577	38.744011	32.719619
H	45.245943	38.745595	34.072666

H	41.617636	38.500356	36.653058
H	40.637458	39.667275	35.777830
H	41.201365	34.308668	34.449641
H	45.734910	36.331111	33.740065
H	45.966438	37.264668	32.261203
H	44.278846	34.608420	30.509296
H	45.872616	34.776036	31.330424
H	45.264717	36.088256	30.299124
H	42.596227	41.063986	35.625020
H	43.841021	39.928340	36.204008
H	43.986731	40.650379	34.580215
H	38.902971	33.809918	35.092885
H	39.568104	34.843526	36.375181
H	38.458978	35.527643	35.160187
H	34.376551	41.071389	34.411461

QM atoms (linking H atom included): 121

IVH4 Cluster2 TS

C	34.945815	41.710412	35.097906
H	34.455944	42.695704	35.154838
H	35.967025	41.838627	34.710994
S	34.985509	41.025471	36.781936
N	36.587356	39.199260	38.497023
C	36.677494	39.861677	39.693295
C	35.884490	38.054642	38.730772
C	36.029693	39.102521	40.748495
C	35.512366	37.968348	40.143983
C	35.551960	37.122414	37.748638
H	34.998721	36.239093	38.066057
C	35.835443	37.214095	36.390404
N	36.505242	38.250321	35.779214
C	36.555730	37.936402	34.438879
C	35.879005	36.670081	34.181342
C	35.448747	36.215224	35.406645
C	37.229953	38.681698	33.477648
H	37.188167	38.316967	32.451356
C	38.002499	39.818635	33.719283
C	38.765141	40.519518	32.697756
C	39.023158	41.482635	34.735584
N	38.173237	40.415620	34.945246
C	39.434169	41.534107	33.341020
C	39.369893	42.420710	35.699222
H	40.011078	43.238871	35.375383
C	38.945532	42.436730	37.029858

C	39.330950	43.431842	38.010327
N	38.119365	41.499099	37.594263
C	37.972313	41.841500	38.908159
C	37.291707	41.095885	39.867710
H	37.306243	41.483917	40.883642
Fe	37.485254	39.767810	36.734106
C	38.718277	43.062460	39.196541
C	38.801770	43.668378	40.517210
H	38.067177	43.303804	41.238838
C	39.702711	44.558869	40.970694
H	40.521394	44.944617	40.362920
H	39.667606	44.883939	42.012639
C	34.755394	36.865655	40.717838
H	34.665355	35.983604	40.075231
C	34.154512	36.805935	41.920638
H	34.161251	37.631895	42.632812
H	33.622852	35.901168	42.225320
C	40.224941	44.604347	37.772171
H	40.358123	44.814557	36.704189
H	39.808477	45.508427	38.244855
H	41.222182	44.437589	38.218178
C	36.006069	39.475606	42.195297
H	35.027951	39.888939	42.500676
H	36.187666	38.593202	42.828303
H	36.778179	40.216849	42.443429
C	34.799018	34.902782	35.716421
H	35.505995	34.225525	36.222906
H	33.930095	35.007444	36.385536
H	34.459438	34.395212	34.803405
C	40.416273	42.485781	32.735901
H	40.161009	42.698984	31.687181
H	40.471727	43.441403	33.272712
H	41.430654	42.049334	32.727280
C	38.790227	40.202721	31.235515
H	37.792627	39.892557	30.895457
H	39.011796	41.128176	30.680176
C	35.717657	35.991291	32.853092
H	36.544419	36.257303	32.182818
H	35.805365	34.903821	32.992310
C	39.805718	39.130256	30.809657
H	39.551361	38.163062	31.279826
H	40.824729	39.386920	31.140131
C	34.388808	36.280549	32.135417
H	34.304562	37.353595	31.888694

H	33.528271	36.053383	32.789537
C	34.202890	35.484317	30.821433
C	39.834797	38.907919	29.280169
O	40.916791	38.558244	28.767432
O	33.088444	35.586099	30.241885
O	38.747487	39.091350	28.658839
O	35.177252	34.799669	30.423675
O	38.895952	38.910913	37.214338
O	43.325151	35.397481	34.345045
O	42.929640	36.746441	31.879147
O	40.902444	35.780102	32.279643
O	43.821540	34.989326	33.054897
O	39.020438	34.685393	32.556782
C	42.337773	36.448911	34.241678
C	42.996405	37.742161	34.793816
C	41.179412	35.936419	35.103147
C	41.932760	38.833219	35.158733
C	41.889155	36.701993	32.792115
C	40.179710	37.038914	35.450672
C	44.101011	38.251404	33.847240
C	40.920226	38.187666	36.074026
C	40.543509	34.707672	34.440265
C	44.171966	36.142151	32.329650
C	44.953928	37.164102	33.175103
C	42.568423	40.079747	35.773814
C	40.065708	35.052687	33.044544
C	39.472065	34.056814	35.313790
C	44.925239	35.648114	31.115649
H	43.466941	37.424743	35.739958
H	41.644076	35.596120	36.043101
H	41.418746	39.137772	34.228050
H	41.382893	37.676994	32.758839
H	39.641965	37.382882	34.548107
H	39.416731	36.658334	36.141312
H	43.647801	38.872210	33.056579
H	44.781007	38.909090	34.407432
H	41.330717	37.952492	37.070064
H	39.850303	38.908147	36.569340
H	41.371936	33.996583	34.283110
H	45.555009	36.605994	33.906660
H	45.660571	37.657839	32.499221
H	44.350046	34.861486	30.609371
H	45.902969	35.253418	31.421826
H	45.100901	36.481101	30.421857

H	41.783019	40.783807	36.087214
H	43.164643	39.814618	36.661353
H	43.227362	40.592970	35.058032
H	39.339276	32.998044	35.058858
H	39.778473	34.096601	36.370325
H	38.500483	34.562964	35.215707
H	34.382041	41.103993	34.389046

QM atoms (linking H atom included): 121

IVH4 Cluster2 Product

C	34.904663	41.704435	35.127166
H	34.423345	42.694455	35.168040
H	35.933890	41.813152	34.757050
S	34.900844	41.023788	36.814512
N	36.361205	39.052399	38.582251
C	36.502584	39.693131	39.786722
C	35.626081	37.926559	38.814051
C	35.828908	38.953030	40.838194
C	35.256026	37.847588	40.227657
C	35.297601	36.992063	37.830843
H	34.732790	36.114805	38.145050
C	35.609919	37.070912	36.475965
N	36.297470	38.100916	35.882046
C	36.361088	37.798353	34.539080
C	35.685265	36.532309	34.267271
C	35.235441	36.073967	35.483424
C	37.034141	38.552585	33.583205
H	36.993047	38.189489	32.555575
C	37.807934	39.694271	33.820334
C	38.572690	40.396320	32.798151
C	38.878285	41.318569	34.845796
N	38.001526	40.271329	35.048589
C	39.274527	41.383319	33.450383
C	39.257545	42.236882	35.815055
H	39.909261	43.048569	35.492394
C	38.853584	42.238259	37.153287
C	39.212765	43.250793	38.124110
N	38.061374	41.276934	37.725990
C	37.897554	41.629327	39.034349
C	37.186837	40.890623	39.979296
H	37.213060	41.265774	40.999941
Fe	37.298882	39.596300	36.851993
C	38.615975	42.870128	39.315428
C	38.683756	43.491806	40.628538

H	37.984960	43.085096	41.361165
C	39.535337	44.440031	41.060896
H	40.319113	44.870243	40.437264
H	39.495503	44.775719	42.099468
C	34.431750	36.789296	40.792986
H	34.265659	35.930524	40.135330
C	33.838726	36.749601	42.000757
H	33.912629	37.555265	42.732002
H	33.243569	35.879196	42.288507
C	40.054088	44.456770	37.860818
H	40.141386	44.675134	36.788477
H	39.619181	45.345095	38.346443
H	41.072762	44.330832	38.270810
C	35.817856	39.322719	42.286083
H	34.850662	39.761799	42.589351
H	35.975437	38.434750	42.917795
H	36.606673	40.044569	42.538782
C	34.569339	34.768514	35.785026
H	35.244335	34.096301	36.338456
H	33.669784	34.890533	36.408698
H	34.270093	34.244848	34.867419
C	40.279605	42.320193	32.860329
H	40.097855	42.463580	31.785323
H	40.279106	43.308010	33.342420
H	41.301073	41.911896	32.957955
C	38.596980	40.098937	31.330911
H	37.621246	39.721654	30.999845
H	38.743350	41.045037	30.785029
C	35.555380	35.863357	32.931934
H	36.425313	36.087911	32.300868
H	35.580743	34.773155	33.074256
C	39.693430	39.113390	30.897232
H	39.515557	38.128442	31.364075
H	40.683859	39.455356	31.236751
C	34.279221	36.215450	32.151460
H	34.253227	37.293923	31.913628
H	33.376428	36.018579	32.755927
C	34.138841	35.443350	30.818500
C	39.768348	38.883394	29.370602
O	40.879811	38.575568	28.892799
O	33.035807	35.542133	30.214835
O	38.689002	39.012763	28.722362
O	35.133474	34.785909	30.429389
O	38.716094	38.583167	37.304091

O	43.296988	35.523787	34.214272
O	43.156818	36.656927	31.620121
O	41.050599	35.902935	32.083202
O	43.763294	34.916340	32.984496
O	39.096713	34.954090	32.419530
C	42.494639	36.702233	33.966567
C	43.348917	37.929493	34.373765
C	41.244724	36.533022	34.838532
C	42.492348	39.225568	34.509897
C	42.096199	36.814444	32.493004
C	40.406296	37.827890	34.875311
C	44.536761	38.151548	33.426775
C	41.272546	38.949820	35.321435
C	40.440337	35.309329	34.382668
C	44.289832	35.922220	32.153610
C	45.223154	36.889993	32.901177
C	43.303141	40.389430	35.070024
C	40.119221	35.384102	32.905473
C	39.193208	35.058016	35.230975
C	44.959124	35.226052	30.992513
H	43.728640	37.674424	35.378306
H	41.604813	36.333321	35.861322
H	42.161771	39.497974	33.486891
H	41.679992	37.812426	32.307316
H	40.000456	38.035314	33.867903
H	39.550714	37.697388	35.546765
H	44.189299	38.737875	32.561024
H	45.291744	38.765692	33.935573
H	41.291146	39.239033	36.378302
H	39.517347	39.106255	37.149069
H	41.124906	34.445697	34.466805
H	45.722044	36.329282	33.703722
H	46.001632	37.200597	32.194026
H	44.254358	34.549154	30.493368
H	45.836830	34.668698	31.346285
H	45.303609	35.981919	30.273888
H	42.628599	41.231591	35.283888
H	43.801971	40.102801	36.010903
H	44.069013	40.724666	34.357237
H	38.787489	34.055266	35.049597
H	39.442445	35.142101	36.299450
H	38.398254	35.784255	35.011115
H	34.344027	41.101183	34.413134

QM atoms (linking H atom included): 121

IVH4 Cluster2 UTS

C	34.889931	41.742346	35.148001
H	34.384137	42.716030	35.248495
H	35.902881	41.898914	34.753236
S	34.972561	40.986253	36.800418
N	36.687301	39.157514	38.474544
C	36.762193	39.815818	39.674694
C	35.997670	38.002952	38.705940
C	36.125277	39.043827	40.727267
C	35.623873	37.906189	40.117911
C	35.663871	37.077682	37.719967
H	35.146881	36.172604	38.036894
C	35.884518	37.212659	36.353543
N	36.479005	38.291415	35.740375
C	36.463479	38.018766	34.387357
C	35.841669	36.724709	34.133190
C	35.484983	36.225861	35.364564
C	37.034214	38.829296	33.414697
H	36.962300	38.486984	32.382379
C	37.763299	39.997495	33.648275
C	38.524744	40.693382	32.625166
C	38.843148	41.619232	34.671907
N	37.970913	40.570194	34.879614
C	39.227612	41.684260	33.272109
C	39.285353	42.492585	35.658203
H	39.940768	43.300166	35.335800
C	38.932677	42.460048	37.008702
C	39.338436	43.437711	37.999242
N	38.131350	41.503192	37.576422
C	38.005702	41.826814	38.895819
C	37.347426	41.062466	39.856274
H	37.357399	41.444087	40.874729
Fe	37.499042	39.788787	36.688411
C	38.742551	43.051711	39.188563
C	38.822556	43.652976	40.511792
H	38.088464	43.282574	41.231442
C	39.717364	44.548434	40.967465
H	40.534287	44.939327	40.360716
H	39.678747	44.872519	42.009580
C	34.854570	36.805412	40.679154
H	34.769982	35.924654	40.034258
C	34.229173	36.751842	41.869436
H	34.228688	37.578982	42.580248

H	33.682186	35.852949	42.163782
C	40.220902	44.619471	37.767407
H	40.353585	44.836146	36.701296
H	39.795937	45.517213	38.244960
H	41.218469	44.458271	38.214207
C	36.084089	39.419233	42.173114
H	35.103504	39.836824	42.464868
H	36.254099	38.537155	42.809535
H	36.855613	40.158292	42.429710
C	34.879734	34.892091	35.670761
H	35.609208	34.233719	36.169679
H	34.010503	34.969863	36.343801
H	34.548314	34.381032	34.756724
C	40.270719	42.576384	32.678490
H	40.074653	42.756419	31.611811
H	40.341477	43.548463	33.182547
H	41.266155	42.101865	32.739460
C	38.614067	40.318199	31.180062
H	37.645147	39.959168	30.807149
H	38.842688	41.218509	30.588997
C	35.679323	36.050664	32.803911
H	36.487433	36.349036	32.124247
H	35.806898	34.965629	32.934579
C	39.687770	39.257637	30.876258
H	39.428173	38.311347	31.384313
H	40.671609	39.567352	31.263101
C	34.333454	36.292935	32.104305
H	34.209502	37.360244	31.850439
H	33.490395	36.042696	32.772553
C	34.159841	35.477094	30.801661
C	39.832536	38.946402	29.368153
O	40.950313	38.575579	28.959681
O	33.046287	35.563702	30.217409
O	38.788599	39.089338	28.664728
O	35.140981	34.793679	30.419210
O	39.001382	38.971320	36.955276
O	43.193244	35.459130	34.445435
O	43.152630	36.683430	31.883614
O	41.118150	35.665164	32.148066
O	43.802642	34.945081	33.236757
O	39.285467	34.464951	32.310237
C	42.288340	36.552283	34.164326
C	42.955756	37.818090	34.731611
C	40.974390	36.237461	34.875257

C	41.992967	39.032619	34.857657
C	42.014158	36.682346	32.663361
C	39.963564	37.353607	34.623533
C	44.213753	38.198714	33.919821
C	40.494709	38.732176	34.933315
C	40.452342	34.885684	34.380030
C	44.299133	36.030104	32.488667
C	45.060047	37.047657	33.356809
C	42.431323	39.964150	35.996368
C	40.219115	34.979497	32.882641
C	39.225408	34.397890	35.150728
C	45.125360	35.436585	31.369421
H	43.264508	37.508180	35.744526
H	41.187395	36.169820	35.954454
H	42.116507	39.607898	33.919209
H	41.497053	37.632175	32.470026
H	39.625401	37.312739	33.571359
H	39.054090	37.176472	35.214160
H	43.898960	38.823648	33.068328
H	44.869133	38.830994	34.536867
H	39.848903	38.969127	36.119853
H	39.954765	39.496191	34.381331
H	41.277372	34.164599	34.504888
H	45.583761	36.488037	34.142097
H	45.832526	37.490674	32.718322
H	44.527166	34.710051	30.804248
H	46.021794	34.952579	31.779680
H	45.450872	36.237146	30.691030
H	41.788530	40.856737	36.041914
H	42.350004	39.442436	36.962303
H	43.476446	40.286486	35.866633
H	39.119116	33.308309	35.076835
H	39.334692	34.641446	36.218647
H	38.298201	34.862966	34.785190
H	34.327792	41.148844	34.427014

QM atoms (linking H atom included): 121

IVH4 Cluster2 UPr

C	34.911364	41.751366	35.126777
H	34.421742	42.736899	35.174591
H	35.936515	41.869861	34.748712
S	34.926526	41.061787	36.810725
N	36.389944	39.082428	38.565216
C	36.543165	39.714023	39.771115

C	35.659293	37.952080	38.796088
C	35.884839	38.964151	40.825480
C	35.307604	37.861664	40.213679
C	35.323496	37.022455	37.812148
H	34.759157	36.145236	38.127374
C	35.634079	37.100397	36.455519
N	36.313291	38.132723	35.860594
C	36.381404	37.828419	34.517692
C	35.715216	36.555808	34.248663
C	35.266068	36.098320	35.465389
C	37.046831	38.587436	33.561462
H	37.010283	38.223117	32.534150
C	37.802513	39.743745	33.795174
C	38.550615	40.454310	32.767620
C	38.834336	41.402028	34.807320
N	37.984214	40.332290	35.018741
C	39.225038	41.466571	33.410633
C	39.228857	42.307237	35.781237
H	39.863097	43.132062	35.456643
C	38.865816	42.277556	37.132373
C	39.233029	43.284523	38.106924
N	38.094426	41.303259	37.708597
C	37.936772	41.650859	39.020188
C	37.227557	40.912415	39.964539
H	37.255647	41.285097	40.986270
Fe	37.311024	39.629663	36.833315
C	38.649464	42.894434	39.301337
C	38.717489	43.514586	40.615341
H	38.008987	43.118091	41.344701
C	39.576682	44.454253	41.050784
H	40.369373	44.873901	40.431020
H	39.532515	44.792207	42.088294
C	34.507223	36.788717	40.785024
H	34.338718	35.934204	40.122184
C	33.941276	36.730984	42.004962
H	34.020796	37.532624	42.740081
H	33.363961	35.851129	42.300321
C	40.067892	44.495427	37.845972
H	40.149606	44.720335	36.774965
H	39.631816	45.377831	38.341277
H	41.088630	44.369397	38.250228
C	35.903571	39.315295	42.278092
H	34.944659	39.752442	42.609171
H	36.072549	38.418242	42.894252

