

The Cartesian coordinates of transition states:

Path 1

IM1:

	x	y	z
C	1.31377	1.9555	0.01964
H	1.92901	1.12523	-0.33654
H	0.55576	2.1295	-0.74763
C	2.20415	3.20096	0.22068
H	2.00329	3.92543	-0.57592
H	1.95405	3.71005	1.15943
C	3.68319	2.80664	0.19252
H	3.86383	2.03442	0.95282
H	3.88095	2.31724	-0.77025
C	4.70757	3.92414	0.38773
H	4.56029	4.4094	1.36221
H	4.56637	4.70145	-0.37556
C	6.11956	3.34031	0.28945
H	6.20407	2.82971	-0.6733
H	6.2258	2.55784	1.05364
C	7.27324	4.33072	0.44653
H	7.1884	5.12632	-0.30703
H	7.1756	4.82558	1.42178
C	8.66968	3.68188	0.3506
H	9.37622	4.30426	0.91351
H	8.658	2.71116	0.86381
C	9.24872	3.52862	-1.06789
H	9.21292	4.51467	-1.55136
H	10.31506	3.282	-0.97154
C	8.62489	2.50075	-2.0305
H	7.56521	2.72404	-2.1927
H	9.10154	2.65957	-3.00544
C	8.8153	1.01601	-1.6401
H	9.00084	0.43319	-2.55169
H	9.72968	0.92553	-1.03936
C	7.65613	0.33759	-0.88857
H	7.41198	0.89649	0.02089
H	7.99885	-0.64984	-0.55534
C	6.38892	0.17258	-1.73904
H	6.08517	1.14617	-2.14033
H	6.61762	-0.45399	-2.61226
C	5.18732	-0.4201	-0.98532
H	4.29532	-0.34504	-1.61861
H	4.98033	0.17372	-0.08907
C	5.3926	-1.87691	-0.57623

H	6.19762	-1.97518	0.157
P	-3.17905	0.10398	-0.45111
O	-1.67129	0.01774	-0.66285
O	-3.74827	-0.41704	0.8546
O	-3.96267	-0.52654	-1.71465
C	-3.80531	-1.91982	-2.06958
H	-4.31425	-2.02719	-3.02905
H	-2.74186	-2.13771	-2.21508
C	-4.42269	-2.89527	-1.06753
H	-4.32786	-3.89085	-1.5108
C	-5.88028	-2.59522	-0.74678
H	-6.27186	-3.34241	-0.05293
H	-5.98178	-1.60555	-0.2955
H	-6.47954	-2.62006	-1.66112
O	-3.65746	-2.96256	0.16765
H	-3.77522	-2.08968	0.6312
H	5.65446	-2.50438	-1.43373
S	3.94571	-2.63825	0.26415
C	2.78983	-2.90665	-1.15784
C	2.52664	-4.38785	-1.45524
H	3.17443	-2.33603	-2.0038
H	3.27353	-5.06737	-1.04425
H	2.4541	-4.57283	-2.53245
C	1.40531	-2.3924	-0.75739
C	1.15243	-4.6338	-0.8383
O	1.13553	-1.1772	-0.6349
O	0.61141	-5.7172	-0.68305
N	0.56545	-3.41482	-0.50435
Ag	-1.48413	-3.2969	0.01978
N	0.57313	1.46255	1.21399
C	-0.61565	2.2898	1.52249
C	1.42553	1.22586	2.4103
Zn	-0.29178	-0.42068	0.74384
C	-1.56608	1.60187	2.53726
H	-1.14002	2.43843	0.57638
H	-0.33446	3.27795	1.90712
C	1.98502	-0.2019	2.47604
H	0.83365	1.43706	3.29836
H	2.263	1.92676	2.44127
N	-1.50062	0.11845	2.50248
N	0.95503	-1.24329	2.25186
H	-2.58538	1.91654	2.30162
H	-1.35705	1.95002	3.55161
H	2.48211	-0.33757	3.44429
H	2.73331	-0.34707	1.69356
C	-0.94547	-0.52591	3.71416
H	-2.42778	-0.24311	2.28223
C	0.08214	-1.61908	3.38085

H	1.42256	-2.08161	1.91992
H	-1.74389	-0.97477	4.31256
H	-0.48178	0.23776	4.34029
H	-0.43899	-2.52779	3.06495
H	0.66262	-1.85269	4.2817
O	-3.52819	1.68476	-0.67253
C	-4.79669	2.22775	-0.67795
C	-4.98059	3.3346	-1.5125
C	-5.83445	1.74034	0.12506
C	-6.21819	3.96066	-1.55806
H	-4.15236	3.68504	-2.11687
C	-7.07583	2.36242	0.07394
H	-5.66213	0.89432	0.77744
C	-7.25367	3.46233	-0.76538
H	-6.39117	4.81611	-2.19723
H	-7.90017	2.00938	0.67925
N	-8.55776	4.11178	-0.81507
O	-8.69307	5.08987	-1.55528
O	-9.46438	3.65266	-0.11497

IM2:

	x	y	z
C	1.14797	1.82514	0.12371
H	1.78601	1.0076	-0.21767
H	0.4159	1.9966	-0.66956
C	2.00857	3.08504	0.37134
H	1.76924	3.84899	-0.37634
H	1.77138	3.53327	1.34383
C	3.49707	2.735	0.29148
H	3.71071	1.92815	1.00647
H	3.69022	2.30421	-0.69979
C	4.48983	3.87213	0.53242
H	4.34228	4.29541	1.53554
H	4.30861	4.68731	-0.18138
C	5.92313	3.35287	0.38345
H	6.02727	2.92469	-0.61764
H	6.06417	2.5177	1.08351
C	7.02931	4.38072	0.62665
H	6.91944	5.2204	-0.07398
H	6.88851	4.80427	1.62986
C	8.46005	3.81216	0.52326
H	9.11733	4.42847	1.14908
H	8.48861	2.8081	0.96646
C	9.08297	3.79302	-0.88465
H	9.00147	4.80732	-1.29919
H	10.15922	3.6011	-0.77478

C	8.54371	2.80235	-1.93292
H	7.47498	2.97192	-2.10221
H	9.02769	3.05941	-2.88303
C	8.81698	1.30816	-1.64326
H	9.03264	0.79777	-2.59102
H	9.73546	1.22817	-1.0473
C	7.69323	0.526	-0.9412
H	7.40669	1.02772	-0.01104
H	8.08628	-0.45549	-0.64851
C	6.44817	0.33303	-1.81815
H	6.13352	1.3004	-2.22634
H	6.70729	-0.28921	-2.68582
C	5.24418	-0.27666	-1.08455
H	4.36289	-0.22161	-1.73482
H	5.0113	0.32264	-0.19908
C	5.4593	-1.7246	-0.65042
H	6.27111	-1.80505	0.07757
P	-3.36676	-0.05499	-0.45558
O	-1.86018	-0.28298	-0.64417
O	-3.99157	-0.07338	0.90512
O	-4.18216	-0.88906	-1.56281
C	-3.87976	-2.26172	-1.92033
H	-4.45997	-2.43492	-2.83092
H	-2.81238	-2.33502	-2.15684
C	-4.25119	-3.29341	-0.84583
H	-4.20696	-4.25952	-1.39363
C	-5.69636	-3.09125	-0.37345
H	-5.97016	-3.88806	0.32423
H	-5.78214	-2.13218	0.14409
H	-6.40413	-3.10561	-1.21048
O	-3.39547	-3.29088	0.25897
H	5.71427	-2.37021	-1.49652
S	4.01411	-2.45484	0.22017
C	2.86126	-2.7698	-1.19193
C	2.71302	-4.25428	-1.5444
H	3.18294	-2.13891	-2.02147
H	3.5112	-4.88875	-1.15823
H	2.65306	-4.40505	-2.62781
C	1.44212	-2.38116	-0.76334
C	1.3624	-4.62992	-0.93794
O	1.07804	-1.19982	-0.59186
O	0.91483	-5.76194	-0.82829
N	0.68175	-3.47816	-0.55816
Ag	-1.37191	-3.45825	-0.08131
N	0.37534	1.30837	1.28491
C	-0.80417	2.15078	1.58856
C	1.20657	1.02764	2.48678
Zn	-0.53607	-0.56219	0.78411

C	-1.75215	1.48487	2.61301
H	-1.33043	2.29275	0.6409
H	-0.51339	3.14218	1.95875
C	1.72518	-0.417	2.53601
H	0.61389	1.24193	3.3736
H	2.06639	1.70061	2.53529
N	-1.7443	0.00322	2.54201
N	0.66932	-1.42588	2.28527
H	-2.76331	1.84277	2.40958
H	-1.49869	1.80185	3.62771
H	2.20539	-0.58165	3.50835
H	2.47898	-0.56785	1.76051
C	-1.23623	-0.69339	3.74209
H	-2.68301	-0.30118	2.27847
C	-0.22341	-1.8007	3.40026
H	1.10574	-2.27266	1.93308
H	-2.0578	-1.14448	4.30711
H	-0.76922	0.03727	4.40514
H	-0.75673	-2.69479	3.06416
H	0.34504	-2.05993	4.30175
O	-3.53785	1.47377	-1.10844
C	-4.66766	2.22897	-1.0114
C	-4.49094	3.6191	-1.07498
C	-5.95281	1.67756	-0.88862
C	-5.58965	4.46194	-1.01317
H	-3.48666	4.01566	-1.1698
C	-7.05344	2.52011	-0.82221
H	-6.08366	0.60391	-0.85801
C	-6.86341	3.90222	-0.88368
H	-5.47583	5.53691	-1.05791
H	-8.0547	2.12072	-0.72886
N	-8.01892	4.78028	-0.81387
O	-7.83186	5.99988	-0.88025
O	-9.137	4.26885	-0.69111

IM3:

	x	y	z
C	1.75288	2.26218	-0.11204
H	2.13741	1.34152	-0.56029
H	1.20401	2.7801	-0.90051
C	2.93577	3.1071	0.40535
H	3.12944	3.92903	-0.29262
H	2.68213	3.57961	1.36235
C	4.19451	2.2457	0.54079
H	3.96349	1.36161	1.14917
H	4.44401	1.85283	-0.45396