H	36.700541	40.031362	42.521844
C	34.608636	34.789190	35.770494
H	35.297623	34.116388	36.306172
H	33.721565	34.905252	36.413184
H	34.292686	34.271040	34.855393
C	40.219548	42.409730	32.812248
H	40.007888	42.580007	31.746607
H	40.243697	43.385060	33.316858
H	41.238904	41.987747	32.866716
C	38.599034	40.133923	31.306458
H	37.629694	39.748656	30.965117
H	38.754118	41.070250	30.746883
C	35.584788	35.882501	32.914989
H	36.446530	36.118065	32.276442
H	35.626667	34.792979	33.058563
C	39.704439	39.143523	30.905721
H	39.523884	38.165900	31.386648
H	40.689975	39.493041	31.252488
C	34.297442	36.216667	32.144371
H	34.255220	37.294026	31.905019
H	33.402353	36.009064	32.756539
C	34.153207	35.440540	30.814254
C	39.796706	38.894418	29.382157
O	40.913269	38.584864	28.919006
O	33.049208	35.539935	30.212508
O	38.723285	39.015281	28.721955
O	35.145813	34.779040	30.426140
O	38.718133	38.588404	37.270080
O	43.289289	35.475708	34.255048
O	43.176393	36.678230	31.689965
O	41.071326	35.895837	32.114736
O	43.770864	34.901528	33.014872
O	39.161455	34.850203	32.408828
C	42.485123	36.657773	34.027907
C	43.331250	37.864152	34.494979
C	41.221083	36.469169	34.868957
C	42.509438	39.165490	34.683637
C	42.105171	36.807717	32.554835
C	40.346989	37.726462	34.854259
C	44.532307	38.117291	33.569466
C	41.123836	38.942282	35.184233
C	40.464840	35.222587	34.397652
C	44.305130	35.930694	32.218006
C	45.226913	36.878222	33.004101

C	43.249810	40.151418	35.592950
C	40.159099	35.311935	32.916206
C	39.218000	34.926067	35.231821
C	44.992029	35.267308	31.047477
H	43.698565	37.553326	35.487728
H	41.555660	36.293775	35.904417
H	42.428525	39.643254	33.679572
H	41.681981	37.808029	32.390831
H	39.856083	37.840172	33.860064
H	39.515831	37.623097	35.565602
H	44.188828	38.730046	32.720373
H	45.280931	38.720529	34.100341
H	39.545312	39.083507	37.165807
H	40.599142	39.797203	35.614249
H	41.174176	34.380114	34.481853
H	45.727883	36.289640	33.785523
H	46.005792	37.216780	32.310525
H	44.299744	34.588177	30.534352
H	45.878250	34.718612	31.393532
H	45.327822	36.041167	30.343719
H	42.668449	41.079628	35.703916
H	43.375199	39.711223	36.593566
H	44.246825	40.393960	35.198934
H	38.837715	33.917449	35.030870
H	39.461777	34.990686	36.302894
H	38.407677	35.638586	35.022080
H	34.351716	41.144506	34.415031

QM atoms (linking H atom included): 121

IVH4 Cluster3 Reactant

C	36.385225	40.785841	34.189028
H	35.847492	41.748248	34.187049
H	37.455200	40.961223	34.016856
S	36.103917	40.019386	35.818554
N	37.380993	38.166852	37.834937
C	37.261078	38.823340	39.038037
C	36.712055	36.984957	37.970884
C	36.507353	38.025194	39.982591
C	36.144839	36.867710	39.309889
C	36.571394	36.044047	36.954723
H	36.039070	35.123133	37.187515
C	37.026148	36.181549	35.654642
N	37.707005	37.269579	35.149056
C	37.960815	36.970942	33.827303

C	37.378123	35.683267	33.471510
C	36.834091	35.176497	34.627180
C	38.733574	37.739878	32.967318
H	38.849192	37.384274	31.943263
C	39.399285	38.913233	33.313564
C	40.204987	39.701208	32.389323
C	40.161433	40.622720	34.462636
N	39.374700	39.491808	34.560964
C	40.707609	40.751776	33.123201
C	40.306686	41.575785	35.456741
H	40.888559	42.461772	35.208021
C	39.706572	41.541120	36.715420
C	39.708858	42.648037	37.649261
N	38.975560	40.488609	37.206519
C	38.508448	40.881287	38.431052
C	37.743250	40.099889	39.290004
H	37.521220	40.512509	40.271323
Fe	38.558973	38.727626	36.263958
C	38.943906	42.240265	38.730519
C	38.588122	42.953729	39.947411
H	37.844873	42.451648	40.573477
C	39.080774	44.115160	40.415654
H	39.856328	44.683493	39.902108
H	38.730747	44.501344	41.375115
C	35.344602	35.735388	39.749887
H	35.242976	34.928667	39.016672
C	34.701628	35.563358	40.920472
H	34.711442	36.298345	41.725336
H	34.124370	34.652500	41.097428
C	40.374521	43.970169	37.444117
H	41.237544	44.083274	38.122984
H	40.721514	44.112402	36.413063
H	39.675492	44.793098	37.665716
C	36.215924	38.391223	41.401640
H	36.748250	39.298124	41.716682
H	35.135464	38.547508	41.567125
H	36.524768	37.582056	42.083605
C	36.244125	33.823679	34.868575
H	36.379158	33.174037	33.994970
H	36.733887	33.320833	35.717195
H	35.165020	33.855490	35.094880
C	41.634521	41.827288	32.649350
H	41.575317	41.935766	31.556730
H	41.418450	42.807839	33.103059

H	42.685593	41.588236	32.891192
C	40.440884	39.412981	30.937020
H	39.599526	38.841642	30.520681
H	40.469969	40.356943	30.371768
C	37.399438	35.054253	32.116252
H	38.362130	35.228647	31.615463
H	37.313395	33.963285	32.237106
C	41.748189	38.660328	30.664510
H	41.746205	37.669991	31.142784
H	42.590251	39.216604	31.116071
C	36.290358	35.504856	31.149239
H	36.380751	36.588872	30.951256
H	35.289408	35.331281	31.575793
C	36.393643	34.750155	29.798836
C	42.113440	38.466702	29.167519
O	42.955428	37.570880	28.930420
O	35.346244	34.372493	29.253481
O	41.582647	39.233403	28.329304
O	37.574724	34.580181	29.363510
O	39.811059	37.828898	36.744180
O	46.202933	36.807423	34.420097
O	45.633204	38.420345	32.144319
O	44.087989	36.757944	32.118576
O	46.950915	36.854124	33.183274
O	42.890976	34.924372	31.890548
C	44.949308	37.532082	34.339387
C	45.146826	38.800593	35.201835
C	43.882115	36.598447	34.917942
C	43.850222	39.464793	35.729040
C	44.590004	37.871461	32.882938
C	42.555799	37.347852	35.084950
C	46.050040	39.808534	34.483947
C	42.742637	38.470016	36.097626
C	43.828716	35.321822	34.074231
C	46.946523	38.174243	32.688737
C	47.271162	39.220010	33.774887
C	44.168875	40.323920	36.957779
C	43.530544	35.639625	32.626634
C	42.938424	34.227096	34.650526
C	47.930912	38.179011	31.536524
H	45.688984	38.420829	36.081135
H	44.231632	36.311049	35.924524
H	43.461133	40.122613	34.928942
H	43.773608	38.608191	32.889251

H	42.195918	37.743848	34.118179
H	41.773649	36.665180	35.437176
H	45.453489	40.364294	33.744906
H	46.411570	40.538238	35.216249
H	42.989269	38.004836	37.069592
H	41.796031	39.002604	36.256040
H	44.871817	34.961483	34.045174
H	47.964498	38.758037	34.493686
H	47.804126	40.047608	33.284510
H	47.822229	39.117704	30.975437
H	47.732950	37.331821	30.868947
H	48.957127	38.093782	31.919508
H	45.065010	40.938784	36.815972
H	43.324272	40.976576	37.229160
H	44.376575	39.669160	37.820647
H	42.946222	33.340005	34.003400
H	43.306160	33.935178	35.646477
H	41.896102	34.553531	34.769083
H	35.991807	40.172590	33.378341

QM atoms (linking H atom included): 121

IVH4 Cluster3 TS

C	36.360546	40.850917	34.169401
H	35.800398	41.800066	34.139570
H	37.427168	41.050449	34.001391
S	36.092303	40.118708	35.817246
N	37.504332	38.290736	37.787673
C	37.388291	38.942619	38.990150
C	36.846740	37.105769	37.922366
C	36.660408	38.126262	39.945540
C	36.309471	36.965706	39.273866
C	36.682507	36.181632	36.890796
H	36.145398	35.261759	37.118406
C	37.128535	36.326944	35.584381
N	37.819090	37.409379	35.078180
C	38.086401	37.107693	33.762866
C	37.507670	35.815185	33.407461
C	36.947392	35.315502	34.559619
C	38.867389	37.882455	32.908797
H	38.993504	37.521534	31.887231
C	39.518292	39.069385	33.246298
C	40.319111	39.861512	32.317840
C	40.208647	40.830501	34.369593
N	39.472149	39.668414	34.484291

C	40.779237	40.942575	33.035784
C	40.296664	41.808813	35.350176
H	40.847420	42.713355	35.093799
C	39.703550	41.762794	36.614348
C	39.730389	42.842278	37.579534
N	38.997654	40.692034	37.105669
C	38.567257	41.044549	38.355219
C	37.847742	40.230942	39.228766
H	37.641737	40.632708	40.217997
Fe	38.605801	38.937941	36.167458
C	39.002645	42.399487	38.674234
C	38.681631	43.074661	39.922429
H	37.960716	42.550880	40.557492
C	39.175866	44.228472	40.406388
H	39.925669	44.820466	39.882559
H	38.853093	44.582017	41.387449
C	35.555046	35.805786	39.724990
H	35.441380	35.010608	38.980707
C	34.977419	35.591836	40.922313
H	35.016728	36.306028	41.744250
H	34.430826	34.663891	41.106161
C	40.403737	44.163836	37.404205
H	41.248466	44.265136	38.107629
H	40.781091	44.310194	36.385491
H	39.703058	44.988766	37.614652
C	36.376582	38.482490	41.367700
H	36.844707	39.429586	41.662252
H	35.291603	38.556285	41.556855
H	36.762432	37.706300	42.049203
C	36.361067	33.959445	34.802007
H	36.415058	33.336252	33.900697
H	36.909234	33.423207	35.594199
H	35.305796	33.993350	35.119414
C	41.701632	42.020613	32.558446
H	41.636343	42.132964	31.466440
H	41.493509	42.999646	33.018091
H	42.754320	41.775901	32.788391
C	40.568678	39.548156	30.872613
H	39.709086	39.007281	30.450834
H	40.643552	40.482652	30.296556
C	37.540342	35.168565	32.061339
H	38.500190	35.348433	31.558048
H	37.467439	34.078603	32.197047
C	41.842980	38.734631	30.618488

H	41.806725	37.763817	31.135996
H	42.714901	39.273323	31.034040
C	36.421121	35.586826	31.091105
H	36.499764	36.666141	30.865669
H	35.425120	35.414544	31.529572
C	36.526698	34.799236	29.761330
C	42.173020	38.456719	29.126764
O	43.001253	37.539750	28.921024
O	35.484583	34.391852	29.227821
O	41.626893	39.180288	28.261519
O	37.709715	34.636984	29.327252
O	39.973231	38.049134	36.753183
O	46.012326	36.910056	34.584790
O	45.347359	38.441458	32.281565
O	44.032903	36.589769	32.160297
O	46.809389	37.063591	33.390730
O	42.967770	34.683927	31.874974
C	44.675976	37.443199	34.429401
C	44.620504	38.732814	35.293364
C	43.750776	36.341911	34.955041
C	43.176123	39.190301	35.684813
C	44.348855	37.747373	32.957263
C	42.319921	36.871363	35.115830
C	45.434921	39.864309	34.646947
C	42.357635	37.995792	36.108648
C	43.871170	35.092822	34.076204
C	46.650144	38.376486	32.903126
C	46.765979	39.435581	34.019054
C	43.202606	40.240092	36.797771
C	43.550533	35.422034	32.633738
C	43.095949	33.895956	34.621820
C	47.694901	38.531089	31.815770
H	45.126209	38.437606	36.227824
H	44.124113	36.077065	35.958518
H	42.709216	39.633473	34.785468
H	43.441466	38.367640	32.922923
H	41.913531	37.219084	34.149088
H	41.664789	36.067388	35.460982
H	44.827706	40.361487	33.872509
H	45.650963	40.618526	35.415922
H	42.598013	37.651374	37.127202
H	41.046631	38.267357	36.360281
H	44.950176	34.856992	34.055452
H	47.455593	39.044077	34.779788

H	47.233618	40.326683	33.579144
H	47.470107	39.433107	31.230897
H	47.694970	37.652865	31.156065
H	48.688384	38.633334	32.274226
H	43.757809	41.141000	36.510906
H	42.178550	40.537502	37.064577
H	43.684351	39.824217	37.698830
H	43.076253	33.071868	33.898122
H	43.562827	33.539881	35.552913
H	42.054950	34.157381	34.857805
H	35.990893	40.210040	33.368963

QM atoms (linking H atom included): 121

IVH4 Cluster3 Product

C	36.302112	40.899027	34.172551
H	35.741393	41.846388	34.119242
H	37.371861	41.092379	34.017448
S	36.003078	40.175085	35.819948
N	37.361102	38.244608	37.811975
C	37.263999	38.894507	39.017661
C	36.696108	37.063701	37.947389
C	36.533209	38.083301	39.974412
C	36.162572	36.928622	39.300779
C	36.543509	36.132761	36.918496
H	36.016272	35.207817	37.150677
C	36.994049	36.272092	35.612614
N	37.667932	37.361581	35.107031
C	37.956268	37.058381	33.796398
C	37.399163	35.755530	33.441772
C	36.837618	35.252279	34.591431
C	38.745581	37.830552	32.945833
H	38.880738	37.461666	31.928184
C	39.406497	39.015969	33.278623
C	40.227022	39.795845	32.355235
C	40.137263	40.752335	34.413056
N	39.364321	39.614070	34.513629
C	40.709958	40.862205	33.080901
C	40.260298	41.712675	35.409148
H	40.843150	42.600622	35.164411
C	39.663157	41.675176	36.673228
C	39.694759	42.759006	37.633651
N	38.934331	40.618546	37.160020
C	38.495817	40.980372	38.401883
C	37.752505	40.173114	39.264430

H	37.551200	40.572432	40.255878
Fe	38.452949	38.886852	36.198817
C	38.947753	42.331138	38.722026
C	38.623374	43.016731	39.963150
H	37.900750	42.497629	40.599567
C	39.121015	44.171775	40.441686
H	39.874533	44.757709	39.915783
H	38.797269	44.534687	41.419268
C	35.397247	35.776987	39.754138
H	35.269999	34.985279	39.008158
C	34.820075	35.566652	40.952525
H	34.866325	36.279775	41.775374
H	34.265042	34.643385	41.135741
C	40.378568	44.075090	37.449679
H	41.229120	44.175481	38.145816
H	40.749402	44.216285	36.427025
H	39.685830	44.906644	37.660323
C	36.275772	38.432172	41.403837
H	36.780019	39.359567	41.704383
H	35.196222	38.541458	41.607072
H	36.641568	37.635238	42.072259
C	36.273026	33.888843	34.838169
H	36.382706	33.248347	33.954584
H	36.799646	33.383709	35.664211
H	35.203724	33.903949	35.106575
C	41.649491	41.928585	32.609899
H	41.599228	42.035263	31.516501
H	41.440913	42.912253	33.060035
H	42.697648	41.681275	32.857014
C	40.487042	39.485015	30.911749
H	39.643514	38.920847	30.489409
H	40.541421	40.419105	30.332130
C	37.456631	35.110968	32.095145
H	38.428547	35.287447	31.613160
H	37.374545	34.020580	32.223564
C	41.784910	38.705849	30.667897
H	41.765056	37.728614	31.173576
H	42.633528	39.263521	31.106618
C	36.363560	35.547288	31.103703
H	36.457264	36.628228	30.890852
H	35.356474	35.382149	31.518172
C	36.487183	34.775957	29.766627
C	42.149242	38.458794	29.177986
O	42.982743	37.546420	28.972657

O	35.449747	34.390006	29.207938
O	41.623629	39.200340	28.314939
O	37.675565	34.604628	29.351382
O	39.875491	37.924802	36.712245
O	46.174598	36.870099	34.486047
O	45.520213	38.422762	32.196267
O	44.113053	36.639522	32.132381
O	46.943474	36.975910	33.266813
O	42.957928	34.780543	31.892264
C	44.864633	37.476385	34.371212
C	44.919259	38.772895	35.223699
C	43.898016	36.430382	34.940942
C	43.519930	39.312235	35.667490
C	44.507905	37.785352	32.907399
C	42.494840	37.033946	35.150355
C	45.759623	39.853869	34.534830
C	42.637208	38.183748	36.079330
C	43.918668	35.170240	34.071192
C	46.838223	38.291589	32.773212
C	47.046968	39.356272	33.871043
C	43.636938	40.337755	36.794447
C	43.587400	35.500963	32.630290
C	43.082966	34.025363	34.638017
C	47.850123	38.384066	31.648599
H	45.443161	38.460265	36.140237
H	44.293398	36.156781	35.933014
H	43.067638	39.803502	34.781658
H	43.633269	38.452830	32.892491
H	42.066625	37.355401	34.181174
H	41.817751	36.276937	35.554638
H	45.148871	40.366624	33.774484
H	46.035888	40.604970	35.285211
H	42.490246	38.003953	37.149954
H	40.691702	38.368014	36.408526
H	44.980549	34.869382	34.031292
H	47.743143	38.943872	34.616262
H	47.537971	40.219932	33.401481
H	47.660885	39.302251	31.075730
H	47.770167	37.512519	30.985776
H	48.864849	38.417233	32.068691
H	44.286215	41.172883	36.519058
H	42.646217	40.739977	37.056671
H	44.066870	39.866908	37.693190
H	43.066098	33.172592	33.947695