C	5.43612	2.91501	1.13002
H	5.21397	3.31195	2.13009
H	5.73454	3.77156	0.51042
C	6.57219	1.8921	1.20149
H	6.71144	1.47914	0.19983
H	6.2426	1.05142	1.82772
C	7.91286	2.39611	1.73397
H	8.25853	3.24849	1.1323
H	7.76239	2.78327	2.75038
C	9.01048	1.31305	1.76433
H	9.74294	1.58707	2.5337
H	8.57528	0.36112	2.09657
C	9.79718	1.11218	0.45583
H	10.18766	2.09194	0.14765
H	10.67913	0.49824	0.68482
C	9.09745	0.47279	-0.75878
H	8.23151	1.07052	-1.0615
H	9.80187	0.54941	-1.596
C	8.70513	-1.01517	-0.6001
H	8.88362	-1.52843	-1.55394
H	9.38944	-1.48254	0.12004
C	7.25662	-1.32263	-0.17937
H	7.01659	-0.82196	0.76456
H	7.18719	-2.39882	0.02199
C	6.21177	-0.93886	-1.2367
H	6.2855	0.13189	-1.45717
H	6.44301	-1.45589	-2.1784
C	4.75761	-1.24246	-0.83635
H	4.07962	-0.77031	-1.5568
H	4.53592	-0.79222	0.13765
C	4.46215	-2.74022	-0.77451
H	5.02845	-3.22443	0.02565
P	-4.73239	-1.19105	0.94469
O	-4.39156	-1.38983	-0.54088
O	-4.57543	0.19088	1.51036
O	-6.23789	-1.77155	1.23784
C	-6.14786	-3.13176	1.70952
H	-7.03349	-3.3406	2.31145
H	-6.11597	-3.81543	0.85444
C	-4.84619	-3.20092	2.52645
H	-4.42605	-4.20899	2.49944
C	-4.99241	-2.71174	3.95847
H	-4.01119	-2.64623	4.4353
H	-5.45979	-1.72297	3.98201
H	-5.61383	-3.40593	4.53229
O	-3.92536	-2.34438	1.80053
H	4.73211	-3.23839	-1.71084
S	2.71776	-3.17307	-0.38926

C	1.86417	-2.77357	-1.98657
C	1.17466	-3.9855	-2.62165
H	2.58909	-2.27278	-2.62893
H	1.55478	-4.94949	-2.28256
H	1.24558	-3.95661	-3.71434
C	0.68939	-1.84559	-1.66828
C	-0.29019	-3.79932	-2.23105
O	0.83615	-0.65477	-1.33204
O	-1.17862	-4.62987	-2.35557
N	-0.48365	-2.5155	-1.73307
Ag	-2.40992	-1.8949	-1.11676
N	0.73118	1.86317	0.89442
C	-0.2115	2.95517	1.21449
C	1.28829	1.22258	2.11009
Zn	-0.55806	0.40223	-0.03112
C	-1.50905	2.4493	1.90661
H	-0.47204	3.42679	0.26576
H	0.25505	3.72204	1.8463
C	1.44762	-0.29179	1.94515
H	0.62413	1.43872	2.94429
H	2.25383	1.65475	2.38392
N	-1.83322	1.0255	1.63362
N	0.21374	-0.93562	1.44781
H	-2.33415	3.06444	1.5406
H	-1.44845	2.60922	2.9868
H	1.76239	-0.72249	2.90398
H	2.22457	-0.5117	1.20889
C	-1.62736	0.10965	2.7883
H	-2.82429	0.94575	1.3872
C	-0.86958	-1.17491	2.41869
H	0.47425	-1.82175	1.02462
H	-2.60134	-0.18106	3.18891
H	-1.10003	0.64314	3.58034
H	-1.56323	-1.87279	1.94571
H	-0.49132	-1.64087	3.33788
O	-1.20872	1.41579	-1.58454
C	-2.18688	2.28561	-1.56032
C	-1.97661	3.61077	-2.04004
C	-3.48106	1.95641	-1.06816
C	-2.98484	4.55379	-2.00019
H	-0.99655	3.86673	-2.42948
C	-4.48797	2.89998	-1.02127
H	-3.67018	0.94775	-0.72509
C	-4.24217	4.20206	-1.48421
H	-2.82195	5.56412	-2.35383
H	-5.4659	2.64824	-0.63047
N	-5.28585	5.18419	-1.43097
O	-5.05054	6.33002	-1.85005

O	-6.39084	4.85669	-0.96706
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TS:

	x	y	z
C	1.17863	1.79339	-0.4004
H	1.81199	0.9178	-0.55545
H	0.47847	1.82226	-1.23922
C	2.05352	3.06598	-0.36006
H	1.89846	3.64746	-1.27539
H	1.74763	3.72072	0.46504
C	3.53444	2.69795	-0.23183
H	3.66692	2.04826	0.64409
H	3.80698	2.07775	-1.096
C	4.52507	3.85751	-0.12568
H	4.28266	4.48079	0.74612
H	4.44151	4.50664	-1.00798
C	5.95095	3.31249	-0.00522
H	6.14663	2.67922	-0.87485
H	5.99364	2.64602	0.86731
C	7.05631	4.36024	0.13194
H	7.04813	5.02898	-0.74029
H	6.8249	4.99225	0.99955
C	8.47008	3.76891	0.31039
H	9.082	4.50513	0.84621
H	8.41964	2.89241	0.96972
C	9.23014	3.42185	-0.98291
H	9.22839	4.31642	-1.62097
H	10.282	3.24613	-0.71841
C	8.76437	2.22633	-1.83452
H	7.72747	2.36919	-2.15639
H	9.35582	2.25332	-2.75784
C	8.94614	0.83234	-1.19001
H	9.23803	0.11834	-1.97119
H	9.79468	0.87493	-0.49474
C	7.72761	0.24312	-0.45789
H	7.3745	0.93758	0.31151
H	8.04981	-0.66107	0.07347
C	6.5646	-0.10772	-1.39581
H	6.30708	0.76659	-2.00419
H	6.8901	-0.88127	-2.10509
C	5.2871	-0.57205	-0.67933
H	4.46654	-0.61099	-1.40556
H	4.99473	0.16585	0.07453
C	5.42797	-1.93548	-0.00572
H	6.15034	-1.90225	0.8144
P	-3.4696	-0.53801	-0.43686

O	-1.94178	-0.70353	-0.67436
O	-4.10211	-0.36958	0.92283
O	-4.37201	-0.96787	-1.72616
C	-4.41773	-2.33038	-2.18396
H	-5.28924	-2.40349	-2.83881
H	-3.50924	-2.53558	-2.76254
C	-4.48593	-3.24724	-0.96469
H	-4.2425	-4.26961	-1.29031
C	-5.86867	-3.24784	-0.3092
H	-5.85349	-3.87395	0.5879
H	-6.14769	-2.23328	-0.01186
H	-6.63111	-3.63928	-0.99192
O	-3.51945	-2.73767	-0.07781
H	5.76867	-2.7005	-0.71025
S	3.88272	-2.53488	0.79126
C	2.87741	-3.00209	-0.68676
C	2.71055	-4.51334	-0.88786
H	3.31469	-2.48921	-1.54488
H	3.37302	-5.11826	-0.26729
H	2.86742	-4.80514	-1.93138
C	1.43498	-2.5191	-0.49514
C	1.24757	-4.76786	-0.52971
O	1.12354	-1.31092	-0.45033
O	0.71609	-5.86454	-0.43401
N	0.58618	-3.55869	-0.35577
Ag	-1.50099	-3.32079	-0.18305
N	0.35207	1.51836	0.80812
C	-0.82827	2.413	0.88562
C	1.1309	1.48715	2.07674
Zn	-0.5526	-0.41563	0.67764
C	-1.81853	1.98913	1.99578
H	-1.32657	2.34297	-0.08374
H	-0.53495	3.4589	1.04201
C	1.62756	0.08179	2.44533
H	0.50677	1.88442	2.87353
H	1.99674	2.15082	2.02216
N	-1.81933	0.53136	2.24704
N	0.56949	-0.95482	2.36516
H	-2.81748	2.30026	1.67998
H	-1.60131	2.52282	2.92509
H	2.06513	0.11926	3.4504
H	2.409	-0.23105	1.75003
C	-1.35039	0.10234	3.57905
H	-2.7512	0.15796	2.03298
C	-0.36702	-1.0783	3.50221
H	1.01915	-1.85435	2.22234
H	-2.19131	-0.19596	4.21379
H	-0.87131	0.94611	4.07931

H	-0.91904	-2.00801	3.33623
H	0.16896	-1.16536	4.45524
O	-3.46864	1.13637	-0.99109
C	-4.49005	1.98939	-0.86281
C	-4.18647	3.3626	-0.99412
C	-5.82704	1.59936	-0.6278
C	-5.17882	4.3206	-0.8904
H	-3.15756	3.64962	-1.18011
C	-6.82121	2.5574	-0.52359
H	-6.07031	0.55088	-0.53286
C	-6.49637	3.91239	-0.65243
H	-4.95329	5.37462	-0.98714
H	-7.85025	2.27235	-0.34618
N	-7.53803	4.90608	-0.54106
O	-7.23102	6.10013	-0.66181
O	-8.69775	4.52616	-0.32887

Path 2

IM1:

	x	y	z
C	-1.65997	-1.52655	-0.09785
H	-1.83136	-0.48209	-0.37265
H	-0.90766	-1.91298	-0.78907
C	-2.93787	-2.34871	-0.30123
H	-3.16614	-2.25816	-1.3714
H	-2.72216	-3.41112	-0.13753
C	-4.19108	-1.96075	0.49256
H	-4.05901	-2.18835	1.55775
H	-4.36131	-0.87775	0.41967
C	-5.42836	-2.69541	-0.03258
H	-5.23284	-3.77644	-0.04459
H	-5.58633	-2.40403	-1.08013
C	-6.71084	-2.4224	0.75853
H	-6.84105	-1.33752	0.87843
H	-6.61803	-2.83202	1.77351
C	-7.94734	-2.99913	0.06269
H	-7.98086	-2.59185	-0.95339
H	-7.83271	-4.08598	-0.05401
C	-9.26744	-2.70088	0.77858
H	-9.27294	-3.21239	1.7504
H	-9.32189	-1.63115	1.00985
C	-8.64415	-0.28701	-2.50517
H	-8.53188	-1.34075	-2.78628
H	-8.96665	0.23458	-3.41666

C	-7.2731	0.23522	-2.05061
H	-6.97642	-0.32397	-1.1537
H	-6.52111	0.00318	-2.81421
C	-7.23799	1.73566	-1.72667
H	-7.23228	2.31282	-2.6616
H	-8.15749	2.01714	-1.20121
C	-6.05044	2.15234	-0.84858
H	-6.1231	1.62722	0.11501
H	-6.14429	3.22104	-0.62147
C	-4.67082	1.87115	-1.45464
H	-4.58014	0.80068	-1.6742
H	-4.57847	2.3908	-2.41884
C	-3.50074	2.26922	-0.54092
H	-2.55771	1.92154	-0.96891
H	-3.61636	1.77317	0.43136
C	-3.40752	3.77864	-0.31458
H	-4.31803	4.16429	0.15125
P	3.96908	-1.04585	-0.04313
O	2.87751	-1.65283	0.82446
O	4.49232	0.35091	0.24605
O	3.5875	-1.14812	-1.60504
C	2.32495	-1.6995	-2.04027
H	2.50673	-2.13956	-3.02196
H	2.00414	-2.48377	-1.35161
C	1.26723	-0.6138	-2.1565
H	0.35386	-1.10053	-2.52416
C	1.66819	0.51445	-3.09815
H	0.88537	1.27537	-3.13655
H	2.5968	0.98122	-2.75945
H	1.81868	0.12198	-4.10784
O	1.01079	-0.08693	-0.83836
H	0.53239	0.80017	-0.8922
H	-3.27737	4.31535	-1.2602
S	-2.08061	4.33538	0.82984
C	-0.60607	4.49379	-0.26378
C	0.40777	5.48582	0.32388
H	-0.96174	4.77531	-1.25762
H	0.06424	5.97912	1.2363
H	0.67912	6.2695	-0.38859
C	0.1984	3.19522	-0.36183
C	1.63522	4.63239	0.62482
O	-0.2533	2.14968	-0.86754
O	2.66375	5.02173	1.15814
N	1.42834	3.33039	0.18801
Ag	3.01579	1.92533	0.20376
N	-1.03308	-1.5167	1.25557
C	-0.87825	-2.87712	1.82002
C	-1.68879	-0.56582	2.1958

Zn	1.04121	-0.87264	1.12024
C	0.00367	-2.89503	3.09049
H	-0.41319	-3.48307	1.03677
H	-1.84567	-3.33289	2.06036
C	-1.04975	0.82853	2.16444
H	-1.64836	-0.9828	3.19982
H	-2.74739	-0.45242	1.95965
N	1.0455	-1.83699	3.08718
N	0.43114	0.80072	2.22312
H	0.4788	-3.8758	3.15615
H	-0.6166	-2.78925	3.98371
H	-1.46358	1.4268	2.98391
H	-1.30806	1.32956	1.23144
C	0.8837	-0.78026	4.12078
H	1.9647	-2.25732	3.16943
C	1.05967	0.63762	3.55525
H	0.78232	1.66807	1.8215
H	1.60477	-0.92086	4.93052
H	-0.10653	-0.8789	4.56673
H	2.12237	0.85487	3.41523
H	0.65628	1.3606	4.27367
O	5.21257	-2.09815	0.13273
C	6.47577	-1.93688	-0.38336
C	7.48197	-2.68789	0.23527
C	6.75971	-1.10847	-1.47655
C	8.78483	-2.61137	-0.23404
H	7.22632	-3.3199	1.07748
C	8.06529	-1.02825	-1.94426
H	5.97488	-0.54299	-1.96136
C	9.06197	-1.77814	-1.31963
H	9.58131	-3.17976	0.2273
H	8.31556	-0.3975	-2.78687
N	10.42896	-1.69146	-1.81478
O	11.29537	-2.36884	-1.25434
O	10.6567	-0.94502	-2.77112
C	-9.72658	-0.15099	-1.42037
H	-10.09381	0.88181	-1.40328
H	-9.26634	-0.31524	-0.44144
C	-10.93814	-1.08403	-1.59144
H	-11.71509	-0.78823	-0.87334
H	-11.36685	-0.90542	-2.58713
C	-10.68602	-2.59605	-1.44031
H	-11.54707	-3.11819	-1.87622
H	-9.82854	-2.89643	-2.05366
C	-10.51877	-3.13499	-0.00563
H	-11.40939	-2.86117	0.57595
H	-10.52152	-4.23215	-0.06297

IM2:

	x	y	z
C	-4.61249	-1.50089	-0.03694
H	-4.36913	-0.45577	-0.24729
H	-4.42811	-2.05368	-0.96069
C	-6.08505	-1.62305	0.39748
H	-6.47603	-2.60077	0.09601
H	-6.16015	-1.58932	1.49133
C	-6.9665	-0.50302	-0.17974
H	-6.86697	-0.47801	-1.27375
H	-8.01841	-0.73638	0.02704
C	-6.63712	0.87988	0.39607
H	-5.61501	1.16311	0.11834
H	-6.64735	0.82388	1.49387
C	-7.59808	1.98939	-0.04661
H	-8.59899	1.76652	0.34424
H	-7.68841	1.98566	-1.142
C	-7.14991	3.38243	0.42561
H	-8.00064	4.07555	0.41182
H	-6.83532	3.31031	1.47486
C	-6.01966	3.97921	-0.42556
H	-5.24378	3.22343	-0.59704
H	-6.42223	4.21879	-1.41822
C	-1.46917	2.99061	0.28027
H	-1.12467	2.65777	1.26916
H	-2.06947	2.17007	-0.13523
C	-0.26577	3.21995	-0.6422
H	0.15446	2.24909	-0.92707
H	-0.61902	3.6717	-1.57857
C	0.85435	4.09445	-0.06048
H	1.61629	4.23314	-0.83448
H	0.46849	5.09736	0.16007
C	1.53956	3.53598	1.20063
H	0.91402	3.71375	2.08462
H	2.46059	4.10861	1.36791
C	1.87224	2.0371	1.13912
H	0.96107	1.46267	1.33222
H	2.1891	1.7573	0.12676
C	2.96031	1.59791	2.13724
H	2.80636	0.55025	2.39957
H	2.88361	2.17094	3.06864
C	4.3497	1.77076	1.52134
H	4.57046	2.82625	1.3348
P	0.18927	-1.25732	-2.60819
O	0.30559	-1.31654	-1.05626
O	-0.78048	-0.28881	-3.19564
O	0.12922	-2.73986	-3.22418
C	-0.13736	-3.8896	-2.38489

H	0.24663	-4.75087	-2.93712
H	0.42561	-3.79055	-1.45218
C	-1.64081	-4.02532	-2.10566
H	-1.72253	-4.85873	-1.37733
C	-2.39994	-4.43102	-3.37308
H	-3.46736	-4.51954	-3.15128
H	-2.27146	-3.66691	-4.14615
H	-2.04611	-5.39049	-3.76683
O	-2.18531	-2.84201	-1.60617
H	4.39289	1.26751	0.55482
S	5.78974	1.18928	2.50167
C	5.69789	-0.65797	2.37822
C	4.82237	-1.34837	3.4288
H	6.74207	-0.97323	2.41158
H	4.50736	-0.69701	4.24572
H	5.32519	-2.217	3.86717
C	5.06135	-1.09544	1.04387
C	3.61201	-1.8232	2.63157
O	5.56608	-0.9193	-0.06142
O	2.57949	-2.27577	3.12312
N	3.83605	-1.66861	1.28324
Ag	2.17675	-1.61423	-0.02141
N	-3.60738	-1.96962	0.94438
C	-3.68261	-3.41363	1.21652
C	-3.5336	-1.11197	2.13883
Zn	-1.58774	-1.9553	-0.0383
C	-2.44887	-3.93712	1.98875
H	-3.72934	-3.89502	0.23669
H	-4.5847	-3.693	1.77797
C	-2.56779	0.0553	1.90673
H	-3.21502	-1.70732	2.9924
H	-4.51195	-0.69968	2.40871
N	-1.18013	-3.21836	1.66223
N	-1.27555	-0.39058	1.34508
H	-2.32888	-4.99487	1.74505
H	-2.61919	-3.88247	3.06708
H	-2.42237	0.6049	2.84411
H	-3.00533	0.74627	1.18525
C	-0.63841	-2.36858	2.7639
H	-0.47537	-3.9031	1.41044
C	-0.30458	-0.93778	2.31567
H	-0.84101	0.38404	0.85223
H	0.28339	-2.80261	3.15276
H	-1.36221	-2.3501	3.57926
H	0.67141	-0.94075	1.82453
H	-0.22185	-0.29565	3.20105
O	1.74454	-0.93612	-3.13643
C	2.36564	0.25903	-2.88122

C	3.64927	0.19952	-2.32482
C	1.76726	1.49011	-3.18381
C	4.32816	1.37314	-2.02883
H	4.09975	-0.75721	-2.09399
C	2.44787	2.66523	-2.89446
H	0.77621	1.50743	-3.61762
C	3.71078	2.59487	-2.30119
H	5.306	1.34083	-1.56919
H	2.0083	3.62937	-3.11082
N	4.38194	3.82526	-1.91531
O	5.47943	3.74178	-1.35491
O	3.81617	4.89886	-2.14932
C	-5.37528	5.24066	0.16902
H	-4.69407	5.67034	-0.57514
H	-6.15251	5.99811	0.33696
C	-4.6128	5.02025	1.48928
H	-5.3249	4.77199	2.28547
H	-4.14799	5.96957	1.78678
C	-3.53704	3.92547	1.43717
H	-4.0093	2.96833	1.18066
H	-3.11702	3.78746	2.44199
C	-2.39171	4.20072	0.45533
H	-1.81897	5.07025	0.80323
H	-2.79337	4.47179	-0.52893