H	43.506336	33.693381	35.598600
H	42.042790	34.327276	34.825075
H	35.946657	40.247066	33.374639

QM atoms (linking H atom included): 121

IVH4 Cluster3 UTS

C	36.229404	40.952672	34.151202
H	35.630173	41.877944	34.133811
H	37.283257	41.192129	33.959211
S	36.037068	40.199819	35.798836
N	37.621783	38.448451	37.740415
C	37.487660	39.097612	38.942721
C	36.971544	37.257528	37.873804
C	36.773419	38.268802	39.899151
C	36.436934	37.107563	39.224390
C	36.816477	36.331125	36.844865
H	36.315300	35.394139	37.083882
C	37.222956	36.497703	35.527802
N	37.853734	37.607773	35.004132
C	38.085719	37.319221	33.675458
C	37.555375	36.001298	33.339696
C	37.042074	35.485050	34.506342
C	38.796593	38.134662	32.800300
H	38.919828	37.777510	31.776938
C	39.400259	39.351765	33.124661
C	40.215782	40.134286	32.204674
C	40.115306	41.097063	34.259645
N	39.351066	39.951531	34.360280
C	40.690509	41.206064	32.928089
C	40.261511	42.040327	35.268613
H	40.829485	42.937508	35.022937
C	39.708886	41.969567	36.550677
C	39.783921	43.019787	37.546026
N	38.987711	40.903885	37.029339
C	38.598538	41.228784	38.298108
C	37.910421	40.396851	39.179860
H	37.714098	40.786030	40.175856
Fe	38.627210	39.164591	36.070910
C	39.062810	42.566533	38.641292
C	38.769550	43.211800	39.911345
H	38.057835	42.675477	40.547113
C	39.269754	44.354630	40.413232
H	40.007276	44.961280	39.889383
H	38.964433	44.680483	41.409250

C	35.665143	35.955846	39.672810
H	35.248786	35.331156	38.873859
C	35.396523	35.584377	40.937842
H	35.785254	36.110610	41.809786
H	34.774749	34.706900	41.131137
C	40.493299	44.325251	37.400938
H	41.296699	44.410861	38.152369
H	40.931957	44.454825	36.405145
H	39.798762	45.165937	37.566084
C	36.468856	38.626509	41.316152
H	36.669088	39.683227	41.531984
H	35.417193	38.408927	41.565410
H	37.091936	38.046236	42.016777
C	36.487389	34.117753	34.759512
H	36.473815	33.514903	33.842805
H	37.094448	33.570670	35.500209
H	35.458487	34.141910	35.155096
C	41.661068	42.249633	32.470622
H	41.622559	42.366637	31.378188
H	41.481372	43.234094	32.929609
H	42.698524	41.962447	32.718945
C	40.520184	39.778112	30.781794
H	39.654636	39.281390	30.319904
H	40.691962	40.690353	30.192500
C	37.602029	35.332165	32.004811
H	38.552608	35.540267	31.496456
H	37.580968	34.243608	32.164450
C	41.752360	38.876977	30.630194
H	41.619084	37.930781	31.179340
H	42.630630	39.375344	31.080668
C	36.463055	35.671387	31.028471
H	36.493219	36.744427	30.764939
H	35.475823	35.474198	31.476442
C	36.593943	34.841359	29.726596
C	42.148353	38.516312	29.172750
O	42.991893	37.597298	29.061865
O	35.561764	34.421308	29.183377
O	41.626417	39.176440	28.243999
O	37.784839	34.661478	29.321166
O	40.142363	38.430324	36.476880
O	46.034639	36.931060	34.511707
O	45.437926	38.398097	32.142754
O	44.176807	36.501890	32.100958
O	46.888231	37.093040	33.353257

O	43.076721	34.605132	31.904845
C	44.719398	37.501799	34.317241
C	44.693111	38.805724	35.151451
C	43.717089	36.484656	34.860634
C	43.279842	39.217069	35.696589
C	44.431893	37.722734	32.824153
C	42.275917	37.022696	34.750797
C	45.427355	39.934675	34.428843
C	42.153502	38.520776	34.951733
C	43.877156	35.154537	34.119555
C	46.719841	38.381106	32.807335
C	46.786468	39.505577	33.865288
C	43.193908	38.991787	37.213949
C	43.646035	35.381214	32.635990
C	43.024637	34.031567	34.703781
C	47.790948	38.501179	31.740319
H	45.306322	38.536815	36.024760
H	43.968515	36.327100	35.921372
H	43.162295	40.298556	35.518925
H	43.515291	38.318357	32.722102
H	41.845965	36.762029	33.768669
H	41.665807	36.481221	35.481204
H	44.808741	40.338663	33.611225
H	45.581391	40.757359	35.143710
H	41.040593	38.606099	35.715830
H	41.851475	39.054459	34.044527
H	44.946006	34.889606	34.194733
H	47.454156	39.167405	34.671621
H	47.257434	40.376330	33.389992
H	47.573016	39.379062	31.116738
H	47.810001	37.599228	31.113836
H	48.773307	38.628987	32.215649
H	43.999180	39.535338	37.734233
H	42.219672	39.331532	37.591380
H	43.285752	37.923147	37.467319
H	43.065744	33.133468	34.074323
H	43.384855	33.773633	35.711278
H	41.971154	34.329098	34.802853
H	35.871645	40.295547	33.358572

QM atoms (linking H atom included): 121

IVH4 Cluster3 UPr

C	36.243385	40.950450	34.151817
H	35.644724	41.874409	34.098452

H	37.301821	41.181586	33.975340
S	36.007362	40.230787	35.810034
N	37.406050	38.343824	37.774189
C	37.313737	38.983973	38.985981
C	36.772521	37.144221	37.914968
C	36.606033	38.157183	39.945073
C	36.251593	36.997990	39.271000
C	36.657872	36.195631	36.897257
H	36.157983	35.257654	37.138537
C	37.110048	36.336806	35.591086
N	37.767210	37.436910	35.087653
C	38.034788	37.151239	33.770172
C	37.497855	35.839879	33.412044
C	36.954751	35.320886	34.563065
C	38.774162	37.961242	32.912291
H	38.920879	37.600075	31.893423
C	39.370869	39.182940	33.238120
C	40.170167	39.974721	32.311616
C	40.031211	40.962630	34.351193
N	39.294642	39.797859	34.464386
C	40.609854	41.069378	33.023722
C	40.173494	41.910393	35.355867
H	40.723618	42.816204	35.101267
C	39.643567	41.827539	36.648471
C	39.690722	42.890661	37.632276
N	38.959781	40.743922	37.138833
C	38.535298	41.081950	38.391911
C	37.798032	40.260888	39.245373
H	37.603187	40.644708	40.244118
Fe	38.487651	39.013132	36.167776
C	38.975198	42.431693	38.729016
C	38.664269	43.087063	39.989664
H	37.968552	42.541801	40.634605
C	39.144138	44.246747	40.473289
H	39.869686	44.857788	39.937584
H	38.834613	44.585616	41.463603
C	35.487618	35.845932	39.729352
H	35.139744	35.173990	38.936643
C	35.147046	35.520616	40.990401
H	35.453737	36.098549	41.862138
H	34.540976	34.631986	41.181922
C	40.363224	44.214176	37.463870
H	41.186161	44.324624	38.190783
H	40.770513	44.351163	36.455070

H	39.654045	45.039194	37.644695
C	36.338653	38.507812	41.371525
H	36.631865	39.537700	41.609867
H	35.272501	38.380330	41.623429
H	36.908036	37.856057	42.054984
C	36.393271	33.953963	34.798491
H	36.460370	33.336734	33.893779
H	36.948047	33.423629	35.590210
H	35.335957	33.969683	35.110549
C	41.551156	42.134610	32.557099
H	41.503447	42.246682	31.464329
H	41.354283	43.115851	33.015777
H	42.595994	41.870959	32.799517
C	40.475765	39.629449	30.885731
H	39.641972	39.065144	30.444366
H	40.562359	40.550333	30.289701
C	37.552724	35.201528	32.062170
H	38.518132	35.395119	31.574087
H	37.492525	34.110541	32.191640
C	41.772829	38.830121	30.709016
H	41.729979	37.875612	31.256916
H	42.613561	39.399369	31.146913
C	36.443191	35.609410	31.076515
H	36.520008	36.687512	30.844372
H	35.442456	35.437188	31.503843
C	36.567382	34.812920	29.753347
C	42.173652	38.514513	29.241501
O	43.034881	37.615562	29.105625
O	35.532622	34.406932	29.204289
O	41.642721	39.191295	28.329326
O	37.756411	34.642822	29.338611
O	39.958231	38.102597	36.709241
O	46.190781	36.809910	34.463321
O	45.772345	38.325320	32.092323
O	44.241648	36.639440	32.101066
O	46.990213	36.764592	33.259516
O	43.015173	34.821054	31.944752
C	44.972129	37.573712	34.287527
C	45.191271	38.876476	35.083188
C	43.842529	36.728206	34.880838
C	43.900863	39.632802	35.501774
C	44.688357	37.816269	32.799381
C	42.510576	37.487363	34.824095
C	46.159697	39.811865	34.359999

C	42.626894	38.926872	35.171306
C	43.801415	35.377521	34.157899
C	47.056792	38.054889	32.696301
C	47.385547	39.145577	33.736977
C	43.967638	40.015568	36.999884
C	43.620942	35.581133	32.664089
C	42.804093	34.388892	34.749949
C	48.074850	37.950585	31.581217
H	45.682670	38.517450	35.999100
H	44.106182	36.546111	35.936487
H	43.881498	40.589136	34.943449
H	43.870720	38.545644	32.704819
H	42.051246	37.386420	33.816280
H	41.767939	37.011489	35.485420
H	45.608055	40.337017	33.569995
H	46.501419	40.570358	35.075434
H	40.712343	38.698221	36.831753
H	41.706726	39.507365	35.203470
H	44.820159	34.963955	34.249641
H	48.032130	38.697954	34.506457
H	47.969015	39.925411	33.225323
H	48.064170	38.879328	30.993384
H	47.815148	37.109070	30.929749
H	49.076980	37.783266	31.999870
H	44.901360	40.556612	37.225891
H	43.116095	40.654525	37.282880
H	43.943774	39.111264	37.630270
H	42.843345	33.430866	34.213924
H	43.041491	34.207901	35.809223
H	41.774561	34.769607	34.712952
H	35.898478	40.277820	33.366531

QM atoms (linking H atom included): 136

IIH10 In- Cluster2 ReactantBigQM

C	44.740351	35.039585	32.982786
H	44.751585	33.946901	33.134113
H	45.796058	35.360657	32.977878
C	44.063022	35.711715	34.165778
C	43.620088	34.929613	35.244851
H	43.707814	33.840394	35.183473
C	43.082250	35.513049	36.400577
H	42.735499	34.875957	37.219453
C	42.993732	36.902345	36.503672
H	42.576153	37.382896	37.390795

C	43.456246	37.695783	35.449578
H	43.404362	38.780977	35.543506
C	43.975547	37.112830	34.292087
H	44.322571	37.767299	33.489847
C	38.840588	43.035213	35.470742
H	38.137584	43.880116	35.548498
H	39.867031	43.423224	35.534417
S	38.513793	41.914998	36.859739
N	39.836698	39.924291	38.471786
C	39.420818	40.233035	39.745541
C	39.183600	38.770228	38.126562
C	38.482586	39.244920	40.237968
C	38.308428	38.335599	39.207287
C	39.339922	38.105895	36.917418
H	38.849156	37.140135	36.810226
C	40.055980	38.574575	35.826345
N	40.686830	39.798200	35.762285
C	41.240145	39.865668	34.500282
C	40.964986	38.655527	33.753027
C	40.221494	37.851080	34.579998
C	41.979029	40.924618	34.001791
H	42.389337	40.837418	32.995936
C	42.326539	42.064881	34.718777
C	43.090918	43.162913	34.157569
C	42.681845	43.466051	36.367444
N	42.047880	42.282477	36.045723
C	43.339509	44.026886	35.199099
C	42.654684	44.063894	37.618546
H	43.183734	45.010250	37.729685
C	41.966477	43.582263	38.731032
C	41.854114	44.293472	39.990217
N	41.234487	42.420820	38.758234
C	40.639716	42.374265	39.989088
C	39.797336	41.369165	40.446480
H	39.410621	41.469158	41.458902
Fe	41.150830	40.989097	37.330696
C	41.009680	43.536901	40.783729
C	40.503831	43.794967	42.127356
H	39.540320	43.335864	42.374840
C	41.106988	44.511594	43.090268
H	42.099472	44.947309	42.970798
H	40.614102	44.634769	44.056491
C	37.390161	37.209816	39.107438
H	37.180111	36.871630	38.086214

C	36.747497	36.578590	40.106708
H	36.903996	36.821351	41.157580
H	36.041416	35.775983	39.882720
C	42.490176	45.607990	40.307561
H	41.850087	46.188360	40.989889
H	43.460258	45.466763	40.815342
H	42.662137	46.212759	39.407030
C	37.845114	39.243393	41.587410
H	36.756351	39.086570	41.518557
H	38.245998	38.425809	42.210881
H	38.021157	40.174546	42.139987
C	39.782724	36.450853	34.298291
H	39.143568	36.396092	33.403475
H	40.663914	35.811547	34.121317
H	39.223670	36.008270	35.133680
C	44.145164	45.285266	35.143720
H	45.216344	45.075136	35.301678
H	44.073276	45.748239	34.147921
H	43.836616	46.029911	35.892844
C	43.459250	43.350386	32.713353
H	42.839426	42.705329	32.077143
H	43.197400	44.388566	32.448898
C	41.465012	38.336934	32.382710
H	42.403435	38.869151	32.174836
H	41.713886	37.264587	32.340998
C	44.930878	43.122398	32.341865
H	45.611025	43.631941	33.040899
H	45.120361	43.586711	31.357423
C	40.471112	38.659423	31.265474
H	40.240822	39.740139	31.261546
H	39.504518	38.152758	31.420428
C	40.985583	38.287191	29.865826
C	45.376758	41.654872	32.191720
O	44.497903	40.768541	32.147065
O	42.223497	38.135646	29.714045
O	46.627299	41.478685	32.075334
O	40.114162	38.173306	28.961619
O	42.489819	40.192151	37.746451
O	47.873867	38.034511	35.113025
O	49.998331	38.087792	36.998073
O	49.429944	40.240721	36.491349
O	49.280996	37.876153	34.820002
O	48.987883	42.368729	36.082458
C	47.651255	38.496699	36.480217

C	47.101460	37.288736	37.283767
C	46.626804	39.634021	36.357645
C	46.530257	37.718104	38.659237
C	48.966225	39.010017	37.082442
C	46.078798	40.053213	37.729995
C	48.134091	36.154014	37.440433
C	45.525204	38.862823	38.505502
C	47.230242	40.798106	35.550636
C	49.910714	37.190038	35.888246
C	49.106937	35.932976	36.279082
C	45.895401	36.546599	39.414263
C	48.584829	41.236365	36.081839
C	46.274405	41.972938	35.392476
C	51.323954	36.907628	35.420267
H	46.259928	36.918413	36.672785
H	45.788673	39.223391	35.772607
H	47.378587	38.086087	39.268102
H	48.821898	39.223313	38.149820
H	45.270150	40.783577	37.583996
H	46.870123	40.561984	38.312906
H	47.596111	35.211851	37.622493
H	48.731851	36.347163	38.343809
H	45.183866	39.190420	39.501139
H	44.629514	38.493135	37.985073
H	47.454184	40.410052	34.540800
H	49.824208	35.152657	36.577438
H	48.592129	35.568576	35.377586
H	46.019504	42.422742	36.361152
H	45.341727	41.633665	34.923000
H	46.720517	42.754307	34.767144
H	46.624703	35.761607	39.661545
H	45.456150	36.894238	40.362835
H	45.088424	36.092309	38.815352
H	51.792514	37.827556	35.046556
H	51.911119	36.554954	36.279922
H	51.325714	36.141885	34.631640
H	38.712924	42.589446	34.484303
H	44.329460	35.229889	31.991313

QM atoms (linking H atom included): 121

IIH10 In- Cluster2 ReactantSmaQM

C	38.859595	43.050804	35.468685
H	38.153939	43.893940	35.541002
H	39.884756	43.442260	35.531471

S	38.531692	41.939501	36.864529
N	39.860875	39.967548	38.471630
C	39.433859	40.269803	39.742838
C	39.212568	38.813032	38.116617
C	38.494208	39.277283	40.224306
C	38.328704	38.372727	39.187915
C	39.389719	38.148030	36.911406
H	38.898738	37.183196	36.795757
C	40.131165	38.612874	35.834914
N	40.758893	39.837277	35.778720
C	41.340529	39.900971	34.529843
C	41.085130	38.686577	33.780923
C	40.321735	37.884581	34.594027
C	42.059745	40.973880	34.030500
H	42.485245	40.891768	33.029240
C	42.367131	42.128763	34.742606
C	43.118548	43.237380	34.184433
C	42.690775	43.537310	36.391944
N	42.073504	42.346253	36.066366
C	43.352284	44.103356	35.227785
C	42.651607	44.131540	37.645241
H	43.174341	45.080607	37.763460
C	41.963437	43.640273	38.753925
C	41.845962	44.342266	40.018235
N	41.237215	42.475430	38.772912
C	40.639877	42.417447	40.001904
C	39.802285	41.404532	40.451171
H	39.410433	41.497882	41.462347
Fe	41.178796	41.047556	37.345119
C	41.003273	43.576786	40.804724
C	40.490449	43.824090	42.147882
H	39.517196	43.378111	42.381221
C	41.096886	44.519071	43.123927
H	42.098094	44.937894	43.018054
H	40.598122	44.641485	44.086935
C	37.414042	37.244430	39.076303
H	37.199095	36.919909	38.051191
C	36.781083	36.597076	40.071680
H	36.945482	36.824501	41.125081
H	36.074587	35.795472	39.844242
C	42.478599	45.656491	40.342977
H	41.864760	46.208178	41.070719
H	43.473927	45.515465	40.799610
H	42.601761	46.287252	39.452096