IM3:

	x	y	z
C	-1.25336	-2.40566	1.96834
H	-1.71476	-1.41832	2.00331
H	-1.32738	-2.74406	0.93
C	-1.99521	-3.38593	2.8781
H	-1.51094	-4.36792	2.85212
H	-1.95641	-3.04211	3.91867
C	-3.46696	-3.5464	2.47042
H	-3.52499	-4.00809	1.47557
H	-3.9346	-4.25627	3.16427
C	-4.2759	-2.24125	2.46947
H	-4.01326	-1.63978	1.591
H	-4.00003	-1.63728	3.3459
C	-5.78753	-2.49686	2.50639
H	-6.02827	-2.98488	3.45971
H	-6.05629	-3.21774	1.72092
C	-6.64268	-1.23224	2.34156
H	-7.65186	-1.41798	2.73196
H	-6.22029	-0.42902	2.96009
C	-6.76675	-0.77082	0.88459

H	-5.76964	-0.6484	0.44876
H	-7.24692	-1.57451	0.31079
C	-4.64557	2.75146	-2.0316
H	-3.76728	2.19251	-1.69044
H	-4.83276	2.40997	-3.05789
C	-4.31009	4.24971	-2.1111
H	-3.53937	4.38483	-2.88014
H	-5.19471	4.78809	-2.47749
C	-3.83537	4.92249	-0.81301
H	-3.59239	5.96921	-1.04209
H	-4.66202	4.95935	-0.0932
C	-2.6171	4.26858	-0.14429
H	-2.87592	3.268	0.21992
H	-2.36053	4.8577	0.74543
C	-1.39333	4.14186	-1.05824
H	-1.6449	3.49708	-1.90589
H	-1.13644	5.12595	-1.47714
C	-0.16476	3.53497	-0.36498
H	0.59133	3.27047	-1.10713
H	-0.45869	2.6053	0.1347
C	0.46561	4.47803	0.65671
H	-0.23014	4.71919	1.46572
P	-1.31963	-0.11659	-0.70875
O	0.19729	-0.43314	-0.75807
O	-1.84191	0.46766	0.56665
O	-1.68891	0.78967	-2.0163
C	-2.18587	-0.04572	-3.08409
H	-2.88196	0.55101	-3.67516
H	-1.35127	-0.375	-3.70771
C	-2.86919	-1.24839	-2.40692
H	-2.75822	-2.14003	-3.0259
C	-4.32411	-1.01398	-2.04119
H	-4.70944	-1.85763	-1.46365
H	-4.43058	-0.10627	-1.44371
H	-4.92926	-0.90576	-2.94656
O	-2.08913	-1.47849	-1.20172
H	0.76551	5.42525	0.19554
S	1.92934	3.81345	1.54696
C	3.29324	3.97822	0.30614
C	4.65191	4.03996	1.01694
H	3.06722	4.85385	-0.30521
H	4.59372	4.24412	2.08813
H	5.29911	4.80149	0.57034
C	3.42442	2.72016	-0.57091
C	5.26157	2.65958	0.76262
O	2.64958	2.39585	-1.46846
O	6.26617	2.21882	1.31363
N	4.52225	1.99383	-0.18557

Ag	4.66962	-0.02775	-0.72634
N	0.19632	-2.21441	2.25756
C	0.96988	-3.46417	2.07844
C	0.44478	-1.53482	3.55927
Zn	1.15425	-0.9366	0.81758
C	2.48968	-3.22125	2.11067
H	0.67838	-3.86208	1.10237
H	0.72219	-4.21671	2.83558
C	0.50038	-0.00711	3.41494
H	1.38028	-1.90475	3.97543
H	-0.33095	-1.78628	4.28666
N	2.8892	-1.89499	1.55466
N	1.42322	0.42993	2.34246
H	2.9746	-4.01489	1.5409
H	2.86517	-3.3048	3.13224
H	0.77974	0.43035	4.3806
H	-0.48714	0.37052	3.13824
C	3.50537	-0.98445	2.56863
H	3.54351	-2.04254	0.7787
C	2.8759	0.41952	2.61569
H	1.18415	1.37921	2.0517
H	4.57232	-0.86992	2.35904
H	3.42802	-1.45669	3.54831
H	3.32002	1.03858	1.83628
H	3.10387	0.87781	3.58525
O	4.32286	-2.11979	-0.98844
C	3.26018	-2.44488	-1.6875
C	2.76019	-1.63563	-2.74702
C	2.53935	-3.63428	-1.3738
C	1.57496	-1.93862	-3.38213
H	3.31417	-0.74251	-3.02165
C	1.34142	-3.93004	-1.99282
H	2.94346	-4.29797	-0.618
C	0.84757	-3.0717	-2.98698
H	1.18303	-1.3021	-4.16494
H	0.77462	-4.81204	-1.72231
N	-0.42266	-3.33859	-3.58196
O	-0.80911	-2.61594	-4.52021
O	-1.11258	-4.27105	-3.13695
C	-7.57299	0.52403	0.70685
H	-7.8741	0.61957	-0.34265
H	-8.50716	0.44035	1.27847
C	-6.83935	1.80414	1.14079
H	-6.56073	1.72452	2.19911
H	-7.54071	2.64698	1.0762
C	-5.5845	2.14944	0.32137
H	-4.83247	1.35656	0.42757
H	-5.12984	3.04486	0.75603

C	-5.86737	2.37789	-1.17029
H	-6.64102	3.15201	-1.27821
H	-6.30626	1.46169	-1.58144

TS:

	x	y	z
C	-3.90521	-1.36828	-1.30242
H	-3.71154	-1.038	-0.27809
H	-3.70342	-0.50901	-1.94702
C	-5.36942	-1.80015	-1.45496
H	-5.4958	-2.36111	-2.38717
H	-5.64812	-2.47813	-0.63993
C	-6.33925	-0.61117	-1.46449
H	-6.16274	-0.0053	-2.36365
H	-7.36043	-1.00275	-1.55476
C	-6.25775	0.29364	-0.22955
H	-5.32089	0.86458	-0.25072
H	-6.21951	-0.32245	0.68
C	-7.45112	1.25214	-0.12893
H	-8.35462	0.65928	0.06245
H	-7.60949	1.74236	-1.10011
C	-7.28868	2.32563	0.95655
H	-8.27168	2.73012	1.23077
H	-6.8891	1.85585	1.86469
C	-6.38862	3.4884	0.52106
H	-5.43817	3.09819	0.13639
H	-6.86666	3.99699	-0.32645
C	-1.62979	3.70378	1.31559
H	-1.7264	2.64429	1.04836
H	-1.2662	4.19675	0.40572
C	-0.54135	3.88122	2.38676
H	0.41599	3.58624	1.94256
H	-0.45235	4.95183	2.61641
C	-0.73256	3.11768	3.7085
H	0.13533	3.32579	4.34933
H	-1.60178	3.51533	4.24579
C	-0.87736	1.59522	3.5613
H	-1.8067	1.35864	3.02702
H	-0.98234	1.1546	4.56129
C	0.29574	0.95249	2.81662
H	0.38138	1.38692	1.81735
H	1.23529	1.17835	3.34042
C	0.1868	-0.56516	2.64155
H	0.96224	-0.88034	1.93672
H	-0.78101	-0.80909	2.18186
C	0.34687	-1.35832	3.94087

H	-0.55024	-1.30749	4.56218
P	1.08981	0.72994	-1.51391
O	1.13048	-0.83714	-1.39475
O	0.86753	1.66638	-0.36621
O	0.89915	1.2714	-3.0467
C	-0.27433	0.91563	-3.79575
H	-0.33512	1.61622	-4.63127
H	-0.14746	-0.10146	-4.1857
C	-1.4856	0.976	-2.86446
H	-2.30436	0.41283	-3.33567
C	-1.95582	2.40049	-2.57851
H	-2.78225	2.38179	-1.8619
H	-1.14176	2.98689	-2.14397
H	-2.29995	2.89361	-3.49381
O	-1.05638	0.36155	-1.67006
H	1.18703	-0.97369	4.52267
S	0.65912	-3.1552	3.66009
C	2.51353	-3.26062	3.71253
C	2.94773	-4.5312	2.9788
H	2.84104	-3.18438	4.74969
H	2.2053	-5.33163	2.94965
H	3.86383	-4.93877	3.41993
C	3.12454	-2.15489	2.84058
C	3.24942	-4.01753	1.56614
O	3.2992	-0.99575	3.20819
O	3.35538	-4.7278	0.56863
N	3.39176	-2.64924	1.58488
Ag	2.79025	-1.48187	-0.09565
N	-2.88821	-2.40031	-1.63448
C	-2.88583	-2.74995	-3.06975
C	-2.95044	-3.582	-0.74121
Zn	-0.84784	-1.55997	-1.38353
C	-1.62868	-3.54812	-3.49465
H	-2.91654	-1.80274	-3.61475
H	-3.77398	-3.32373	-3.36149
C	-2.07372	-3.40856	0.50559
H	-2.6337	-4.45997	-1.30093
H	-3.97585	-3.78567	-0.42073
N	-0.43537	-3.27064	-2.65098
N	-0.70386	-2.9587	0.17593
H	-1.40227	-3.28737	-4.53026
H	-1.83762	-4.6205	-3.48068
H	-2.05622	-4.35221	1.0636
H	-2.50634	-2.64446	1.15728
C	-0.02251	-4.40459	-1.77397
H	0.34445	-3.01444	-3.24683
C	0.23565	-3.98836	-0.31939
H	-0.28842	-2.56731	1.01879

H	0.88949	-4.86631	-2.16152
H	-0.79742	-5.17056	-1.814
H	1.2336	-3.55692	-0.23862
H	0.21553	-4.88048	0.31735
O	2.85176	0.7914	-1.67017
C	3.58834	1.90012	-1.4924
C	4.89857	1.72632	-1.00391
C	3.12445	3.19554	-1.79826
C	5.73214	2.81667	-0.82257
H	5.23477	0.72164	-0.77049
C	3.95557	4.28847	-1.61406
H	2.12271	3.32826	-2.18363
C	5.25282	4.0954	-1.12742
H	6.7392	2.6973	-0.44477
H	3.61732	5.29015	-1.84569
N	6.11595	5.24006	-0.93548
O	7.26397	5.04863	-0.51376
O	5.67225	6.36493	-1.20045
C	-6.11053	4.51542	1.62675
H	-5.58944	5.37489	1.18866
H	-7.06596	4.90359	2.00458
C	-5.29298	3.97794	2.81405
H	-5.88857	3.24181	3.36774
H	-5.11219	4.80546	3.51314
C	-3.94509	3.34193	2.44012
H	-4.11227	2.43596	1.84202
H	-3.45894	3.00451	3.36039
C	-3.01349	4.28169	1.66364
H	-2.88611	5.21619	2.22959
H	-3.51305	4.56526	0.7298

Path 3

IM1:

	x	y	z
C	-0.77925	-3.70681	0.43404
H	-0.50691	-3.09068	-0.4292
C	-3.58677	3.09151	0.4074
H	-4.2895	3.04483	1.25094
P	1.69787	0.38657	-0.09674
O	0.28541	-0.2046	0.04891
O	2.2918	1.15822	1.0424
O	1.75298	1.27993	-1.43174
C	1.01489	0.9131	-2.61792
H	1.72563	0.53567	-3.3571

H	0.28227	0.13894	-2.38444
C	0.31877	2.13864	-3.1732
H	-0.16308	1.83531	-4.10682
C	1.22406	3.33651	-3.39761
H	0.64969	4.18382	-3.77995
H	1.71923	3.62899	-2.4679
H	1.99192	3.082	-4.1335
O	-0.78463	2.47546	-2.25153
H	-3.91619	3.90246	-0.24787
N	-0.0111	-3.1814	1.60283
C	1.45395	-3.36051	1.45004
C	-0.53095	-3.67706	2.90651
Zn	-0.17352	-1.06991	1.72251
C	2.27849	-2.51725	2.45563
H	1.69347	-3.04794	0.43197
H	1.74564	-4.41014	1.55782
C	-1.61179	-2.75364	3.49039
H	0.303	-3.77172	3.59937
H	-0.95522	-4.67899	2.80225
N	1.58025	-1.28289	2.91552
N	-1.22375	-1.31601	3.46826
H	3.21095	-2.23442	1.96474
H	2.54945	-3.11845	3.32594
H	-1.84318	-3.07509	4.51128
H	-2.52484	-2.83391	2.89597
C	1.14402	-1.30669	4.34138
H	2.16954	-0.47068	2.74558
C	-0.30881	-0.8416	4.54059
H	-2.07099	-0.756	3.50687
H	1.79271	-0.66757	4.94506
H	1.26408	-2.32092	4.72173
H	-0.35682	0.24919	4.51785
H	-0.6583	-1.17494	5.52358
O	2.59459	-0.94445	-0.47561
C	3.93018	-0.93474	-0.81251
C	4.41087	-2.11287	-1.39505
C	4.77326	0.1596	-0.58456
C	5.74521	-2.20145	-1.76355
H	3.72939	-2.93977	-1.55621
C	6.10816	0.0727	-0.95988
H	4.39492	1.05449	-0.10839
C	6.57851	-1.10271	-1.54457
H	6.14309	-3.09877	-2.21823
H	6.785	0.90131	-0.79916
N	7.97986	-1.1869	-1.93564
O	8.38032	-2.23818	-2.4429
O	8.69893	-0.203	-1.7412
Zn	-0.62472	3.42361	-0.44864

N	-2.24303	3.48063	0.93132
N	-0.53476	5.48976	-0.30567
N	0.52239	3.40434	1.33436
C	-1.77762	2.54826	1.98904
C	-2.26253	4.8929	1.42241
C	-1.79795	5.89776	0.36006
C	0.74668	5.74548	0.39773
H	-0.49098	5.93854	-1.21622
C	-0.31755	2.81473	2.41512
C	0.96574	4.80688	1.59341
H	1.33725	2.79338	1.21718
H	-1.85174	1.54346	1.57702
H	-2.43282	2.60011	2.86714
H	-1.63276	4.96352	2.30661
H	-3.27308	5.16139	1.74457
H	-1.69551	6.88364	0.82638
H	-2.54959	5.97572	-0.42882
H	1.53129	5.58666	-0.34574
H	0.80727	6.78338	0.74295
H	0.12756	1.86391	2.70548
H	-0.28286	3.46293	3.29269
H	2.02853	4.81745	1.84679
H	0.43207	5.18613	2.46511
H	-1.8313	-3.51166	0.64806
C	-0.55769	-5.18434	0.1046
H	0.51336	-5.36122	-0.03799
H	-0.87007	-5.81255	0.94729
C	-1.28588	-5.65467	-1.16638
H	-0.98711	-5.02045	-2.01245
H	-0.90584	-6.65682	-1.39425
C	-2.82277	-5.72382	-1.09432
H	-3.12655	-6.09924	-0.10717
H	-3.1624	-6.47656	-1.81747
C	-3.5699	-4.4196	-1.40342
H	-3.36991	-3.66056	-0.63723
H	-3.18525	-4.00916	-2.34528
C	-5.08631	-4.62372	-1.50384
H	-5.43668	-5.12685	-0.59271
H	-5.30158	-5.31028	-2.33471
C	-5.88252	-3.32589	-1.69503
H	-6.95606	-3.5576	-1.68296
H	-5.70259	-2.67016	-0.83278
C	-5.54921	-2.5794	-2.99183
H	-4.49847	-2.26789	-2.97828
H	-5.64542	-3.2751	-3.83635
C	-6.43616	-1.3545	-3.25922
H	-6.12385	-0.89723	-4.2075
H	-7.47302	-1.6856	-3.40417

C	-6.41013	-0.28009	-2.16064
H	-7.02047	0.57122	-2.48962
H	-6.89149	-0.66255	-1.25139
C	-5.00529	0.21664	-1.80588
H	-4.43471	-0.59477	-1.33555
H	-4.46187	0.47777	-2.72479
C	-5.01417	1.42814	-0.86876
H	-5.66274	1.22508	-0.00643
H	-5.45259	2.28894	-1.39069
C	-3.60806	1.78001	-0.37213
H	-3.2426	0.95239	0.24521
H	-2.92931	1.84836	-1.22967
H	-1.47495	2.92701	-2.76118

IM2:

	x	y	z
C	0.87569	3.78073	0.40561
H	0.60274	3.17216	-0.46278
C	3.43393	-3.12648	0.58512
H	4.10912	-3.02918	1.44827
P	-1.60495	-0.31338	-0.15146
O	-0.19876	0.29506	0.01294
O	-2.28759	-0.9252	1.03464
O	-1.58695	-1.37054	-1.34774
C	-0.88314	-1.10101	-2.5943
H	-1.62808	-0.7759	-3.32649
H	-0.15151	-0.3077	-2.43037
C	-0.16863	-2.3788	-3.0309
H	0.30188	-2.11648	-3.99546
C	-1.15777	-3.52004	-3.29354
H	-0.6116	-4.41392	-3.60775
H	-1.72212	-3.76094	-2.38619
H	-1.8738	-3.25682	-4.07999
O	0.84653	-2.72125	-2.12915
H	3.79163	-3.96998	-0.013
N	0.07661	3.26971	1.55851
C	-1.38432	3.44063	1.36711
C	0.56665	3.76403	2.87347
Zn	0.23165	1.16226	1.685
C	-2.22749	2.61255	2.37011
H	-1.59545	3.10493	0.34949
H	-1.68494	4.49061	1.44454
C	1.63209	2.8372	3.48234
H	-0.28281	3.85979	3.54699
H	0.99562	4.76502	2.78013
N	-1.5441	1.37807	2.84658

N	1.24366	1.39942	3.44967
H	-3.15883	2.33546	1.87242
H	-2.50268	3.22402	3.23197
H	1.83952	3.15776	4.50864
H	2.5592	2.917	2.90999
C	-1.14016	1.39368	4.27894
H	-2.11837	0.56194	2.64058
C	0.3078	0.92246	4.50281
H	2.08946	0.83838	3.50189
H	-1.80185	0.75338	4.86748
H	-1.26389	2.40644	4.66268
H	0.35198	-0.16837	4.47478
H	0.64113	1.24898	5.49376
O	-2.4542	0.98214	-0.73822
C	-3.80039	0.97757	-1.01002
C	-4.39299	2.23773	-1.15832
C	-4.55334	-0.1954	-1.15363
C	-5.74644	2.33361	-1.44583
H	-3.78261	3.12645	-1.04948
C	-5.9089	-0.09957	-1.44046
H	-4.08968	-1.16698	-1.04863
C	-6.49084	1.16031	-1.58175
H	-6.22777	3.29526	-1.56335
H	-6.51568	-0.98764	-1.55738
N	-7.91295	1.25398	-1.8814
O	-8.40901	2.3773	-2.00645
O	-8.55501	0.20604	-1.99604
Zn	0.54715	-3.45388	-0.4438
N	2.07531	-3.4941	1.07365
N	0.45588	-5.54648	-0.1549
N	-0.70567	-3.38564	1.30539
C	1.55423	-2.50438	2.04251
C	2.07061	-4.87145	1.63973
C	1.6695	-5.9272	0.60229
C	-0.86363	-5.77215	0.47441
H	0.46759	-6.02937	-1.04821
C	0.07383	-2.74841	2.40382
C	-1.16528	-4.77311	1.60218
H	-1.50925	-2.78057	1.12699
H	1.65052	-1.52977	1.56954
H	2.15896	-2.49138	2.95931
H	1.3862	-4.90055	2.48535
H	3.05936	-5.12077	2.03924
H	1.5403	-6.89169	1.10768
H	2.46909	-6.04071	-0.13388
H	-1.60037	-5.65729	-0.32504
H	-0.95176	-6.79045	0.87196
H	-0.38531	-1.7847	2.62594