C	37.849710	39.268169	41.570472
H	36.764323	39.091495	41.496523
H	38.262473	38.459869	42.198498
H	38.007906	40.203546	42.121259
C	39.840421	36.502724	34.287319
H	39.142971	36.494716	33.434246
H	40.689907	35.851674	34.023863
H	39.327932	36.037823	35.140264
C	44.149008	45.367548	35.176383
H	45.221588	45.163037	35.332141
H	44.075553	45.833255	34.181796
H	43.836487	46.107660	35.928136
C	43.486732	43.434846	32.740977
H	42.858805	42.801480	32.100578
H	43.235774	44.478258	32.489476
C	41.572545	38.382168	32.401070
H	42.503939	38.924327	32.183099
H	41.821112	37.309519	32.339367
C	44.954007	43.193992	32.358471
H	45.645394	43.677412	33.064678
H	45.142455	43.677135	31.382975
C	40.550133	38.708229	31.307388
H	40.329221	39.790989	31.305384
H	39.584186	38.210796	31.494438
C	41.017096	38.323044	29.894617
C	45.368496	41.723318	32.161391
O	44.465779	40.868194	32.055619
O	42.246425	38.140733	29.713940
O	46.616371	41.514030	32.068573
O	40.123609	38.226435	29.011381
O	42.525094	40.275249	37.774402
O	47.800993	38.000247	35.152360
O	49.925300	38.072323	37.034329
O	49.367855	40.221739	36.500678
O	49.207774	37.835325	34.859576
O	48.928525	42.348945	36.081763
C	47.580250	38.484502	36.510371
C	47.028726	37.292874	37.336849
C	46.558579	39.623178	36.365331
C	46.461055	37.754410	38.702462
C	48.898142	39.001491	37.106749
C	45.994056	40.062167	37.725027
C	48.056603	36.157044	37.509193
C	45.442770	38.882847	38.518514

C	47.172354	40.776731	35.549769
C	49.833364	37.159315	35.936624
C	49.019686	35.913197	36.344545
C	45.852344	36.601025	39.503752
C	48.525345	41.216793	36.084053
C	46.223561	41.954273	35.373636
C	51.246008	36.860909	35.476127
H	46.185331	36.912433	36.735294
H	45.722675	39.209327	35.776309
H	47.307403	38.154535	39.293330
H	48.754537	39.228651	38.171492
H	45.182233	40.784535	37.558715
H	46.777578	40.584422	38.306428
H	47.516073	35.221027	37.713462
H	48.661943	36.363700	38.404092
H	45.090020	39.228984	39.503638
H	44.548577	38.498474	38.001763
H	47.401302	40.377148	34.545362
H	49.730695	35.128766	36.646159
H	48.494829	35.544908	35.450454
H	45.971275	42.423092	36.334000
H	45.289160	41.614251	34.908240
H	46.676069	42.720196	34.734789
H	46.600132	35.847184	39.789503
H	45.398552	36.977083	40.434176
H	45.062310	36.096146	38.923178
H	51.721638	37.772100	35.089807
H	51.828991	36.517435	36.342574
H	51.243249	36.083281	34.699126
H	38.735426	42.597476	34.485250

QM atoms (linking H atom included): 136

IIH10 In- Cluster2 TS BigQM

C	44.743247	34.996963	32.948573
H	44.760001	33.902384	33.085278
H	45.796523	35.326323	32.948787
C	44.056077	35.650754	34.134940
C	43.590198	34.855895	35.194705
H	43.667971	33.766807	35.118086
C	43.039046	35.427686	36.350250
H	42.673195	34.783245	37.154927
C	42.964364	36.815647	36.472996
H	42.540001	37.298962	37.354547
C	43.456550	37.619688	35.441178

H	43.416753	38.701380	35.562944
C	43.980912	37.049964	34.281425
H	44.338176	37.712183	33.490586
C	39.030312	42.953398	35.525234
H	38.352577	43.810785	35.660831
H	40.066062	43.322336	35.552913
S	38.747569	41.828212	36.915575
N	39.996116	39.794425	38.457224
C	39.578059	40.124516	39.726305
C	39.285552	38.680221	38.095780
C	38.596041	39.175419	40.207295
C	38.389375	38.277878	39.171090
C	39.397424	38.028077	36.875813
H	38.855931	37.091707	36.754554
C	40.128780	38.483643	35.790368
N	40.816560	39.674910	35.737757
C	41.344526	39.752724	34.467841
C	41.010513	38.567452	33.706627
C	40.246063	37.778102	34.528640
C	42.084388	40.805391	33.956848
H	42.460891	40.726301	32.938203
C	42.440417	41.942479	34.669368
C	43.131338	43.078505	34.088472
C	42.806509	43.347341	36.317961
N	42.217711	42.137422	36.013492
C	43.384990	43.944996	35.128080
C	42.800331	43.945573	37.570213
H	43.300957	44.908106	37.666268
C	42.140493	43.453794	38.692767
C	41.998197	44.189537	39.934957
N	41.441641	42.270178	38.744270
C	40.819650	42.246903	39.963941
C	39.967387	41.254992	40.426115
H	39.567243	41.371581	41.430634
Fe	41.348164	40.823567	37.311863
C	41.156564	43.436279	40.734283
C	40.616508	43.723400	42.059236
H	39.655925	43.252569	42.295891
C	41.181064	44.476185	43.018442
H	42.167383	44.928594	42.911284
H	40.664655	44.613399	43.970808
C	37.428546	37.188127	39.067666
H	37.192641	36.871617	38.044857
C	36.780390	36.564361	40.068421

H	36.964965	36.783792	41.120070
H	36.042298	35.789865	39.847072
C	42.594174	45.528956	40.227155
H	41.927972	46.109881	40.883741
H	43.560138	45.428907	40.752520
H	42.764266	46.115948	39.314607
C	37.948281	39.198511	41.551537
H	36.860414	39.041860	41.476861
H	38.342741	38.392305	42.193651
H	38.119881	40.139504	42.088867
C	39.748734	36.401570	34.228478
H	39.076517	36.388259	33.356419
H	40.598844	35.736385	34.003230
H	39.206027	35.957679	35.073646
C	44.137568	45.235274	35.061858
H	45.210469	45.078704	35.262796
H	44.077306	45.671291	34.053626
H	43.776751	45.983643	35.784136
C	43.432968	43.286276	32.630228
H	42.820544	42.607799	32.023599
H	43.108756	44.308903	32.374274
C	41.477911	38.254741	32.325624
H	42.427404	38.762376	32.109321
H	41.695115	37.176286	32.264333
C	44.896567	43.127905	32.192348
H	45.577151	43.724401	32.816614
H	44.999302	43.536925	31.171022
C	40.477894	38.624439	31.229619
H	40.277546	39.711130	31.250794
H	39.500747	38.139577	31.386730
C	40.973063	38.266560	29.821368
C	45.421955	41.681335	32.112018
O	44.587130	40.754153	32.088603
O	42.210564	38.124292	29.656566
O	46.682863	41.557666	32.032561
O	40.093718	38.153435	28.924703
O	42.739196	39.847964	37.734308
O	47.551664	38.288623	35.210497
O	49.554636	38.246994	37.227526
O	49.267361	40.401847	36.542113
O	48.947031	37.963418	35.024247
O	49.092732	42.528288	35.962773
C	47.299523	38.872586	36.525291
C	46.550848	37.801778	37.353940

C	46.422366	40.096440	36.246582
C	45.919790	38.385394	38.646868
C	48.631059	39.279092	37.182214
C	45.836495	40.699356	37.532515
C	47.442925	36.584070	37.674404
C	45.171397	39.692501	38.439837
C	47.207033	41.125113	35.415579
C	49.427323	37.288129	36.173863
C	48.458336	36.165623	36.602047
C	45.093962	37.348135	39.417476
C	48.567683	41.447671	36.008498
C	46.399701	42.382590	35.152244
C	50.822956	36.821486	35.808874
H	45.732260	37.473473	36.694113
H	45.585057	39.735587	35.626348
H	46.771601	38.659239	39.310718
H	48.452335	39.583961	38.223589
H	45.104926	41.475858	37.265509
H	46.639540	41.223307	38.093560
H	46.797500	35.718728	37.885439
H	47.999356	36.789310	38.602681
H	44.877926	40.142880	39.399606
H	43.885914	39.621476	37.989153
H	47.431472	40.652750	34.442770
H	49.061196	35.341498	37.013831
H	47.961546	35.781135	35.698784
H	46.199908	42.928298	36.080906
H	45.433586	42.111477	34.714797
H	46.923294	43.060714	34.473202
H	45.716553	36.516330	39.775413
H	44.630547	37.811135	40.301066
H	44.296772	36.935058	38.783760
H	51.404878	37.657598	35.396161
H	51.327882	36.472313	36.720296
H	50.773935	36.004951	35.074363
H	38.853091	42.524556	34.538951
H	44.330881	35.199898	31.960221

QM atoms (linking H atom included): 121

IIH10 In- Cluster2 TS SmaQM

C	39.057494	42.966008	35.518879
H	38.377751	43.822240	35.649799
H	40.092669	43.335852	35.545740
S	38.775462	41.850187	36.916135

N	40.026981	39.835732	38.463382
C	39.592211	40.165097	39.726030
C	39.328407	38.717514	38.092754
C	38.603895	39.214923	40.192646
C	38.418207	38.313244	39.155913
C	39.460674	38.065189	36.874625
H	38.927686	37.124739	36.747092
C	40.204362	38.523160	35.797429
N	40.881467	39.720036	35.748402
C	41.429583	39.798317	34.487833
C	41.115038	38.608362	33.723837
C	40.341790	37.815991	34.537339
C	42.142027	40.870634	33.976152
H	42.517990	40.806339	32.955034
C	42.468097	42.015195	34.691032
C	43.137934	43.165188	34.113050
C	42.829377	43.412041	36.347988
N	42.248506	42.200260	36.037508
C	43.393211	44.024599	35.158168
C	42.828749	43.998596	37.606177
H	43.325075	44.963129	37.707447
C	42.169414	43.496591	38.724636
C	42.022191	44.224094	39.971602
N	41.466440	42.314839	38.764250
C	40.838557	42.283595	39.981803
C	39.978242	41.293066	40.433003
H	39.568036	41.408304	41.433908
Fe	41.380986	40.874987	37.328160
C	41.173689	43.467637	40.760463
C	40.619494	43.748210	42.080951
H	39.647354	43.291249	42.297064
C	41.181825	44.479365	43.057415
H	42.177231	44.916013	42.969566
H	40.652104	44.612415	44.003053
C	37.467668	37.216204	39.040484
H	37.257498	36.889980	38.015270
C	36.803034	36.593791	40.031293
H	36.961602	36.823064	41.085234
H	36.077703	35.810657	39.798502
C	42.623568	45.558437	40.275496
H	41.971912	46.127009	40.956712
H	43.601286	45.448287	40.776597
H	42.773993	46.160669	39.369078
C	37.931437	39.241916	41.524924

H	36.844380	39.089767	41.429565
H	38.310024	38.434829	42.175735
H	38.098081	40.182947	42.063775
C	39.817577	36.453314	34.218013
H	39.129707	36.472946	33.357854
H	40.647839	35.775133	33.960560
H	39.280478	36.002586	35.063317
C	44.142647	45.317082	35.099432
H	45.214654	45.159610	35.306765
H	44.088897	45.754343	34.091528
H	43.776776	46.062814	35.821925
C	43.421435	43.388037	32.653653
H	42.795714	42.721562	32.046740
H	43.103884	44.416233	32.416690
C	41.569224	38.312489	32.332319
H	42.502246	38.846028	32.101832
H	41.804610	37.237817	32.253941
C	44.876626	43.219945	32.192772
H	45.574004	43.794250	32.818766
H	44.965856	43.646305	31.177213
C	40.533795	38.664368	31.260280
H	40.323082	39.748969	31.279824
H	39.566608	38.171136	31.450896
C	40.987865	38.297723	29.840067
C	45.372719	41.766855	32.069783
O	44.516276	40.867523	31.963454
O	42.218485	38.137123	29.647876
O	46.632975	41.610909	32.036575
O	40.088417	38.192790	28.963353
O	42.765971	39.884302	37.729845
O	47.464233	38.323452	35.311380
O	49.482674	38.303551	37.311440
O	49.217322	40.450048	36.585299
O	48.856157	37.983888	35.118808
O	49.067727	42.556724	35.934007
C	47.232116	38.941687	36.611952
C	46.481361	37.899168	37.473666
C	46.371842	40.175373	36.321798
C	45.882993	38.522537	38.762165
C	48.572944	39.346668	37.250683
C	45.837138	40.821650	37.609067
C	47.356452	36.671583	37.804672
C	45.163050	39.841972	38.536019
C	47.160136	41.160140	35.443322

C	49.337221	37.325606	36.278137
C	48.358855	36.222471	36.733670
C	45.023376	37.534909	39.556863
C	48.528566	41.485512	36.017058
C	46.365284	42.414327	35.134818
C	50.725836	36.834750	35.918797
H	45.648570	37.570595	36.833889
H	45.501947	39.822008	35.743048
H	46.751886	38.775676	39.409470
H	48.404814	39.673821	38.286542
H	45.120005	41.611592	37.344724
H	46.668136	41.331535	38.141849
H	46.700605	35.818576	38.032185
H	47.920709	36.883601	38.726548
H	44.856840	40.306771	39.484007
H	43.896535	39.743436	38.045912
H	47.373344	40.649236	34.487736
H	48.954981	35.398845	37.156007
H	47.851307	35.828591	35.840362
H	46.159701	42.991506	36.042557
H	45.402826	42.134120	34.695316
H	46.899056	43.063817	34.436497
H	45.564845	36.610093	39.799817
H	44.712420	37.987632	40.508894
H	44.115360	37.274080	38.995791
H	51.313518	37.654871	35.482916
H	51.230505	36.506698	36.838268
H	50.666347	35.998379	35.207774
H	38.879281	42.532467	34.534831

QM atoms (linking H atom included): 136

IIH10 In- Cluster2 ProductBigQM

C	44.714671	35.085956	32.923974
H	44.681063	34.001095	33.121106
H	45.783253	35.359976	32.898735
C	44.078944	35.841822	34.077710
C	43.602735	35.140140	35.196540
H	43.639769	34.046660	35.189530
C	43.106839	35.808318	36.325033
H	42.734002	35.229791	37.175308
C	43.099166	37.204375	36.366537
H	42.722329	37.755891	37.230385
C	43.589484	37.911865	35.264917
H	43.591763	39.001939	35.273962

C	44.062952	37.248669	34.133479
H	44.427157	37.850065	33.299009
C	38.784078	43.047524	35.465191
H	38.089715	43.900822	35.522781
H	39.813835	43.423527	35.545119
S	38.422082	41.929176	36.849848
N	39.780353	39.913231	38.516929
C	39.344419	40.235650	39.779860
C	39.133646	38.759233	38.166340
C	38.406349	39.243593	40.269748
C	38.247132	38.326481	39.243350
C	39.299368	38.098422	36.952827
H	38.802025	37.135685	36.841532
C	40.012015	38.560512	35.850575
N	40.643135	39.780895	35.773418
C	41.183938	39.849797	34.505517
C	40.910499	38.633119	33.768481
C	40.170814	37.832007	34.603337
C	41.928960	40.907201	34.004405
H	42.331105	40.814081	32.995993
C	42.301160	42.046064	34.718129
C	43.083902	43.134297	34.162851
C	42.658164	43.442549	36.372624
N	42.027752	42.262276	36.045008
C	43.329507	43.998710	35.206784
C	42.610818	44.041126	37.628477
H	43.145320	44.984903	37.743245
C	41.904309	43.578687	38.742488
C	41.799067	44.296501	40.000150
N	41.149700	42.431656	38.778860
C	40.554375	42.394801	40.006982
C	39.709353	41.386547	40.467621
H	39.314156	41.496981	41.476250
Fe	41.029765	41.011647	37.340753
C	40.942755	43.555015	40.797343
C	40.453292	43.817273	42.145784
H	39.479670	43.381138	42.396579
C	41.085029	44.506683	43.110045
H	42.089664	44.913010	42.985877
H	40.604264	44.635266	44.081095
C	37.338202	37.194067	39.139331
H	37.166925	36.830628	38.119658
C	36.663325	36.580978	40.129005
H	36.776140	36.851920	41.178437