H	-0.00851	-3.3565	3.30736
H	-2.243	-4.77762	1.78469
H	-0.69223	-5.10723	2.52634
H	1.91891	3.55822	0.63622
C	0.70196	5.26359	0.07264
H	-0.36328	5.47921	-0.06151
H	1.04569	5.88379	0.90899
C	1.43652	5.69784	-1.2078
H	1.09163	5.08213	-2.04995
H	1.10824	6.71964	-1.42891
C	2.9761	5.68285	-1.16027
H	3.31641	6.04678	-0.18073
H	3.34374	6.41204	-1.89382
C	3.64687	4.33804	-1.4731
H	3.42843	3.59915	-0.69266
H	3.2171	3.93722	-2.39947
C	5.16876	4.46197	-1.61592
H	5.56843	4.96435	-0.72484
H	5.39647	5.12009	-2.46628
C	5.89387	3.12183	-1.7999
H	6.9771	3.30114	-1.83008
H	5.71343	2.49661	-0.91541
C	5.48014	2.35995	-3.06417
H	4.41843	2.09448	-3.0036
H	5.57348	3.03028	-3.92933
C	6.30458	1.09196	-3.33237
H	5.93554	0.62366	-4.25457
H	7.34729	1.37582	-3.52758
C	6.27969	0.04844	-2.20438
H	6.84544	-0.83376	-2.53201
H	6.80942	0.43585	-1.32445
C	4.87229	-0.38589	-1.78464
H	4.34668	0.46099	-1.3242
H	4.28813	-0.65791	-2.67493
C	4.87042	-1.56433	-0.80611
H	5.54682	-1.34881	0.03224
H	5.27517	-2.45338	-1.30845
C	3.46636	-1.8628	-0.27112
H	3.12985	-0.99558	0.30853
H	2.76701	-1.9764	-1.10729

IM3:

	x	y	z
C	1.83827	-4.4819	0.43052
H	2.15766	-4.08971	-0.53933
H	2.47131	-5.35177	0.66056

C	0.39028	-4.96612	0.34088
H	0.42175	-5.834	-0.3301
H	0.06091	-5.36627	1.3073
C	-0.65683	-3.98712	-0.19799
H	-0.83664	-3.17006	0.50801
H	-0.2871	-3.51464	-1.11404
C	-1.99529	-4.68366	-0.46598
H	-2.26809	-5.28236	0.41474
H	-1.87347	-5.39848	-1.2915
C	-3.14639	-3.72391	-0.78142
H	-2.87051	-3.09319	-1.63337
H	-3.28682	-3.04371	0.06948
C	-4.4551	-4.47113	-1.06518
H	-4.34439	-5.03929	-1.99972
H	-4.5976	-5.22035	-0.27408
C	-5.73517	-3.62533	-1.14845
H	-6.57761	-4.32391	-1.22824
H	-5.88627	-3.09123	-0.20291
C	-5.82619	-2.64362	-2.33097
H	-5.42854	-3.13939	-3.22744
H	-6.888	-2.45599	-2.5395
C	-5.14548	-1.27213	-2.17909
H	-4.06873	-1.39153	-2.03192
H	-5.25392	-0.75306	-3.13935
C	-5.73245	-0.37001	-1.0693
H	-5.71726	0.67115	-1.4173
H	-6.79117	-0.62146	-0.92438
C	-5.01213	-0.4013	0.28913
H	-5.0513	-1.40267	0.73395
H	-5.55715	0.25694	0.97883
C	-3.54988	0.04467	0.19633
H	-2.96745	-0.70927	-0.33738
H	-3.49843	0.94623	-0.42543
C	-2.89173	0.30704	1.5592
H	-1.80363	0.25833	1.45486
H	-3.17266	-0.49414	2.25291
C	-3.28919	1.64679	2.18838
H	-3.30176	1.58467	3.28347
P	-0.19155	0.33429	-1.20311
O	0.35046	0.18848	0.20994
O	-1.15214	1.51853	-1.38563
O	0.91684	0.44475	-2.37696
C	0.91769	-0.75472	-3.19591
H	1.15708	-0.45658	-4.21684
H	1.67478	-1.43223	-2.79929
C	-0.49704	-1.34806	-3.07289
H	-0.4674	-2.43698	-3.13916
C	-1.51047	-0.76821	-4.04433

H	-2.51207	-1.13664	-3.81184
H	-1.51932	0.32428	-3.99352
H	-1.25633	-1.06825	-5.06512
O	-0.88549	-1.04347	-1.69677
H	-4.30178	1.90715	1.87158
N	2.14207	-3.41499	1.43041
C	3.61446	-3.21872	1.45074
C	1.61937	-3.70845	2.78727
Zn	1.5545	-1.37463	0.87424
C	4.07616	-1.98915	2.26933
H	3.91526	-3.09171	0.41184
H	4.11434	-4.11387	1.84529
C	0.30662	-2.96769	3.09584
H	2.37758	-3.42946	3.51716
H	1.46011	-4.78318	2.91988
N	3.07296	-0.88748	2.32959
N	0.32331	-1.56409	2.63167
H	4.98625	-1.60804	1.80186
H	4.34513	-2.28151	3.28722
H	0.1131	-3.02529	4.17339
H	-0.5232	-3.45928	2.58791
C	2.43071	-0.69592	3.65913
H	3.5265	-0.02302	2.05136
C	0.90768	-0.5667	3.55317
H	-0.62576	-1.2771	2.4144
H	2.82342	0.19995	4.14684
H	2.69073	-1.53912	4.29977
H	0.65674	0.41451	3.14523
H	0.47022	-0.63782	4.55626
O	2.72852	-1.41088	-0.73531
C	3.61706	-0.49242	-0.9995
C	4.72485	-0.81153	-1.83721
C	3.53794	0.83928	-0.49034
C	5.6972	0.12262	-2.12901
H	4.78668	-1.81846	-2.23677
C	4.51271	1.77325	-0.77897
H	2.67217	1.1236	0.09699
C	5.59717	1.41796	-1.59554
H	6.54091	-0.12535	-2.76074
H	4.4492	2.78326	-0.39375
N	6.6076	2.38901	-1.89499
O	7.55261	2.0602	-2.63177
O	6.50528	3.52785	-1.40794
Zn	-1.63199	2.91288	-0.17626
N	-2.40771	2.79725	1.80884
N	-2.85415	4.57286	-0.43763
N	-0.26307	4.2629	0.73256
C	-1.13669	2.75904	2.57911

C	-3.13927	4.08407	2.00586
C	-3.79674	4.57207	0.70993
C	-1.90201	5.70793	-0.54579
H	-3.39134	4.52412	-1.29864
C	-0.13999	3.8654	2.16746
C	-0.77655	5.64795	0.50013
H	0.64403	4.1694	0.28691
H	-0.69087	1.78375	2.38237
H	-1.33291	2.83067	3.65601
H	-2.44802	4.83277	2.38431
H	-3.90834	3.96637	2.77483
H	-4.21628	5.57047	0.87424
H	-4.61459	3.90092	0.43727
H	-1.47596	5.64973	-1.55012
H	-2.42115	6.66812	-0.45107
H	0.86965	3.49184	2.34669
H	-0.26347	4.75023	2.79504
H	0.03681	6.29555	0.16552
H	-1.12422	6.0511	1.45093

TS:

	x	y	z
C	-1.6182	3.05123	0.5351
H	-1.70816	2.37256	-0.31789
C	4.52619	-0.98362	0.72592
H	4.88527	-0.59772	1.69162
P	-0.63466	-0.96673	-0.82272
O	0.2214	-0.11743	0.15887
O	-0.8395	-2.44255	-0.62509
O	-0.75124	-0.38355	-2.32907
C	0.37381	-0.17776	-3.20746
H	-0.04573	-0.07757	-4.21058
H	0.86486	0.75795	-2.92137
C	1.3546	-1.34107	-3.07592
H	2.29394	-1.03741	-3.56665
C	0.84581	-2.63077	-3.72114
H	1.56518	-3.43959	-3.55328
H	-0.10973	-2.92421	-3.27914
H	0.71766	-2.50833	-4.80206
O	1.52075	-1.44836	-1.68772
H	5.39409	-1.3899	0.19809
N	-1.91411	2.2414	1.75466
C	-3.30268	1.72527	1.7733
C	-1.56236	2.9475	3.01868
Zn	-0.70335	0.49674	1.71721
C	-3.47666	0.4242	2.61678

H	-3.57059	1.51301	0.73962
H	-3.99635	2.48718	2.14188
C	-0.12115	2.67516	3.46641
H	-2.26472	2.63732	3.79069
H	-1.69108	4.02736	2.90834
N	-2.19477	-0.22911	3.00868
N	0.23051	1.2328	3.42189
H	-4.04271	-0.29064	2.0177
H	-4.06512	0.62825	3.51432
H	0.02209	3.08458	4.47252
H	0.57552	3.18249	2.79456
C	-1.76212	0.06087	4.41004
H	-2.29811	-1.23305	2.89795
C	-0.26285	0.37326	4.52585
H	1.24269	1.15176	3.38411
H	-1.99057	-0.79078	5.055
H	-2.35071	0.89893	4.78118
H	0.31291	-0.55356	4.47242
H	-0.07141	0.8341	5.50136
O	-2.13555	-0.25601	-0.35849
C	-3.35001	-0.71746	-0.77242
C	-4.15473	0.14059	-1.5344
C	-3.81826	-1.98106	-0.38221
C	-5.43403	-0.25444	-1.90212
H	-3.76242	1.1066	-1.83018
C	-5.09472	-2.38234	-0.75251
H	-3.16706	-2.62791	0.19008
C	-5.88832	-1.51335	-1.50519
H	-6.07578	0.38976	-2.48834
H	-5.48448	-3.34955	-0.46377
N	-7.23012	-1.93223	-1.88684
O	-7.91956	-1.15056	-2.54872
O	-7.61643	-3.04957	-1.5309
Zn	2.43292	-2.75138	-0.72066
N	3.59711	-2.12028	0.97645
N	3.51262	-4.51233	-0.65898
N	1.26635	-3.63511	0.82829
C	2.53125	-1.74844	1.93704
C	4.33721	-3.33681	1.40696
C	4.67913	-4.25374	0.2249
C	2.53275	-5.54088	-0.22452
H	3.86139	-4.78132	-1.57456
C	1.43751	-2.83464	2.06528
C	1.63663	-5.06596	0.93598
H	0.3245	-3.49613	0.45128
H	2.07467	-0.83872	1.55323
H	2.95562	-1.53363	2.92738
H	3.73587	-3.87649	2.13612