H	35.972678	35.766460	39.898874
C	42.460239	45.599271	40.315645
H	41.845476	46.180700	41.019394
H	43.441101	45.440726	40.796583
H	42.618345	46.210398	39.416533
C	37.757639	39.246259	41.613355
H	36.664083	39.129945	41.536945
H	38.123184	38.405997	42.227796
H	37.963997	40.162295	42.180130
C	39.727854	36.431828	34.324550
H	39.082238	36.378024	33.434147
H	40.606115	35.791725	34.139144
H	39.173783	35.990571	35.164219
C	44.133831	45.258146	35.152268
H	45.207723	45.048883	35.290421
H	44.046509	45.731834	34.162590
H	43.835663	45.994768	35.913327
C	43.462885	43.316963	32.720776
H	42.853103	42.661770	32.084880
H	43.193946	44.350841	32.446060
C	41.417062	38.304639	32.402718
H	42.370766	38.814102	32.209991
H	41.643806	37.227522	32.362007
C	44.939353	43.100141	32.361521
H	45.608106	43.626477	33.058946
H	45.133100	43.555346	31.373641
C	40.452611	38.654754	31.269774
H	40.241912	39.739848	31.271999
H	39.473740	38.165393	31.399212
C	40.989766	38.287392	29.877192
C	45.407355	41.637257	32.234866
O	44.546624	40.731772	32.229852
O	42.230793	38.140204	29.741185
O	46.659306	41.482035	32.099530
O	40.130625	38.174098	28.961415
O	42.552972	40.179250	37.830533
O	47.943503	38.083714	35.079185
O	49.994116	38.075906	37.047690
O	49.507964	40.238261	36.505355
O	49.355963	37.887631	34.841012
O	49.160401	42.374401	36.053266
C	47.683058	38.547554	36.438340
C	47.071264	37.348392	37.210984
C	46.695449	39.712343	36.276061

C	46.443977	37.780702	38.570715
C	48.987610	39.027572	37.089286
C	46.094349	40.142811	37.630954
C	48.067765	36.188191	37.409182
C	45.579645	38.986097	38.408314
C	47.352255	40.872394	35.507946
C	49.927985	37.184267	35.930322
C	49.079777	35.946148	36.286270
C	45.702422	36.633984	39.264315
C	48.713356	41.258688	36.062092
C	46.439722	42.086073	35.380114
C	51.350708	36.873224	35.512184
H	46.247037	37.002963	36.564559
H	45.873098	39.322493	35.657137
H	47.300861	38.061118	39.227025
H	48.808808	39.254032	38.149733
H	45.291130	40.874768	37.462746
H	46.874116	40.691543	38.209891
H	47.499330	35.259747	37.568404
H	48.633414	36.366391	38.336524
H	44.629783	39.071851	38.941012
H	43.179187	40.204498	37.090217
H	47.570921	40.503405	34.489933
H	49.766051	35.148874	36.610661
H	48.593324	35.595458	35.363758
H	46.237839	42.538951	36.359893
H	45.479024	41.792889	34.936291
H	46.899451	42.854286	34.748827
H	46.379731	35.812890	39.538007
H	45.229513	36.993680	40.191452
H	44.909841	36.233770	38.612639
H	51.846653	37.785971	35.156197
H	51.902232	36.509489	36.390708
H	51.365045	36.109419	34.721691
H	38.671737	42.599030	34.478125
H	44.298818	35.254921	31.930704

QM atoms (linking H atom included): 121

IIH10 In- Cluster2 ProductSmaQM

C	38.823242	43.112441	35.483844
H	38.124823	43.962003	35.529790
H	39.849613	43.500073	35.564340
S	38.485959	42.024265	36.891530
N	39.769499	39.977881	38.511528

C	39.348735	40.289169	39.781642
C	39.121710	38.831829	38.141334
C	38.415331	39.290567	40.258912
C	38.242928	38.389657	39.216496
C	39.305563	38.164975	36.934286
H	38.796897	37.210996	36.807536
C	40.094590	38.603577	35.877902
N	40.770331	39.805128	35.828761
C	41.351338	39.876518	34.579270
C	41.080666	38.667717	33.832566
C	40.292013	37.877221	34.639436
C	42.054182	40.956541	34.065028
H	42.485974	40.865641	33.067902
C	42.322511	42.127903	34.758531
C	43.072172	43.238223	34.203947
C	42.592642	43.573654	36.400617
N	41.992767	42.376038	36.072875
C	43.275929	44.121807	35.240518
C	42.536502	44.179921	37.649162
H	43.054860	45.130954	37.767166
C	41.849458	43.684227	38.755984
C	41.748198	44.372275	40.028711
N	41.126404	42.515235	38.789229
C	40.544878	42.440225	40.028558
C	39.720266	41.423666	40.491201
H	39.341194	41.513838	41.506934
Fe	41.071061	41.077305	37.366304
C	40.922260	43.597644	40.825971
C	40.444618	43.832015	42.184093
H	39.480091	43.378959	42.439375
C	41.076025	44.519574	43.149593
H	42.072318	44.943742	43.019948
H	40.603637	44.627844	44.127212
C	37.341923	37.251309	39.107256
H	37.183547	36.885303	38.086440
C	36.662094	36.633498	40.090902
H	36.759943	36.906655	41.141246
H	35.981485	35.812269	39.853898
C	42.392868	45.678817	40.360574
H	41.779770	46.235887	41.084827
H	43.382564	45.523157	40.825094
H	42.530748	46.308374	39.471318
C	37.784454	39.267354	41.611083
H	36.688653	39.165612	41.546103

H	38.148413	38.407924	42.199875
H	38.008292	40.167755	42.195889
C	39.796797	36.503474	34.319308
H	39.145195	36.504533	33.431211
H	40.645323	35.834338	34.101238
H	39.230793	36.055504	35.147216
C	44.076061	45.383405	35.187288
H	45.145125	45.176122	35.362135
H	44.021320	45.837641	34.186273
H	43.756657	46.132325	35.926759
C	43.460871	43.421879	32.763955
H	42.850845	42.771127	32.123791
H	43.197721	44.458461	32.496049
C	41.570186	38.355757	32.453655
H	42.510403	38.884910	32.241334
H	41.802859	37.279498	32.391460
C	44.935413	43.197349	32.400736
H	45.613763	43.682320	33.118314
H	45.133011	43.688092	31.430783
C	40.560525	38.701241	31.353045
H	40.351999	39.786231	31.359927
H	39.587517	38.212976	31.527669
C	41.030061	38.325328	29.937602
C	45.368033	41.731849	32.200669
O	44.479974	40.864728	32.078844
O	42.257048	38.126604	29.757475
O	46.620400	41.539407	32.120648
O	40.138217	38.252382	29.050710
O	42.613064	40.278666	37.976382
O	47.866527	38.000494	35.130749
O	49.945305	38.078083	37.063068
O	49.386019	40.220999	36.514706
O	49.279434	37.845807	34.870049
O	48.949762	42.347512	36.096581
C	47.611813	38.474749	36.486413
C	47.057227	37.269363	37.290591
C	46.580623	39.601281	36.316481
C	46.460439	37.710466	38.658498
C	48.911469	39.001230	37.112557
C	45.948761	40.024328	37.657875
C	48.088185	36.138904	37.478301
C	45.529604	38.864300	38.487301
C	47.198348	40.779759	35.540452
C	49.889421	37.171975	35.956600

C	49.083358	35.912978	36.337687
C	45.818041	36.552804	39.427484
C	48.546205	41.215628	36.093064
C	46.247575	41.961650	35.397496
C	51.314173	36.895941	35.521030
H	46.225802	36.890326	36.673433
H	45.777038	39.178791	35.691053
H	47.321923	38.063157	39.272399
H	48.742584	39.228065	38.174653
H	45.077838	40.668925	37.471542
H	46.682292	40.650720	38.217748
H	47.547898	35.197572	37.658227
H	48.667957	36.340887	38.391246
H	44.657192	38.974064	39.137411
H	42.739640	39.397447	37.593209
H	47.434179	40.412618	34.525311
H	49.797243	35.137080	36.654114
H	48.587457	35.542895	35.427968
H	46.007118	42.408047	36.371783
H	45.307850	41.635397	34.932596
H	46.697423	42.740471	34.772401
H	46.555777	35.792609	39.720819
H	45.343597	36.922767	40.349834
H	45.041889	36.061874	38.819531
H	51.783044	37.817028	35.150651
H	51.887066	36.552231	36.393887
H	51.336921	36.126105	34.736536
H	38.721651	42.633489	34.510010

QM atoms (linking H atom included): 136

IIH10 In- Cluster1 ReactantBigQM

C	38.965775	52.083148	38.811036
H	38.811084	52.246173	37.731337
H	39.991009	52.426896	39.039072
C	38.874245	50.600062	39.123247
C	38.590203	49.687313	38.096507
H	38.391661	50.060712	37.087165
C	38.571176	48.306934	38.333380
H	38.340787	47.626402	37.510001
C	38.854259	47.816242	39.610373
H	38.860768	46.744110	39.817031
C	39.151824	48.713149	40.642698
H	39.396710	48.319716	41.630939
C	39.158243	50.089552	40.404679

H	39.412267	50.772722	41.219169
C	37.244760	44.869666	46.581219
H	37.104231	44.178031	47.427159
H	38.239005	45.329761	46.653700
S	37.102634	43.901380	45.046374
N	38.080311	43.707243	42.210550
C	38.323683	42.365009	42.044421
C	37.076885	44.017435	41.336191
C	37.466093	41.802338	41.020004
C	36.665749	42.841843	40.576776
C	36.502483	45.274967	41.229708
H	35.744399	45.422518	40.462692
C	36.781123	46.358625	42.045076
N	37.689297	46.386401	43.080458
C	37.617895	47.658876	43.610309
C	36.616327	48.441027	42.909271
C	36.111705	47.632118	41.924814
C	38.439044	48.161045	44.609955
H	38.278260	49.194015	44.919274
C	39.476678	47.468495	45.228105
C	40.336003	48.026353	46.261466
C	40.864390	45.864062	45.793389
N	39.808542	46.162845	44.960160
C	41.213639	47.020625	46.604647
C	41.457726	44.612278	45.896436
H	42.227282	44.494000	46.658063
C	41.140133	43.482079	45.143000
C	41.722935	42.169223	45.348765
N	40.189520	43.441540	44.153532
C	40.116098	42.141429	43.741950
C	39.243598	41.638463	42.782810
H	39.306542	40.575291	42.560307
Fe	39.114666	45.006328	43.432051
C	41.069589	41.317733	44.473486
C	41.242310	39.889881	44.241029
H	40.839643	39.510708	43.295166
C	41.828529	38.985485	45.044822
H	42.223868	39.238705	46.028761
H	41.905162	37.946711	44.717699
C	35.608273	42.849705	39.577074
H	35.180480	43.835245	39.369238
C	35.098307	41.810131	38.890891
H	35.441336	40.783743	39.017927
H	34.297892	41.972407	38.165284

C	42.812821	41.831031	46.310857
H	43.484565	41.078183	45.872060
H	43.405172	42.711725	46.588874
H	42.405936	41.418742	47.250353
C	37.497964	40.393520	40.534171
H	37.603041	40.366089	39.437665
H	38.341289	39.830865	40.948308
H	36.568946	39.849023	40.775250
C	35.139645	48.005506	40.858638
H	34.439805	47.191316	40.613609
H	34.548092	48.869390	41.182645
H	35.671752	48.276244	39.930494
C	42.340593	47.117369	47.582950
H	43.229006	47.574173	47.114155
H	42.070412	47.775089	48.422426
H	42.642558	46.140238	47.988479
C	40.274834	49.412508	46.839009
H	39.250727	49.809776	46.791860
H	40.512004	49.353520	47.912222
C	36.232812	49.848084	43.206165
H	37.071496	50.398490	43.648152
H	36.011322	50.374440	42.264278
C	41.229161	50.440995	46.206843
H	40.952173	50.626320	45.153858
H	42.259385	50.054301	46.171153
C	35.027846	49.974802	44.148343
H	35.251457	49.493020	45.117625
H	34.137688	49.462506	43.748258
C	34.678489	51.446636	44.419381
C	41.277934	51.815088	46.933564
O	42.201651	52.592772	46.582899
O	33.505125	51.736463	44.742194
O	40.408850	52.046362	47.808257
O	35.631444	52.264326	44.296649
O	40.158930	45.555693	42.332172
O	42.944039	50.601061	40.351203
O	45.404706	50.041572	39.043920
O	45.666001	49.485121	41.236566
O	43.986942	51.558935	40.047309
O	46.004583	49.275241	43.391591
C	43.410249	49.230913	40.190819
C	42.731748	48.663922	38.918394
C	42.978885	48.502319	41.470770
C	42.921044	47.132996	38.814663

C	44.936549	49.192969	40.033314
C	43.140582	46.983573	41.349375
C	43.191213	49.377179	37.631501
C	42.458001	46.441750	40.098404
C	43.708563	49.115036	42.677564
C	44.583120	51.197759	38.820534
C	43.516753	50.868553	37.752329
C	42.225849	46.536969	37.592990
C	45.208711	49.260750	42.478199
C	43.387921	48.428873	44.001760
C	45.507556	52.340898	38.462232
H	41.657038	48.862317	39.067163
H	41.903642	48.713992	41.589654
H	44.004521	46.940860	38.696659
H	45.240524	48.176900	39.752485
H	42.695193	46.502342	42.231098
H	44.215363	46.727938	41.348165
H	42.414458	49.254126	36.861690
H	44.086996	48.866710	37.247998
H	42.635911	45.359013	40.017374
H	41.369321	46.564920	40.211197
H	43.372725	50.162664	42.743606
H	43.897084	51.217287	36.780159
H	42.612929	51.450183	37.982868
H	43.848743	48.966413	44.840042
H	43.761845	47.395962	44.010669
H	42.301115	48.394481	44.160151
H	42.632517	46.924201	36.648240
H	42.362364	45.445667	37.576012
H	41.144512	46.752383	37.621385
H	46.172456	52.019502	37.648383
H	44.933450	53.218617	38.139356
H	46.117369	52.609923	39.334781
H	36.491142	45.652723	46.664578
H	38.276315	52.731383	39.351871

QM atoms (linking H atom included): 121

IIH10 In- Cluster1 ReactantSmaQM

C	37.235829	44.854434	46.602589
H	37.093207	44.164852	47.450020
H	38.230436	45.313810	46.675152
S	37.095696	43.883940	45.069365
N	38.093785	43.688680	42.237690
C	38.337074	42.346837	42.070740

C	37.094819	44.001839	41.359716
C	37.483398	41.786845	41.041341
C	36.685837	42.827525	40.596280
C	36.523461	45.261164	41.250689
H	35.766934	45.408666	40.481874
C	36.797966	46.343425	42.069676
N	37.700837	46.367417	43.109656
C	37.625847	47.636766	43.644293
C	36.624606	48.421887	42.943447
C	36.125395	47.616992	41.952292
C	38.442527	48.136306	44.649445
H	38.278484	49.167814	44.962158
C	39.481417	47.444258	45.266387
C	40.345223	48.005399	46.294642
C	40.874974	45.842949	45.825861
N	39.814906	46.139334	44.997733
C	41.226695	47.001701	46.633830
C	41.471838	44.592179	45.923545
H	42.247177	44.475169	46.679132
C	41.152379	43.461146	45.171827
C	41.740369	42.149324	45.371554
N	40.197358	43.419111	44.187070
C	40.127368	42.120683	43.770622
C	39.255362	41.619010	42.809948
H	39.321104	40.556899	42.582906
Fe	39.122646	44.981126	43.469573
C	41.086367	41.298447	44.496162
C	41.263620	39.871878	44.259497
H	40.867537	39.494726	43.309821
C	41.845958	38.967069	45.065473
H	42.230693	39.219841	46.053854
H	41.927507	37.929143	44.737279
C	35.633161	42.837280	39.591159
H	35.201938	43.822554	39.387435
C	35.130373	41.800019	38.895758
H	35.475564	40.773590	39.018450
H	34.333050	41.963823	38.167004
C	42.835631	41.811729	46.327536
H	43.502248	41.055456	45.887031
H	43.431486	42.692500	46.598067
H	42.433738	41.404230	47.271279
C	37.515095	40.379184	40.553205
H	37.631445	40.353350	39.457794
H	38.352745	39.813996	40.975032

H	36.581586	39.837973	40.783713
C	35.141289	47.989366	40.894820
H	34.435542	47.175727	40.664333
H	34.555237	48.856901	41.221145
H	35.656950	48.255256	39.956240
C	42.357674	47.101000	47.607442
H	43.244674	47.556492	47.134609
H	42.091220	47.761300	48.446245
H	42.660856	46.125061	48.014429
C	40.283124	49.393959	46.867821
H	39.257022	49.786729	46.824235
H	40.525762	49.340467	47.940351
C	36.233063	49.827035	43.245763
H	37.072300	50.384508	43.678325
H	35.995870	50.350190	42.305641
C	41.229699	50.424029	46.225287
H	40.946981	50.600813	45.172266
H	42.261704	50.042309	46.187289
C	35.035993	49.953140	44.198689
H	35.275880	49.488911	45.172784
H	34.147195	49.425767	43.815677
C	34.675901	51.427473	44.447379
C	41.275087	51.803861	46.941791
O	42.197611	52.580968	46.586761
O	33.496145	51.718171	44.744967
O	40.403961	52.040462	47.813136
O	35.628130	52.247255	44.330889
O	40.176136	45.526410	42.379428
O	42.955076	50.592035	40.374549
O	45.418121	50.028127	39.073277
O	45.668461	49.479506	41.268289
O	44.000561	51.547720	40.072753
O	46.004147	49.255080	43.422194
C	43.418027	49.222752	40.214041
C	42.742714	48.660828	38.937884
C	42.980251	48.491434	41.491991
C	42.920640	47.128934	38.832193
C	44.945112	49.182803	40.062516
C	43.133498	46.972380	41.366647
C	43.208647	49.373555	37.652375
C	42.449635	46.438009	40.113690
C	43.709512	49.095879	42.704462
C	44.601479	51.187173	38.848565
C	43.541011	50.863039	37.773334

C	42.228961	46.538710	37.605603
C	45.209713	49.244847	42.507514
C	43.388430	48.401737	44.023941
C	45.529564	52.330961	38.498177
H	41.668641	48.866386	39.081975
H	41.905242	48.706888	41.612842
H	44.003457	46.928871	38.719654
H	45.250264	48.165816	39.786429
H	42.684742	46.490421	42.246319
H	44.206641	46.710701	41.364778
H	42.433419	49.254037	36.880396
H	44.102309	48.858658	37.269725
H	42.622259	45.354763	40.030921
H	41.360297	46.563297	40.227614
H	43.373645	50.143310	42.775588
H	43.930024	51.207584	36.803032
H	42.640507	51.452326	37.996685
H	43.850312	48.933765	44.865256
H	43.762785	47.369189	44.025317
H	42.301854	48.366495	44.182518
H	42.637841	46.929774	36.663389
H	42.364179	45.447265	37.583233
H	41.147082	46.752798	37.629572
H	46.194085	52.013218	37.682362
H	44.956779	53.211769	38.180789
H	46.138726	52.594103	39.373069
H	36.483280	45.638834	46.682922

QM atoms (linking H atom included): 136

IIH10 In- Cluster1 TS BigQM

C	38.937357	52.136336	38.789493
H	38.767464	52.286614	37.710145
H	39.963988	52.485686	39.001911
C	38.840011	50.661229	39.129573
C	38.478595	49.732479	38.143296
H	38.248302	50.086170	37.133134
C	38.421284	48.360584	38.423677
H	38.129616	47.663660	37.634316
C	38.750186	47.897159	39.699055
H	38.738806	46.834835	39.946442
C	39.135891	48.811523	40.685698
H	39.428113	48.431739	41.664607
C	39.172426	50.178016	40.409242
H	39.489099	50.875010	41.188845

C	37.481040	44.988917	46.480590
H	37.375818	44.310743	47.341672
H	38.465164	45.472713	46.534708
S	37.368479	43.978845	44.972133
N	38.140648	43.808526	42.045786
C	38.415061	42.472520	41.873595
C	37.084962	44.090976	41.225029
C	37.529465	41.886440	40.886545
C	36.676249	42.901776	40.484528
C	36.462561	45.327766	41.142899
H	35.657807	45.443752	40.419715
C	36.763734	46.429993	41.925053
N	37.721418	46.496818	42.909767
C	37.638292	47.761273	43.447455
C	36.585539	48.512997	42.790511
C	36.059136	47.688195	41.830341
C	38.466153	48.282986	44.432301
H	38.278471	49.304860	44.760716
C	39.513093	47.601989	45.041314
C	40.316284	48.137056	46.130818
C	40.892089	45.990844	45.634400
N	39.883153	46.307607	44.750893
C	41.181092	47.126784	46.494899
C	41.487231	44.741902	45.753778
H	42.210885	44.614869	46.558331
C	41.199710	43.618488	44.982170
C	41.749499	42.301283	45.233769
N	40.297309	43.576506	43.944555
C	40.210669	42.265110	43.559771
C	39.353293	41.754258	42.594873
H	39.416784	40.691956	42.372150
Fe	39.180471	45.148794	43.219120
C	41.117724	41.441446	44.349856
C	41.243952	39.999881	44.184152
H	40.725643	39.579956	43.315167
C	41.897378	39.117371	44.963360
H	42.416177	39.405004	45.877324
H	41.898653	38.059425	44.691621
C	35.552923	42.870675	39.559573
H	34.977199	43.799973	39.505256
C	35.128027	41.852067	38.788764
H	35.618598	40.879686	38.756310
H	34.247893	41.978127	38.154203
C	42.780770	41.966352	46.259008

H	43.501788	41.241695	45.854580
H	43.331983	42.853153	46.592154
H	42.323648	41.521119	47.159790
C	37.559534	40.470909	40.417027
H	37.747483	40.426106	39.331749
H	38.350236	39.882044	40.895852
H	36.596158	39.962982	40.592340
C	35.036200	48.044833	40.807113
H	34.415177	47.188655	40.502972
H	34.369671	48.821934	41.199922
H	35.527173	48.435096	39.899531
C	42.242623	47.196381	47.545911
H	43.177257	47.619310	47.140063
H	41.933939	47.867964	48.360039
H	42.487399	46.213741	47.976570
C	40.216304	49.504715	46.748927
H	39.195835	49.900318	46.650512
H	40.389836	49.410545	47.831947
C	36.170884	49.907554	43.107033
H	37.007167	50.483383	43.520862
H	35.897731	50.428600	42.175455
C	41.212991	50.541380	46.202594
H	40.986266	50.776563	45.147366
H	42.233020	50.133417	46.193782
C	35.000209	49.992369	44.097832
H	35.276127	49.496895	45.047000
H	34.104112	49.469859	43.725597
C	34.636530	51.451808	44.414753
C	41.289220	51.879017	46.986238
O	42.238553	52.641761	46.670948
O	33.463037	51.723931	44.751563
O	40.425539	52.097780	47.867877
O	35.582735	52.280410	44.311649
O	40.150643	45.817456	41.928484
O	42.784888	50.314096	40.655676
O	45.112678	49.645763	39.167625
O	45.633124	49.391008	41.366769
O	43.743225	51.245637	40.105595
O	46.197865	49.549739	43.476151
C	43.285841	48.949271	40.634874
C	42.477508	48.198755	39.555717
C	43.026329	48.411628	42.046353
C	42.652958	46.664253	39.662881
C	44.787764	48.924355	40.303980

C	43.242229	46.901324	42.154402
C	42.781875	48.713957	38.131507
C	42.523951	46.130079	41.079943
C	43.850987	49.214718	43.057262
C	44.223345	50.733686	38.880807
C	43.072714	50.217419	37.987532
C	41.748767	45.908992	38.693486
C	45.312437	49.374332	42.668862
C	43.719347	48.691627	44.480140
C	45.052389	51.856108	38.287534
H	41.429939	48.433115	39.788782
H	41.960478	48.603862	42.253138
H	43.698321	46.440474	39.363110
H	45.099550	47.886943	40.118104
H	42.911054	46.551756	43.144288
H	44.328520	46.679387	42.105892
H	41.930504	48.472136	37.478128
H	43.647110	48.162856	37.728150
H	42.741763	45.056138	41.133086
H	41.248129	46.037319	41.487556
H	43.466778	50.245427	43.022951
H	43.351602	50.401011	36.938260
H	42.178636	50.824286	38.197573
H	44.098313	49.422201	45.198585
H	44.293046	47.764974	44.608569
H	42.666674	48.487007	44.711221
H	42.010621	46.109925	37.644277
H	41.839048	44.825225	38.860036
H	40.697154	46.186892	38.847910
H	45.680634	51.459051	37.479749
H	44.406487	52.649979	37.890354
H	45.704801	52.279205	39.063730
H	36.709271	45.755062	46.554489
H	38.249433	52.781869	39.335491

QM atoms (linking H atom included): 121

IIH10 In- Cluster1 TS SmaQM

C	37.490918	44.962904	46.511392
H	37.381682	44.288048	47.374505
H	38.473438	45.450372	46.569302
S	37.386989	43.944733	45.007359
N	38.150907	43.786144	42.075018
C	38.438943	42.455309	41.890801
C	37.091076	44.065477	41.259211

C	37.556368	41.868639	40.901381
C	36.692074	42.878626	40.509709
C	36.463955	45.300121	41.179917
H	35.660157	45.414652	40.455169
C	36.762597	46.402528	41.963227
N	37.714411	46.468375	42.953266
C	37.628698	47.732099	43.491086
C	36.577167	48.484664	42.830438
C	36.057624	47.660993	41.864815
C	38.455353	48.256859	44.475889
H	38.263925	49.278171	44.803649
C	39.507596	47.581112	45.080565
C	40.311918	48.119806	46.167296
C	40.899678	45.978100	45.663272
N	39.885598	46.290525	44.785376
C	41.184144	47.113987	46.526076
C	41.503638	44.732746	45.774426
H	42.231174	44.607936	46.575741
C	41.223658	43.610803	44.997579
C	41.780534	42.296353	45.245473
N	40.323336	43.566449	43.958517
C	40.243276	42.255597	43.569725
C	39.387799	41.742743	42.604101
H	39.460303	40.682160	42.375741
Fe	39.185801	45.127633	43.253255
C	41.153507	41.435228	44.358942
C	41.282463	39.993780	44.195812
H	40.764349	39.571148	43.327951
C	41.934789	39.114047	44.979137
H	42.451029	39.404378	45.893615
H	41.935939	38.055029	44.711955
C	35.567782	42.844394	39.585693
H	34.962727	43.756647	39.565835
C	35.175492	41.840993	38.778494
H	35.697765	40.887407	38.707792
H	34.290729	41.960866	38.149307
C	42.809530	41.965164	46.274090
H	43.530395	41.237237	45.875976
H	43.361183	42.853043	46.603237
H	42.349745	41.526530	47.176812
C	37.598893	40.457380	40.420951
H	37.820378	40.421129	39.341499
H	38.374073	39.862682	40.916990
H	36.629975	39.949515	40.562357

C	35.032771	48.014773	40.840571
H	34.389138	47.165020	40.566253
H	34.388030	48.816867	41.220025
H	35.517937	48.371490	39.916605
C	42.251053	47.187016	47.571123
H	43.185321	47.602581	47.157004
H	41.949940	47.865495	48.382637
H	42.493704	46.205996	48.006318
C	40.209295	49.489483	46.781322
H	39.185760	49.878942	46.690711
H	40.394261	49.400950	47.862803
C	36.159317	49.879184	43.146505
H	36.996454	50.457875	43.553936
H	35.878348	50.396341	42.214902
C	41.194730	50.530293	46.221388
H	40.956103	50.760356	45.167791
H	42.216188	50.127192	46.203553
C	34.993666	49.972369	44.141263
H	35.274840	49.491715	45.096182
H	34.097431	49.441969	43.780183
C	34.627524	51.436075	44.436683
C	41.276072	51.871771	46.998091
O	42.224794	52.631765	46.673729
O	33.454167	51.710869	44.771525
O	40.417608	52.096182	47.883372
O	35.571652	52.265443	44.317921
O	40.137708	45.813557	41.966635
O	42.755950	50.227779	40.682378
O	45.089465	49.561717	39.202748
O	45.615604	49.324752	41.403444
O	43.709588	51.160425	40.126406
O	46.176881	49.522354	43.510383
C	43.269448	48.867696	40.679204
C	42.465058	48.099044	39.612196
C	43.015204	48.348748	42.097345
C	42.642772	46.567009	39.738945
C	44.770420	48.847640	40.345770
C	43.253091	46.842690	42.226392
C	42.759424	48.602968	38.182425
C	42.534291	46.052365	41.165968
C	43.830906	49.180380	43.092930
C	44.191258	50.638978	38.906444
C	43.043749	50.105110	38.020688
C	41.716012	45.797038	38.803869

C	45.292470	49.333520	42.705186
C	43.694042	48.691281	44.526380
C	45.010442	51.764029	38.304535
H	41.419719	48.333253	39.847336
H	41.945560	48.526033	42.298947
H	43.680738	46.340191	39.418339
H	45.086660	47.810566	40.166279
H	42.934521	46.501121	43.223261
H	44.341719	46.633771	42.170789
H	41.904793	48.353194	37.536263
H	43.623169	48.049014	37.780431
H	42.754055	44.979884	41.234610
H	41.261376	45.979144	41.566135
H	43.441552	50.208208	43.030647
H	43.320086	50.277373	36.968770
H	42.148424	50.711479	38.225654
H	44.068261	49.439864	45.228936
H	44.267027	47.768563	44.679256
H	42.640372	48.491818	44.756000
H	41.871903	46.075486	37.751664
H	41.895476	44.716286	38.894128
H	40.664272	45.978069	39.068752
H	45.646089	51.366223	37.503083
H	44.358270	52.548755	37.899307
H	45.656325	52.200366	39.078953
H	36.716656	45.727181	46.578223

QM atoms (linking H atom included): 136

IIH10 In- Cluster1 ProductBigQM

C	38.977788	52.087079	38.791726
H	38.823852	52.265078	37.714191
H	40.001998	52.430744	39.025227
C	38.893908	50.598586	39.079895
C	38.607494	49.703955	38.037353
H	38.396169	50.095087	37.037297
C	38.601242	48.319447	38.247356
H	38.367363	47.651025	37.415146
C	38.901900	47.809273	39.512250
H	38.909427	46.733164	39.694836
C	39.200733	48.685256	40.561418
H	39.457086	48.268296	41.537070
C	39.191875	50.066426	40.349553
H	39.446931	50.736133	41.175118
C	37.408875	44.884273	46.645953

H	37.265135	44.242978	47.528449
H	38.406029	45.341663	46.700079
S	37.294642	43.828964	45.170069
N	38.117113	43.729502	42.185836
C	38.380809	42.387894	42.018579
C	37.076490	44.031989	41.348876
C	37.512942	41.825012	41.006900
C	36.672303	42.851442	40.598161
C	36.489655	45.285482	41.240189
H	35.713341	45.415292	40.489067
C	36.799960	46.390632	42.017111
N	37.715609	46.440301	43.041790
C	37.665196	47.716503	43.555751
C	36.667238	48.493661	42.845184
C	36.149701	47.672723	41.874828
C	38.480790	48.221845	44.561047
H	38.325637	49.257370	44.863430
C	39.494190	47.516611	45.200622
C	40.336949	48.058714	46.252852
C	40.859016	45.886285	45.804281
N	39.825002	46.202817	44.946654
C	41.197644	47.042690	46.616270
C	41.448164	44.633753	45.925006
H	42.206416	44.518325	46.697963
C	41.143657	43.504167	45.166485
C	41.735056	42.193848	45.366942
N	40.213294	43.454461	44.159141
C	40.153706	42.157975	43.729674
C	39.305890	41.658872	42.749926
H	39.381743	40.600905	42.510889
Fe	39.103115	45.033340	43.448562
C	41.102690	41.341640	44.475829
C	41.283767	39.914780	44.246753
H	40.865479	39.528663	43.310400
C	41.885455	39.016448	45.046814
H	42.294192	39.276024	46.023495
H	41.955651	37.974717	44.727726
C	35.567765	42.835312	39.649986
H	34.977292	43.756423	39.619555
C	35.176663	41.838493	38.834261
H	35.685234	40.876738	38.776391
H	34.308073	41.972107	38.185346
C	42.819887	41.862653	46.336921
H	43.504546	41.119713	45.901560

H	43.399278	42.749559	46.621904
H	42.410193	41.442201	47.271717
C	37.552738	40.419990	40.511613
H	37.769417	40.394904	39.431270
H	38.334842	39.828319	40.998421
H	36.587133	39.905886	40.652280
C	35.175755	48.048624	40.810817
H	34.545004	47.206170	40.489184
H	34.514238	48.843350	41.175928
H	35.708211	48.422113	39.919049
C	42.307526	47.132097	47.614597
H	43.213868	47.563960	47.156361
H	42.034742	47.807534	48.438839
H	42.583926	46.155363	48.038433
C	40.282482	49.445282	46.828334
H	39.263881	49.853166	46.762074
H	40.501091	49.385485	47.905456
C	36.269213	49.898054	43.139639
H	37.099098	50.460036	43.583846
H	36.036804	50.422203	42.198688
C	41.258620	50.460490	46.210017
H	41.005297	50.641731	45.150673
H	42.285731	50.063043	46.196462
C	35.064456	49.999348	44.087682
H	35.300559	49.501902	45.046157
H	34.177496	49.484145	43.684270
C	34.701356	51.461540	44.391741
C	41.308155	51.836985	46.930541
O	42.229167	52.613657	46.570197
O	33.521954	51.737584	44.705214
O	40.444600	52.070684	47.809905
O	35.651805	52.286781	44.305857
O	40.314162	45.652946	42.200578
O	42.949362	50.601458	40.341908
O	45.432511	50.048527	39.077766
O	45.639185	49.469202	41.272124
O	44.004453	51.557365	40.078832
O	45.931729	49.198192	43.428447
C	43.412934	49.231691	40.170399
C	42.759052	48.693773	38.873814
C	42.944587	48.487856	41.427644
C	42.958361	47.160348	38.729441
C	44.941628	49.190439	40.048313
C	43.098534	46.963264	41.300517

C	43.238188	49.431098	37.607720
C	42.612032	46.448392	39.993927
C	43.649787	49.072173	42.662679
C	44.624441	51.215038	38.858557
C	43.576772	50.915801	37.763495
C	42.223176	46.581584	37.520943
C	45.155222	49.211229	42.498907
C	43.290609	48.362925	43.964415
C	45.562682	52.360157	38.541354
H	41.681534	48.878433	39.011765
H	41.867932	48.698053	41.520825
H	44.046207	47.006240	38.541849
H	45.251837	48.176611	39.762769
H	42.541931	46.474285	42.111370
H	44.171543	46.703273	41.446066
H	42.468799	49.331141	36.827114
H	44.133038	48.919065	37.223910
H	42.230575	45.425738	39.936448
H	40.105666	45.352094	41.302624
H	43.322245	50.121865	42.740452
H	43.977298	51.278527	36.804667
H	42.674900	51.501842	37.988302
H	43.751191	48.869787	44.822031
H	43.637062	47.320586	43.954080
H	42.201054	48.353165	44.102114
H	42.596592	46.996141	36.574364
H	42.371009	45.492748	37.472765
H	41.142847	46.787092	37.593026
H	46.237389	52.054029	37.729477
H	44.998969	53.249754	38.232386
H	46.159591	52.603242	39.430350
H	36.660726	45.676477	46.673397
H	38.287303	52.727947	39.339983