H	5.26457	-3.06	1.91959
H	5.09518	-5.19255	0.6073
H	5.43878	-3.77899	-0.40094
H	1.91658	-5.75341	-1.10179
H	3.04043	-6.46742	0.06658
H	0.49666	-2.33359	2.30192
H	1.65554	-3.50365	2.90087
H	0.74383	-5.69746	0.95641
H	2.15039	-5.2236	1.88557
H	-0.56749	3.3368	0.60343
C	-2.50823	4.27618	0.31426
H	-3.55095	3.94423	0.26787
H	-2.43835	4.96671	1.16296
C	-2.18336	5.04151	-0.9827
H	-2.02741	4.32446	-1.80092
H	-3.07549	5.61678	-1.25462
C	-0.99829	6.02006	-0.92375
H	-1.12173	6.68241	-0.05564
H	-1.0595	6.66887	-1.80757
C	0.4045	5.4	-0.89687
H	0.57039	4.85602	0.04094
H	0.48175	4.65879	-1.70271
C	1.51196	6.45136	-1.0391
H	1.43071	7.15968	-0.20403
H	1.34043	7.03647	-1.95371
C	2.9318	5.86849	-1.07418
H	3.65891	6.68645	-0.98214
H	3.07954	5.22917	-0.19352
C	3.24122	5.08031	-2.35272
H	2.5661	4.22038	-2.43374
H	3.02009	5.71837	-3.21885
C	4.69571	4.59878	-2.45791
H	4.83062	4.10132	-3.42767
H	5.36172	5.47196	-2.46506
C	5.14755	3.63722	-1.34798
H	6.18514	3.33796	-1.5471
H	5.16408	4.15763	-0.38163
C	4.27963	2.38148	-1.22681
H	3.27428	2.65706	-0.88205
H	4.1464	1.93134	-2.22091
C	4.85837	1.32815	-0.27762
H	5.05713	1.78283	0.70255
H	5.82937	0.98659	-0.66182
C	3.91319	0.13646	-0.11072
H	2.97758	0.48548	0.33764
H	3.63651	-0.25838	-1.09424

Path 4

IM1:

	x	y	z
C	-4.27044	3.22132	0.40132
H	-4.0316	4.27471	0.21285
C	4.29853	-0.54508	-2.56409
H	4.05327	-0.60547	-3.63959
P	0.73699	-0.68124	1.83578
O	0.61714	-0.22176	0.38364
O	0.72236	-2.13575	2.18825
O	2.03683	0.01712	2.48282
C	2.38605	1.37924	2.16084
H	1.78999	2.05688	2.77907
H	2.17919	1.57311	1.10593
C	3.86021	1.58069	2.45375
H	4.07363	2.64163	2.26867
C	4.26122	1.20245	3.87216
H	5.33012	1.37699	4.028
H	4.04209	0.149	4.06139
H	3.71191	1.81191	4.59595
O	4.59071	0.80144	1.48016
H	5.39086	-0.53215	-2.48631
O	-0.42982	0.14392	2.708
C	-1.76176	-0.14472	2.68651
C	-2.28861	-1.32662	2.14016
C	-2.61166	0.81416	3.26012
C	-3.6595	-1.54605	2.16968
H	-1.62888	-2.07833	1.72788
C	-3.97816	0.59054	3.30234
H	-2.1812	1.71979	3.6707
C	-4.4903	-0.59178	2.7571
H	-4.07954	-2.44145	1.73338
H	-4.64984	1.31306	3.74618
N	-5.92057	-0.83483	2.8113
O	-6.35215	-1.89905	2.35421
O	-6.6444	0.03653	3.30506
N	3.83687	-1.74725	-1.85304
N	5.53368	-3.12419	0.15989
N	2.5889	-3.25324	0.25461
C	2.38677	-1.9438	-1.92577
C	4.62039	-2.93933	-2.19772
C	5.83552	-3.16402	-1.27965
C	4.87048	-4.29047	0.76183
H	6.4009	-2.96514	0.66078
C	1.86536	-3.08393	-1.02124
C	3.39235	-4.4853	0.3599

H	1.92722	-3.16901	1.02363
H	1.91875	-1.01511	-1.59942
H	2.04755	-2.14243	-2.95915
H	3.97284	-3.81378	-2.1616
H	4.98998	-2.88662	-3.23261
H	6.29982	-4.11976	-1.5689
H	6.57177	-2.37528	-1.46159
H	4.92988	-4.14236	1.84442
H	5.39943	-5.2279	0.52711
H	0.81592	-2.85958	-0.80707
H	1.87063	-4.03099	-1.57224
H	2.95189	-5.16324	1.10055
H	3.3511	-5.01656	-0.59423
H	-4.21665	3.08518	1.49047
C	-3.21282	2.32944	-0.25673
H	-3.33777	2.35596	-1.3478
H	-3.37533	1.2877	0.04387
C	-1.76532	2.71372	0.07381
H	-1.09795	1.9845	-0.40611
H	-1.58783	2.61477	1.15289
C	-1.36719	4.12019	-0.38824
H	-1.76875	4.29673	-1.39659
H	-1.83054	4.87553	0.25933
C	0.14766	4.33887	-0.41792
H	0.58943	3.6404	-1.14366
H	0.5733	4.07075	0.55779
C	0.54112	5.77509	-0.79334
H	-0.08502	6.10053	-1.63491
H	0.30363	6.44851	0.04195
C	2.0144	5.9303	-1.19314
H	2.19295	6.94947	-1.56091
H	2.20453	5.26446	-2.04424
C	3.00844	5.62474	-0.06648
H	2.74252	4.67526	0.41122
H	2.91067	6.3894	0.71529
C	4.47416	5.55399	-0.52442
H	5.09881	5.32866	0.35024
H	4.79539	6.53949	-0.88669
C	4.75197	4.50186	-1.61461
H	5.83749	4.41815	-1.75696
H	4.34794	4.84119	-2.57702
C	4.17052	3.12596	-1.28634
H	3.07599	3.1918	-1.25711
H	4.47983	2.82487	-0.27693
C	4.55881	2.00774	-2.2588
H	4.39654	2.32971	-3.29603
H	5.63247	1.79581	-2.16203
C	3.74688	0.74441	-1.9542

H	2.70675	0.90659	-2.25899
H	3.73004	0.614	-0.86541
N	-2.73135	-1.059	-2.0467
C	-3.66515	-2.03544	-1.82022
C	-3.0279	-0.30899	-3.15822
C	-4.75542	-1.977	-2.91187
O	-3.64034	-2.84563	-0.89728
C	-4.33354	-0.78927	-3.78842
O	-2.34164	0.61987	-3.58057
H	-4.71175	-2.91744	-3.46844
H	-5.06086	0.02506	-3.7868
H	-4.15974	-1.07079	-4.83054
S	-6.464	-1.96598	-2.23927
C	-6.34685	-0.83444	-0.79882
H	-7.33438	-0.91628	-0.33301
H	-5.62631	-1.25948	-0.09699
C	-6.01649	0.62479	-1.10676
H	-6.657	0.98928	-1.91853
H	-4.98543	0.69743	-1.4594
C	-5.71211	2.9665	-0.06719
H	-6.37231	3.64972	0.47987
H	-5.8036	3.24157	-1.12705
C	-6.20352	1.51873	0.12791
H	-5.67611	1.08131	0.98164
H	-7.2668	1.51447	0.39618
Ag	-1.08421	-0.65902	-0.82122
Ag	4.03642	-1.32713	0.63311
H	5.53696	0.87245	1.66433

IM2:

	x	y	z
C	-4.28992	3.04429	0.9341
H	-4.14164	4.12782	1.01639
C	4.13374	0.24376	-2.54587
H	3.79509	0.49506	-3.56905
P	0.61722	-1.40302	2.02639
O	0.60216	-0.29396	0.96907
O	0.50436	-2.84215	1.61624
O	1.85754	-1.22161	3.01287
C	2.39147	0.07637	3.39099
H	2.15384	0.21264	4.45181
H	1.90358	0.8563	2.80209
C	3.90806	0.12743	3.14565
H	4.21601	1.05172	3.68471
C	4.61062	-1.04626	3.85021
H	5.69493	-0.93681	3.7478

H	4.31503	-1.98868	3.37615
H	4.36793	-1.09972	4.91913
O	4.24058	0.23702	1.80711
H	5.22846	0.21172	-2.57605
O	-0.61236	-1.00754	3.10473
C	-1.94075	-1.0984	2.82296
C	-2.46747	-1.99541	1.87782
C	-2.79492	-0.26117	3.5599
C	-3.84111	-2.06823	1.69106
H	-1.80411	-2.64249	1.3199
C	-4.16677	-0.33825	3.37964
H	-2.36376	0.43027	4.27446
C	-4.67911	-1.25089	2.45132
H	-4.25778	-2.74978	0.96256
H	-4.84236	0.291	3.94358
N	-6.11672	-1.35152	2.27838
O	-6.55372	-2.18807	1.48001
O	-6.84075	-0.59188	2.93097
N	3.67639	-1.09736	-2.16076
N	5.3835	-2.97985	-0.64578
N	2.46247	-3.13019	-0.51672
C	2.22538	-1.2579	-2.22957
C	4.43016	-2.15696	-2.83614
C	5.66156	-2.62629	-2.042
C	4.7401	-4.2672	-0.36866
H	6.25238	-2.94121	-0.12524
C	1.72012	-2.60944	-1.68015
C	3.25297	-4.34745	-0.77274
H	1.80258	-3.27389	0.2467
H	1.78175	-0.4585	-1.63248
H	1.83894	-1.14254	-3.26063
H	3.7735	-3.00581	-3.01944
H	4.77548	-1.83185	-3.82985
H	6.11831	-3.4632	-2.59577
H	6.39631	-1.81535	-2.01574
H	4.8227	-4.41797	0.71238
H	5.25948	-5.10774	-0.85864
H	0.67185	-2.46466	-1.39682
H	1.71548	-3.35876	-2.47996
H	2.82249	-5.20002	-0.23339
H	3.18545	-4.59997	-1.83439
H	-4.25263	2.64999	1.95969
C	-3.1424	2.4251	0.13047
H	-3.25228	2.68457	-0.93089
H	-3.21032	1.3319	0.18326
C	-1.74374	2.85793	0.5846
H	-1.00417	2.27838	0.01473
H	-1.58887	2.59019	1.63921