QM atoms (linking H atom included): 121

IIH10 In- Cluster1 ProductSmaQM

C	37.312847	44.833682	46.673840
H	37.165499	44.193483	47.556653
H	38.310371	45.290505	46.728777
S	37.200811	43.786744	45.192149
N	38.082333	43.688369	42.229910
C	38.350682	42.349045	42.057543
C	37.055011	43.997218	41.380032
C	37.495584	41.791216	41.031909

C	36.665477	42.822130	40.612066
C	36.465159	45.250608	41.278544
H	35.691000	45.383370	40.525581
C	36.762347	46.350786	42.068360
N	37.673608	46.399723	43.096574
C	37.614642	47.671251	43.618744
C	36.616860	48.449475	42.906842
C	36.105468	47.631409	41.930461
C	38.420824	48.174170	44.633420
H	38.262568	49.208978	44.936882
C	39.439225	47.471936	45.268256
C	40.307208	48.025961	46.293202
C	40.824967	45.850301	45.850290
N	39.765666	46.155498	45.020099
C	41.179858	47.015310	46.643266
C	41.428889	44.603063	45.955813
H	42.206548	44.497025	46.710041
C	41.117288	43.468412	45.206953
C	41.724437	42.162291	45.390842
N	40.170009	43.413356	44.216472
C	40.121692	42.121323	43.773218
C	39.276555	41.622063	42.790537
H	39.357690	40.565277	42.548310
Fe	39.054910	44.986572	43.515850
C	41.088570	41.310029	44.501737
C	41.280839	39.886881	44.259112
H	40.859847	39.504322	43.322344
C	41.897672	38.990119	45.048814
H	42.306915	39.251262	46.024678
H	41.981391	37.951536	44.722904
C	35.598126	42.820283	39.622333
H	35.097029	43.783962	39.487874
C	35.151021	41.795092	38.872871
H	35.565536	40.788824	38.924682
H	34.329440	41.948084	38.169163
C	42.821091	41.834100	46.348918
H	43.509123	41.099091	45.905291
H	43.395785	42.723854	46.634273
H	42.423192	41.405521	47.285259
C	37.546175	40.390063	40.525430
H	37.703885	40.376922	39.434635
H	38.367328	39.817689	40.969376
H	36.604886	39.846523	40.714207
C	35.129662	48.007024	40.866415

H	34.462728	47.178077	40.583706
H	34.502681	48.837316	41.213604
H	35.656669	48.333504	39.953527
C	42.312069	47.118010	47.614056
H	43.198261	47.567593	47.134226
H	42.049247	47.784655	48.448737
H	42.612734	46.142941	48.024342
C	40.256625	49.415572	46.863347
H	39.235604	49.819493	46.811141
H	40.491148	49.360558	47.937535
C	36.222357	49.855123	43.201259
H	37.060218	50.418838	43.628020
H	35.975540	50.374384	42.261392
C	41.219365	50.435209	46.227556
H	40.943778	50.617685	45.173645
H	42.247060	50.041312	46.193636
C	35.030852	49.973102	44.162372
H	35.278266	49.498854	45.129754
H	34.140700	49.447243	43.780619
C	34.670314	51.442960	44.430885
C	41.277548	51.811913	46.949756
O	42.204199	52.584586	46.595588
O	33.493671	51.727950	44.746375
O	40.411238	52.050029	47.825234
O	35.619250	52.266152	44.312874
O	40.286387	45.592816	42.293887
O	42.955287	50.576251	40.412405
O	45.409029	50.012124	39.099458
O	45.674808	49.482578	41.299055
O	43.998973	51.531896	40.107171
O	46.019767	49.284640	43.453792
C	43.422508	49.207251	40.257877
C	42.745567	48.638678	38.985256
C	42.987328	48.488575	41.542590
C	42.952320	47.103262	38.869778
C	44.948436	49.172638	40.100345
C	43.130746	46.959803	41.442072
C	43.189596	49.356244	37.695207
C	42.618435	46.423171	40.154887
C	43.723130	49.095254	42.749284
C	44.590564	51.171936	38.878069
C	43.518534	50.847268	37.813780
C	42.207903	46.492550	37.683603
C	45.221822	49.257711	42.542906

C	43.419958	48.393503	44.069944
C	45.514986	52.314305	38.515972
H	41.669694	48.817070	39.142062
H	41.913205	48.704715	41.662101
H	44.038771	46.949889	38.675492
H	45.257830	48.154603	39.829389
H	42.587868	46.487320	42.272033
H	44.205579	46.699189	41.573191
H	42.405741	49.232843	36.932460
H	44.081672	48.845845	37.302274
H	42.186386	45.420491	40.131722
H	40.068611	45.303973	41.394154
H	43.379119	50.139437	42.826715
H	43.893523	51.195269	36.839046
H	42.620260	51.434883	38.050503
H	43.887760	48.928473	44.906111
H	43.803199	47.363867	44.066096
H	42.335414	48.350075	44.239398
H	42.575466	46.876330	36.722059
H	42.354260	45.402326	37.671843
H	41.127148	46.698171	37.751936
H	46.175842	51.993141	37.698573
H	44.940044	53.192797	38.196026
H	46.128207	52.582794	39.386226
H	36.569538	45.630458	46.700415

QM atoms (linking H atom included): 121

IIH10 Out Cluster2 Re

C	41.798413	47.423016	40.286555
H	42.768486	47.659048	40.747984
H	41.962973	46.973659	39.297499
S	40.953568	46.258123	41.390442
N	38.667300	44.403465	41.439678
C	39.098783	43.347333	42.206093
C	37.616894	44.962921	42.113165
C	38.278457	43.204931	43.394528
C	37.347911	44.228776	43.342811
C	36.908386	46.077518	41.686196
H	36.081391	46.410464	42.311566
C	37.146135	46.798835	40.525180
N	38.122168	46.523317	39.593331
C	37.958070	47.454217	38.589246
C	36.842541	48.343176	38.887517
C	36.357603	47.940147	40.110552

C	38.780136	47.566010	37.473564
H	38.564034	48.375003	36.777959
C	39.867482	46.748527	37.181531
C	40.746521	46.929382	36.036571
C	41.338433	45.120477	37.266905
N	40.257260	45.659426	37.930912
C	41.647570	45.891930	36.076658
C	42.092128	44.043815	37.712925
H	42.956592	43.762535	37.112591
C	41.875541	43.325345	38.884753
C	42.750769	42.275757	39.371317
N	40.842054	43.544487	39.760754
C	41.022292	42.671144	40.795348
C	40.207148	42.565816	41.915860
H	40.452876	41.787329	42.634330
Fe	39.328874	44.881052	39.560557
C	42.221324	41.868555	40.582724
C	42.688578	40.845254	41.508581
H	41.924806	40.419907	42.169406
C	43.937689	40.365659	41.632108
H	44.772906	40.744553	41.040708
H	44.147137	39.569004	42.349620
C	36.301959	44.585810	44.295126
H	36.008093	45.642639	44.299747
C	35.677015	43.764471	45.156647
H	35.866583	42.690400	45.192795
H	34.924165	44.155496	45.846141
C	43.964454	41.756076	38.672846
H	44.048872	40.668172	38.822074
H	43.942847	41.962858	37.594980
H	44.885260	42.224640	39.061409
C	38.435686	42.149733	44.440255
H	38.202765	42.543423	45.441817
H	37.754223	41.300714	44.261260
H	39.449847	41.728693	44.458448
C	35.187718	48.504546	40.851220
H	35.253908	48.337175	41.937027
H	35.115601	49.588002	40.685352
H	34.240867	48.048130	40.513658
C	42.725781	45.603295	35.081171
H	42.324145	45.047414	34.217569
H	43.142110	46.539031	34.678124
H	43.552360	45.011488	35.496933
C	40.705721	48.046435	35.034257

H	39.962829	48.800409	35.316897
H	41.674293	48.577317	35.068019
C	36.286222	49.428196	38.009237
H	36.636270	49.302533	36.977294
H	35.191294	49.309146	37.953428
C	40.425474	47.597578	33.593840
H	39.608005	46.861641	33.582023
H	41.280030	47.048805	33.167074
C	36.589288	50.871135	38.444217
H	37.675139	51.062129	38.409253
H	36.293708	51.047232	39.492138
C	35.886891	51.944976	37.580301
C	40.053726	48.719304	32.601188
O	39.791611	49.860612	33.041545
O	35.910525	53.123720	38.002388
O	40.031664	48.376128	31.383830
O	35.348050	51.564921	36.506855
O	38.307885	43.884122	38.813198
O	38.391810	44.467067	34.950421
O	36.080854	44.487483	33.294622
O	36.995932	42.385158	33.258327
O	38.325700	44.901363	33.569122
O	38.190993	40.570213	32.923892
C	37.192930	43.745385	35.336207
C	36.418023	44.668290	36.306215
C	37.669677	42.459401	36.024876
C	35.288112	43.938465	37.075274
C	36.365943	43.400115	34.094557
C	36.476835	41.703810	36.627731
C	35.885367	45.936129	35.610748
C	35.732296	42.578321	37.634253
C	38.528027	41.646299	35.046261
C	37.081433	45.531103	33.346631
C	36.734645	46.521784	34.477476
C	34.752866	44.805994	38.220362
C	37.883727	41.455778	33.688588
C	39.066260	40.336166	35.620474
C	37.160011	46.162118	31.971971
H	37.183541	44.954522	37.042635
H	38.314768	42.779427	36.858383
H	34.457553	43.761425	36.363660
H	35.404227	42.966962	34.400742
H	36.837123	40.797577	37.135481
H	35.797627	41.347703	35.830195

H	35.740408	46.720295	36.370154
H	34.887927	45.710027	35.202312
H	34.845920	42.044249	38.015968
H	36.401524	42.759569	38.489289
H	39.389785	42.290298	34.792641
H	36.173389	47.351415	34.021535
H	37.671281	46.952749	34.852800
H	38.262551	39.714400	36.040217
H	39.786590	40.545042	36.425150
H	39.564493	39.743553	34.844740
H	35.571063	45.058566	38.914159
H	34.307489	45.747100	37.863227
H	33.983822	44.261556	38.791085
H	37.442047	45.409305	31.227525
H	36.173801	46.564798	31.702541
H	37.902294	46.970911	31.947161
H	41.253566	48.358758	40.161673

QM atoms (linking H atom included): 121

IIH10 Out Cluster2 TS

C	41.760869	47.371095	40.225740
H	42.739409	47.594249	40.675728
H	41.914756	46.923665	39.233480
S	40.940615	46.191866	41.328293
N	38.613513	44.421589	41.484313
C	39.047993	43.365448	42.246873
C	37.578839	44.999561	42.162769
C	38.235566	43.235665	43.441853
C	37.312509	44.267685	43.394926
C	36.876746	46.120452	41.739587
H	36.068331	46.472234	42.378339
C	37.095888	46.819986	40.560219
N	38.038152	46.518412	39.602806
C	37.881081	47.451023	38.599136
C	36.785844	48.356498	38.913913
C	36.316769	47.968656	40.149538
C	38.690050	47.556343	37.472716
H	38.480705	48.371231	36.782775
C	39.767580	46.728960	37.177595
C	40.661917	46.912782	36.045027
C	41.240685	45.096522	37.273782
N	40.143249	45.626953	37.919290
C	41.562780	45.875089	36.092285
C	42.003031	44.029154	37.725700

H	42.875302	43.757179	37.133009
C	41.789868	43.318419	38.901268
C	42.675968	42.281030	39.393711
N	40.755145	43.528365	39.778425
C	40.947856	42.668235	40.824103
C	40.145127	42.569082	41.951937
H	40.394648	41.794870	42.673330
Fe	39.222625	44.865093	39.578009
C	42.155631	41.877742	40.610353
C	42.642310	40.868352	41.541257
H	41.889273	40.444156	42.214818
C	43.897471	40.401653	41.657325
H	44.723996	40.780878	41.053744
H	44.122600	39.616278	42.382737
C	36.268809	44.625917	44.348447
H	35.975840	45.682828	44.353887
C	35.640710	43.803333	45.206739
H	35.828682	42.728844	45.239612
H	34.887512	44.193273	45.896358
C	43.891262	41.767999	38.692741
H	43.982543	40.680326	38.840891
H	43.864824	41.974550	37.614936
H	44.810686	42.241830	39.078335
C	38.391824	42.180267	44.487800
H	38.166085	42.575620	45.490459
H	37.704746	41.334429	44.313260
H	39.404219	41.754537	44.500057
C	35.162343	48.549245	40.901834
H	35.239227	48.386010	41.987411
H	35.097411	49.632422	40.730756
H	34.206862	48.099290	40.579379
C	42.656069	45.594152	35.111033
H	42.265842	45.046978	34.236612
H	43.080284	46.532385	34.722268
H	43.475761	44.997196	35.533454
C	40.641968	48.036707	35.048878
H	39.889995	48.784965	35.320759
H	41.607471	48.571160	35.110588
C	36.232783	49.442207	38.035197
H	36.568802	49.305040	36.999840
H	35.135801	49.338098	37.992492
C	40.402029	47.600400	33.596458
H	39.602505	46.846805	33.553571
H	41.278199	47.076434	33.182030

C	36.562034	50.883390	38.454516
H	37.650366	51.056677	38.407327
H	36.279209	51.073128	39.503384
C	35.868835	51.959055	37.587072
C	40.025884	48.723247	32.606626
O	39.749107	49.860425	33.048235
O	35.906293	53.140318	38.001387
O	40.016286	48.385253	31.386936
O	35.322221	51.578207	36.517741
O	38.135762	43.686377	38.883944
O	38.470954	44.555079	34.774498
O	36.075466	44.478061	33.243919
O	37.031695	42.400547	33.231718
O	38.320012	44.947444	33.388288
O	38.196569	40.564613	32.911028
C	37.308654	43.833360	35.250641
C	36.559871	44.789485	36.218615
C	37.868314	42.593637	35.965027
C	35.513299	44.067860	37.102706
C	36.424627	43.426040	34.066884
C	36.771092	41.874074	36.759964
C	35.943660	46.000976	35.500780
C	36.102967	42.822072	37.717862
C	38.637006	41.706165	34.975620
C	37.054236	45.545856	33.210139
C	36.734272	46.568783	34.320141
C	34.919507	44.980096	38.181716
C	37.928905	41.479037	33.655836
C	39.134384	40.390955	35.578273
C	37.062457	46.138989	31.817339
H	37.355558	45.141423	36.889514
H	38.586268	42.970757	36.709051
H	34.678543	43.739871	36.444639
H	35.490194	42.982789	34.440950
H	37.206136	41.031446	37.311240
H	36.016597	41.425643	36.079203
H	35.800731	46.806222	36.237538
H	34.940497	45.722661	35.140871
H	35.448379	42.335311	38.454167
H	37.116628	43.286981	38.469403
H	39.514055	42.297432	34.654442
H	36.140087	47.372820	33.860112
H	37.674728	47.028183	34.649752
H	38.307543	39.798387	35.995637

H	39.850773	40.589029	36.389215
H	39.619008	39.771046	34.815995
H	35.715426	45.353411	38.841407
H	34.390583	45.843784	37.753385
H	34.203177	44.417821	38.801654
H	37.320586	45.373525	31.077352
H	36.063912	46.531310	31.582482
H	37.797192	46.953034	31.749925
H	41.216248	48.308608	40.113826

QM atoms (linking H atom included): 121

IIH10 Out Cluster2 Product

C	41.819632	47.400834	40.250374
H	42.793737	47.643693	40.698111
H	41.980219	46.949999	39.260846
S	41.016373	46.215731	41.358302
N	38.627116	44.397664	41.464013
C	39.073831	43.344197	42.228468
C	37.599995	44.986345	42.149801
C	38.261736	43.215841	43.421298
C	37.338968	44.251158	43.378499
C	36.905157	46.117447	41.735096
H	36.097805	46.467262	42.376257
C	37.124944	46.824450	40.559183
N	38.077170	46.539140	39.609077
C	37.915876	47.460535	38.597573
C	36.807277	48.353946	38.905141
C	36.335332	47.963641	40.139167
C	38.728405	47.563972	37.473376
H	38.508860	48.365987	36.771742
C	39.819948	46.749396	37.188203
C	40.705478	46.927732	36.049663
C	41.320712	45.132660	37.296772
N	40.222393	45.664818	37.942278
C	41.620520	45.900396	36.103047
C	42.089904	44.069767	37.749675
H	42.956891	43.794866	37.150916
C	41.876644	43.351684	38.922902
C	42.748705	42.299298	39.409711
N	40.838966	43.553321	39.795416
C	41.008077	42.675842	40.830089
C	40.183725	42.559897	41.941732
H	40.425693	41.779966	42.659459
Fe	39.316703	44.919049	39.601903

C	42.211659	41.879805	40.614891
C	42.674441	40.846928	41.531788
H	41.909120	40.425249	42.192842
C	43.919757	40.355487	41.649786
H	44.757154	40.728878	41.057884
H	44.123906	39.553792	42.363374
C	36.297311	44.606956	44.335047
H	35.999381	45.662226	44.337928
C	35.675899	43.784319	45.197919
H	35.870154	42.711210	45.235490
H	34.921998	44.173104	45.887149
C	43.965954	41.785788	38.712756
H	44.046975	40.695371	38.845805
H	43.951256	42.009886	37.638224
H	44.884725	42.246407	39.115673
C	38.417105	42.161650	44.468809
H	38.209641	42.564980	45.472278
H	37.715695	41.325345	44.306271
H	39.423604	41.722389	44.469024
C	35.169566	48.533080	40.882013
H	35.234854	48.361034	41.966959
H	35.102213	49.617315	40.718947
H	34.220242	48.082190	40.543696
C	42.707324	45.621182	35.114518
H	42.314561	45.062302	34.248700
H	43.118492	46.560188	34.713872
H	43.535091	45.034784	35.535452
C	40.665973	48.039789	35.042157
H	39.911986	48.785922	35.314623
H	41.628836	48.580476	35.087795
C	36.248339	49.435824	38.025703
H	36.588018	49.302321	36.991204
H	35.152135	49.325117	37.981289
C	40.412101	47.588933	33.596879
H	39.608309	46.838492	33.570013
H	41.282337	47.057411	33.179718
C	36.568081	50.878416	38.449697
H	37.655397	51.058538	38.405061
H	36.282594	51.062856	39.498936
C	35.869273	51.953486	37.585018
C	40.033299	48.708377	32.603369
O	39.758673	49.847034	33.042523
O	35.906659	53.134609	38.000153
O	40.020411	48.366975	31.384884

O	35.318362	51.572161	36.518261
O	38.156691	43.747950	38.750793
O	38.390629	44.515030	34.841853
O	36.057425	44.502872	33.218787
O	36.984716	42.405126	33.209908
O	38.305884	44.919117	33.453874
O	38.173608	40.581237	32.901237
C	37.196391	43.802013	35.257625
C	36.435241	44.750116	36.215011
C	37.694227	42.538012	35.967893
C	35.308282	44.047772	37.017826
C	36.356563	43.430209	34.034087
C	36.526926	41.776686	36.616845
C	35.896600	46.006181	35.504021
C	35.659553	42.658435	37.444222
C	38.534589	41.697913	34.998199
C	37.061135	45.547664	33.235449
C	36.734501	46.564336	34.349666
C	34.869905	44.893218	38.224906
C	37.876069	41.482715	33.650929
C	39.060189	40.393528	35.597984
C	37.125401	46.153059	31.849804
H	37.207489	45.042230	36.940421
H	38.337994	42.882683	36.789975
H	34.424645	43.967643	36.340420
H	35.400522	42.995521	34.360647
H	36.923471	40.960123	37.238392
H	35.922825	41.262291	35.831883
H	35.767888	46.805076	36.251149
H	34.892870	45.778635	35.112785
H	35.020495	42.191131	38.200874
H	37.415542	43.460958	39.305033
H	39.402543	42.325217	34.725110
H	36.173836	47.388798	33.883279
H	37.677473	46.996493	34.707622
H	38.248030	39.780622	36.015326
H	39.769166	40.612823	36.409984
H	39.567059	39.787108	34.838471
H	35.728580	45.071523	38.889227
H	34.467527	45.871237	37.920498
H	34.090450	44.369915	38.801401
H	37.389183	45.385850	31.113577
H	36.140852	46.563453	31.587343
H	37.876825	46.952957	31.806184

H	41.257657	48.327265	40.132148
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QM atoms (linking H atom included): 121

IIH10 Out Cluster1 Re

C	44.332348	45.658061	39.332134
H	45.390854	45.422906	39.525965
H	44.019165	45.166933	38.401011
S	43.353637	45.043919	40.739017
N	40.604704	44.331590	41.276208
C	40.789484	43.207243	42.047194
C	40.047182	45.273014	42.097646
C	40.344057	43.437975	43.406939
C	39.885693	44.744202	43.445677
C	39.667966	46.546810	41.692788
H	39.162582	47.174575	42.426566
C	39.872633	47.094221	40.434512
N	40.522450	46.478211	39.388974
C	40.518701	47.390449	38.356275
C	39.843576	48.619184	38.755341
C	39.436841	48.423795	40.053541
C	41.068790	47.172060	37.099388
H	41.029361	47.990767	36.380614
C	41.651740	45.983140	36.672154
C	42.211823	45.782838	35.343358
C	42.313901	43.895692	36.596255
N	41.748569	44.838160	37.430860
C	42.599858	44.464133	35.293052
C	42.630429	42.597064	36.964336
H	43.105594	41.971855	36.208393
C	42.425209	42.028821	38.219718
C	42.847599	40.693768	38.587010
N	41.830675	42.664491	39.281016
C	41.849390	41.777369	40.320329
C	41.358683	42.025699	41.597343
H	41.408244	41.212165	42.318137
Fe	40.985488	44.505606	39.280624
C	42.477629	40.526056	39.912280
C	42.641404	39.382096	40.795342
H	42.407141	39.570721	41.848276
C	43.004666	38.126070	40.478564
H	43.222003	37.808515	39.458354
H	43.058749	37.365507	41.260113
C	39.410343	45.528046	44.579565
H	39.551146	46.612314	44.489576

C	38.858061	45.069745	45.716820
H	38.634652	44.014769	45.884052
H	38.594464	45.765440	46.516904
C	43.572445	39.735123	37.700546
H	44.430815	39.295134	38.233065
H	42.913609	38.906153	37.392070
H	43.960395	40.215113	36.792709
C	40.410142	42.447785	44.523302
H	39.457791	41.901814	44.637442
H	41.189606	41.690652	44.359283
H	40.613726	42.948138	45.482639
C	38.632697	49.342308	40.917689
H	38.352585	50.250748	40.366418
H	37.703515	48.856679	41.256176
H	39.177779	49.658659	41.823148
C	43.183681	43.754299	34.114080
H	42.388371	43.436860	33.421902
H	43.827565	44.432189	33.535103
H	43.767866	42.863212	34.383891
C	42.345140	46.800179	34.250647
H	42.060424	47.800045	34.602825
H	43.406560	46.894581	33.968359
C	39.622806	49.833932	37.908395
H	39.481598	49.555423	36.855759
H	38.674485	50.300583	38.216580
C	41.527730	46.472465	32.994088
H	40.488983	46.246686	33.262405
H	41.897594	45.554861	32.506551
C	40.728546	50.898988	37.996027
H	41.683989	50.480597	37.631977
H	40.902320	51.207378	39.039389
C	40.419145	52.161633	37.160958
C	41.533545	47.582894	31.922053
O	42.351243	48.514784	32.040432
O	39.726917	51.996968	36.112542
O	40.683681	47.453591	30.991576
O	40.888153	53.245777	37.568670
O	39.530429	44.004719	38.814198
O	38.877757	44.588747	35.052761
O	36.394362	45.355780	33.900130
O	36.550080	43.074901	33.886393
O	38.647132	44.958066	33.674358
O	37.083727	40.983656	33.445026
C	37.619256	44.338475	35.739779

C	37.417112	45.512349	36.724305
C	37.777765	42.992241	36.452390
C	36.275138	45.244323	37.737044
C	36.479163	44.235976	34.723716
C	36.554026	42.721641	37.339215
C	37.224667	46.865331	36.006025
C	36.374998	43.844132	38.362324
C	38.108936	41.916472	35.410363
C	37.662440	45.977212	33.618856
C	37.948848	47.071017	34.669006
C	36.237526	46.310924	38.838322
C	37.197187	41.921075	34.190884
C	38.272993	40.513354	35.987018
C	37.637854	46.451689	32.183375
H	38.361338	45.537699	37.291870
H	38.647950	43.092115	37.119010
H	35.319230	45.301324	37.181231
H	35.520707	44.176031	35.255927
H	36.684075	41.766697	37.866461
H	35.640382	42.597814	36.731239
H	37.540736	47.671027	36.686361
H	36.147720	47.009018	35.823704
H	35.470861	43.658405	38.965661
H	37.239599	43.832101	39.045541
H	39.077310	42.218575	34.974257
H	37.621997	48.036586	34.252768
H	39.037701	47.139405	34.801052
H	38.423584	39.792802	35.178172
H	37.382938	40.191768	36.546640
H	39.139636	40.479309	36.665376
H	35.460959	46.073474	39.582844
H	37.207676	46.352548	39.362160
H	36.019236	47.314599	38.445080
H	36.799594	47.150390	32.048401
H	38.585526	46.938605	31.906127
H	37.475860	45.590628	31.519857
H	44.230143	46.735671	39.204156

QM atoms (linking H atom included): 121

IIH10 Out Cluster1 TS

C	44.246743	45.625768	39.275173
H	45.299447	45.362845	39.461089
H	43.918215	45.151029	38.339864
S	43.276985	45.001060	40.677403

N	40.562761	44.383555	41.373458
C	40.737335	43.249198	42.128244
C	40.046758	45.340151	42.198970
C	40.311560	43.486003	43.493685
C	39.886432	44.804379	43.545391
C	39.691465	46.625475	41.801824
H	39.233816	47.271632	42.550366
C	39.852264	47.158294	40.529346
N	40.432509	46.523820	39.453384
C	40.440100	47.437961	38.421320
C	39.809885	48.681069	38.843089
C	39.435728	48.495747	40.154362
C	40.970540	47.219696	37.154518
H	40.950736	48.047687	36.446460
C	41.525769	46.023133	36.716651
C	42.107205	45.817397	35.396996
C	42.173894	43.923061	36.646844
N	41.588627	44.866089	37.467905
C	42.488395	44.496514	35.353539
C	42.499074	42.627074	37.015626
H	42.984117	42.006750	36.263057
C	42.306024	42.063715	38.273406
C	42.754113	40.737207	38.642568
N	41.710929	42.688532	39.340490
C	41.753431	41.809463	40.386982
C	41.282975	42.057715	41.670770
H	41.339772	41.244471	42.391087
Fe	40.855049	44.547334	39.356402
C	42.399412	40.567259	39.971580
C	42.596541	39.426553	40.852197
H	42.388362	39.618111	41.909860
C	42.958745	38.171888	40.526412
H	43.150168	37.855270	39.500526
H	43.042666	37.411641	41.305830
C	39.429935	45.587177	44.686981
H	39.592894	46.668971	44.606472
C	38.865466	45.130022	45.818879
H	38.619122	44.078249	45.975201
H	38.615494	45.823772	46.624959
C	43.492584	39.793494	37.750409
H	44.345012	39.346192	38.286156
H	42.840113	38.968722	37.418047
H	43.890950	40.290259	36.855860
C	40.359585	42.484865	44.601095

H	39.398666	41.952392	44.707182
H	41.127507	41.717850	44.428715
H	40.569187	42.972538	45.565439
C	38.646423	49.419805	41.026555
H	38.347974	50.319260	40.470352
H	37.727823	48.930482	41.388375
H	39.203423	49.749768	41.919097
C	43.090814	43.784431	34.185684
H	42.304348	43.477862	33.478472
H	43.753824	44.457032	33.622738
H	43.660600	42.887093	34.466173
C	42.271376	46.829479	34.301049
H	41.957133	47.825557	34.636518
H	43.343462	46.938840	34.065534
C	39.589010	49.897476	37.997588
H	39.404392	49.619686	36.950879
H	38.664925	50.389771	38.338927
C	41.515100	46.483445	33.009608
H	40.474725	46.222567	33.229249
H	41.933278	45.582519	32.530272
C	40.720739	50.937380	38.033978
H	41.654344	50.491287	37.646917
H	40.933528	51.260036	39.065551
C	40.412580	52.190770	37.185838
C	41.521927	47.596606	31.939822
O	42.325798	48.538788	32.072847
O	39.710650	52.018654	36.144696
O	40.689356	47.458733	30.994115
O	40.891992	53.277009	37.575591
O	39.276185	43.892474	39.049181
O	38.974601	44.659781	34.823052
O	36.386889	45.371346	33.879221
O	36.584160	43.097189	33.884661
O	38.619323	45.015992	33.471234
O	37.096477	41.003695	33.430135
C	37.789426	44.404834	35.618606
C	37.655544	45.599737	36.597889
C	38.052241	43.074231	36.329104
C	36.651787	45.323173	37.743313
C	36.563625	44.266648	34.709047
C	36.962322	42.804056	37.372551
C	37.344175	46.929970	35.884784
C	36.879521	43.953244	38.342251
C	38.265762	41.960935	35.296818

C	37.615843	46.015448	33.486880
C	37.954977	47.132396	34.494481
C	36.674728	46.404557	38.828085
C	37.261928	41.951380	34.151620
C	38.407301	40.571078	35.915820
C	37.487435	46.474371	32.053966
H	38.652697	45.668906	37.056270
H	38.990474	43.197746	36.890171
H	35.630526	45.310156	37.303940
H	35.655666	44.198724	35.325350
H	37.191749	41.879865	37.914333
H	35.972304	42.632325	36.903217
H	37.685592	47.757441	36.524570
H	36.250891	47.029375	35.792248
H	36.274281	43.753064	39.236668
H	38.104532	44.007226	38.830018
H	39.208486	42.207336	34.778059
H	37.567652	48.080618	34.090838
H	39.047672	47.233630	34.542949
H	38.530311	39.821996	35.129329
H	37.512515	40.287037	36.488845
H	39.276305	40.536560	36.591434
H	35.958792	46.162812	39.629174
H	37.676263	46.469241	39.276834
H	36.406173	47.393655	38.432186
H	36.629959	47.155639	31.960984
H	38.412551	46.978808	31.735689
H	37.314725	45.604556	31.405522
H	44.158935	46.706819	39.167072

QM atoms (linking H atom included): 121

IIH10 Out Cluster1 Product

C	44.322841	45.649963	39.292026
H	45.381973	45.411798	39.471853
H	43.996270	45.164601	38.361544
S	43.358611	45.018850	40.695731
N	40.554616	44.349664	41.368886
C	40.743732	43.216184	42.124573
C	40.034960	45.308280	42.191888
C	40.310000	43.452444	43.486411
C	39.874331	44.769401	43.535906
C	39.681797	46.596529	41.795093
H	39.208898	47.236603	42.539337
C	39.856551	47.135071	40.525798

N	40.464313	46.511447	39.459035
C	40.463378	47.415177	38.416600
C	39.809406	48.649721	38.828535
C	39.426558	48.464784	40.138657
C	41.002115	47.194287	37.153703
H	40.958870	48.012533	36.435303
C	41.590202	46.008069	36.725759
C	42.156409	45.799176	35.400738
C	42.277472	43.912942	36.664097
N	41.699115	44.860959	37.485212
C	42.558813	44.482911	35.361126
C	42.604590	42.617491	37.034187
H	43.083992	41.994393	36.280216
C	42.398123	42.049296	38.290283
C	42.823019	40.715124	38.659715
N	41.791138	42.667298	39.352763
C	41.804919	41.785141	40.397071
C	41.308035	42.029982	41.672527
H	41.354691	41.215220	42.391542
Fe	40.965389	44.547585	39.373309
C	42.443601	40.540146	39.982903
C	42.605050	39.389322	40.857742
H	42.371316	39.572988	41.911676
C	42.963318	38.134039	40.531079
H	43.178708	37.823528	39.508254
H	43.018826	37.367158	41.306382
C	39.412313	45.550312	44.676998
H	39.556090	46.634075	44.589011
C	38.866183	45.090384	45.816780
H	38.640992	44.035623	45.983196
H	38.611595	45.785017	46.620649
C	43.556395	39.763164	37.772250
H	44.404167	39.311078	38.311536
H	42.897410	38.942456	37.441878
H	43.960040	40.254755	36.877127
C	40.365638	42.455570	44.597950
H	39.402629	41.930349	44.719775
H	41.126327	41.683239	44.419095
H	40.591809	42.946148	45.557305
C	38.635723	49.391348	41.006569
H	38.330920	50.286036	40.446313
H	37.721906	48.901054	41.378289
H	39.197932	49.729727	41.892822
C	43.147300	43.771120	34.185907

H	42.351491	43.458324	33.492232
H	43.796123	44.446151	33.609619
H	43.725469	42.877411	34.460330
C	42.291859	46.809871	34.300632
H	41.963872	47.800995	34.637723
H	43.359932	46.937824	34.056537
C	39.586570	49.864378	37.979961
H	39.416907	49.583699	36.931683
H	38.653924	50.348179	38.309505
C	41.532554	46.454416	33.013465
H	40.496179	46.179103	33.238292
H	41.962034	45.561513	32.529061
C	40.710008	50.913636	38.030543
H	41.650246	50.475508	37.650610
H	40.910979	51.233103	39.065545
C	40.402936	52.169707	37.184498
C	41.526043	47.574276	31.949189
O	42.325400	48.520145	32.084528
O	39.702714	51.999371	36.142040
O	40.690382	47.438048	31.006409
O	40.882219	53.255095	37.576740
O	39.325724	43.922329	38.876559
O	38.908930	44.662410	34.890316
O	36.369803	45.396640	33.839401
O	36.546567	43.116309	33.860037
O	38.611752	45.000936	33.519214
O	37.080311	41.022269	33.431116
C	37.685541	44.421594	35.636119
C	37.524654	45.619217	36.600554
C	37.895826	43.094668	36.367068
C	36.423384	45.381666	37.666804
C	36.500520	44.291141	34.677519
C	36.730719	42.817380	37.330802
C	37.302398	46.960168	35.869417
C	36.424300	43.984987	38.204941
C	38.172126	41.989214	35.342356
C	37.623461	46.015961	33.485276
C	37.953782	47.135681	34.492342
C	36.486637	46.419823	38.796836
C	37.215076	41.971289	34.157708
C	38.330335	40.599943	35.956525
C	37.546737	46.461332	32.044459
H	38.488899	45.653906	37.129431
H	38.791384	43.218645	36.991008

H	35.443698	45.526179	37.154065
H	35.566704	44.232747	35.255080
H	36.966762	41.941623	37.950931
H	35.819765	42.517665	36.764203
H	37.663201	47.775633	36.514350
H	36.218230	47.108755	35.744007
H	35.847885	43.802400	39.118021
H	38.549184	44.269110	39.348707
H	39.128696	42.260694	34.862684
H	37.593601	48.087495	34.071955
H	39.046799	47.218114	34.565327
H	38.494102	39.858026	35.169466
H	37.431065	40.290904	36.509164
H	39.185170	40.586931	36.650596
H	35.708557	46.223859	39.550766
H	37.467216	46.385206	39.298770
H	36.337989	47.442587	38.422893
H	36.699226	47.150088	31.919207
H	38.485119	46.953074	31.745284
H	37.381361	45.586318	31.400730
H	44.211813	46.727972	39.175251