C	-1.45686	4.35111	0.37314
H	-1.90416	4.66838	-0.57988
H	-1.94705	4.94845	1.15252
C	0.0386	4.67533	0.33915
H	0.49624	4.10794	-0.48444
H	0.51288	4.30946	1.2588
C	0.33711	6.16907	0.14266
H	-0.34689	6.56515	-0.61986
H	0.11191	6.71568	1.06892
C	1.77896	6.4507	-0.30216
H	1.88842	7.51229	-0.56052
H	1.95693	5.89385	-1.2307
C	2.84376	6.07667	0.73645
H	2.62704	5.0837	1.14461
H	2.77491	6.7693	1.58548
C	4.28163	6.0838	0.19292
H	4.9632	5.82084	1.01272
H	4.55268	7.10165	-0.11778
C	4.52639	5.11978	-0.98291
H	5.60103	5.10385	-1.20781
H	4.03677	5.5007	-1.88837
C	4.03981	3.69264	-0.71907
H	2.95245	3.69839	-0.57602
H	4.46531	3.32823	0.22654
C	4.3714	2.69344	-1.83138
H	4.03826	3.09229	-2.79965
H	5.46122	2.5716	-1.9047
C	3.7119	1.33709	-1.56538
H	2.62335	1.47022	-1.58413
H	3.96511	1.0068	-0.55085
N	-2.26748	-0.50694	-2.12189
C	-3.15106	-1.5415	-2.27968
C	-2.43915	0.46714	-3.07472
C	-4.07845	-1.25845	-3.48087
O	-3.20026	-2.55001	-1.57956
C	-3.60694	0.10961	-3.99269
O	-1.75387	1.48316	-3.1724
H	-3.90719	-2.04333	-4.22268
H	-4.37593	0.88186	-3.92257
H	-3.26588	0.08042	-5.03112
S	-5.86191	-1.43999	-3.07566
C	-5.98871	-0.71342	-1.39501
H	-7.00647	-0.96568	-1.08139
H	-5.31014	-1.26504	-0.74137
C	-5.74943	0.79075	-1.28652
H	-6.39163	1.32274	-1.9984
H	-4.71697	1.0177	-1.5611
C	-5.68746	2.78906	0.34725

H	-6.42818	3.23823	1.01899
H	-5.78225	3.32254	-0.60848
C	-6.02344	1.29913	0.13609
H	-5.43807	0.70612	0.84611
H	-7.07635	1.10993	0.37644
Ag	-0.87272	-0.37569	-0.56581
Ag	3.86793	-1.37534	0.44047

IM3:

	x	y	z
C	4.77879	2.04623	-0.40212
H	4.90215	3.12753	-0.55053
C	-3.7581	-0.9891	2.37344
H	-3.46806	-1.14074	3.42819
P	-1.79622	1.35329	-2.24741
O	-0.47059	0.60705	-2.2076
O	-3.05899	0.56404	-1.94713
O	-1.9688	2.11105	-3.69199
C	-1.52332	3.47756	-3.56611
H	-2.02285	4.06912	-4.33443
H	-0.4387	3.52484	-3.71172
C	-1.91115	3.90637	-2.14154
H	-1.21926	4.66262	-1.76449
C	-3.35119	4.37483	-2.01056
H	-3.60301	4.5302	-0.959
H	-4.03761	3.63298	-2.42939
H	-3.48833	5.31957	-2.54547
O	-1.70143	2.7146	-1.33794
H	-4.85071	-0.92358	2.35428
O	0.49569	-2.6869	-2.0348
C	1.71616	-2.31788	-2.15062
C	2.78758	-2.95574	-1.42449
C	2.0951	-1.21382	-3.00166
C	4.08633	-2.51567	-1.51553
H	2.52799	-3.77093	-0.75992
C	3.39439	-0.77485	-3.08655
H	1.30482	-0.70411	-3.54113
C	4.40713	-1.41798	-2.34414
H	4.87955	-2.99334	-0.95323
H	3.66098	0.06897	-3.71105
N	5.74132	-0.96065	-2.42698
O	6.62871	-1.53924	-1.76099
O	6.00824	0.01965	-3.15889
N	-3.35715	-2.15108	1.56166
N	-4.70509	-2.92033	-0.96263
N	-1.8348	-3.51426	-0.47855

C	-2.01756	-2.62518	1.91403
C	-4.35706	-3.2245	1.52174
C	-5.34214	-3.10517	0.34729
C	-4.07336	-4.0753	-1.61285
H	-5.39194	-2.53612	-1.60158
C	-1.43191	-3.66931	0.93593
C	-2.75346	-4.56145	-0.97291
H	-0.99189	-3.45912	-1.05166
H	-1.36412	-1.75337	1.92637
H	-1.99569	-3.06008	2.93043
H	-3.84149	-4.18245	1.46117
H	-4.94336	-3.26052	2.4519
H	-5.99344	-3.99397	0.36615
H	-5.98017	-2.22975	0.50586
H	-3.87341	-3.76294	-2.64254
H	-4.74833	-4.94581	-1.65893
H	-0.34577	-3.58618	1.00054
H	-1.69256	-4.6781	1.27681
H	-2.24753	-5.17416	-1.72837
H	-2.99003	-5.23689	-0.14659
H	5.14051	1.57221	-1.32361
C	3.28546	1.72969	-0.24573
H	2.9548	1.97343	0.77124
H	3.12824	0.65204	-0.36658
C	2.4111	2.49189	-1.25644
H	1.45043	1.98027	-1.37959
H	2.90207	2.45987	-2.23893
C	2.1347	3.95082	-0.85294
H	3.07157	4.44394	-0.55648
H	1.76255	4.50829	-1.72361
C	1.10751	4.05841	0.27935
H	1.40233	3.41405	1.11532
H	0.16011	3.64745	-0.08382
C	0.89782	5.47943	0.81346
H	1.8376	5.83508	1.25677
H	0.67658	6.16382	-0.01913
C	-0.23127	5.56728	1.85418
H	-0.1517	6.50706	2.41657
H	-0.09866	4.76068	2.58725
C	-1.62942	5.48393	1.22887
H	-1.67364	4.62558	0.55324
H	-1.78149	6.37268	0.60157
C	-2.78349	5.37974	2.23699
H	-3.73003	5.52147	1.69752
H	-2.71547	6.20657	2.95708
C	-2.86214	4.04448	2.99696
H	-3.74043	4.07105	3.65627
H	-1.99234	3.93033	3.65732

C	-2.95339	2.82536	2.07335
H	-1.99956	2.68171	1.55694
H	-3.69831	3.01935	1.28807
C	-3.32121	1.51885	2.78398
H	-2.67358	1.37465	3.65933
H	-4.35031	1.58206	3.16566
C	-3.17255	0.32099	1.84219
H	-2.10701	0.19512	1.62281
H	-3.66056	0.54704	0.88486
N	0.90098	-0.78035	1.59225
C	1.49462	-1.87907	2.15498
C	0.80897	0.25298	2.49467
C	1.85995	-1.59213	3.62647
O	1.69201	-2.95848	1.60189
C	1.48405	-0.11858	3.81358
O	0.26299	1.33226	2.27294
H	1.22853	-2.23849	4.24361
H	2.35315	0.52604	3.96424
H	0.79903	0.05083	4.64821
S	3.56432	-2.10917	4.07241
C	4.54936	-1.65847	2.58793
H	5.55535	-2.0109	2.84017
H	4.1905	-2.25481	1.74512
C	4.57451	-0.17283	2.23434
H	4.78537	0.41565	3.13556
H	3.58804	0.13163	1.87846
C	5.68348	1.6309	0.76816
H	6.71505	1.89053	0.50018
H	5.43919	2.24217	1.64859
C	5.63284	0.14313	1.16845
H	5.47	-0.47942	0.28145
H	6.61077	-0.1558	1.56765
Ag	0.16612	-0.49678	-0.40336
Ag	-2.83216	-1.3794	-0.80833

TS:

	x	y	z
C	2.4647	2.56585	-2.28395
H	2.03201	3.20585	-3.06369
C	-4.95173	-0.27273	2.1388
H	-4.94635	0.27663	3.09966
P	0.0616	-1.04566	-0.81045
O	-0.43395	-0.08774	0.27613
O	-0.15623	-2.53132	-0.74162
O	0.08767	-0.42415	-2.31137

C	-1.04268	0.12169	-3.02263
H	-0.70774	0.21575	-4.06003
H	-1.25166	1.11906	-2.62174
C	-2.28833	-0.7546	-2.86673
H	-3.09984	-0.21173	-3.40199
C	-2.12153	-2.11791	-3.5535
H	-3.02666	-2.71479	-3.39444
H	-1.27768	-2.65514	-3.11311
H	-1.95978	-2.01399	-4.6336
O	-2.51008	-0.82787	-1.50463
H	-5.96827	-0.65882	2.00432
O	1.75305	-0.85182	-0.566
C	2.71617	-1.64612	-1.07839
C	3.83586	-1.88789	-0.26173
C	2.65917	-2.17447	-2.38034
C	4.89906	-2.63311	-0.74571
H	3.84903	-1.47457	0.74161
C	3.71982	-2.92706	-2.86181
H	1.79636	-1.97081	-3.00067
C	4.83272	-3.14772	-2.04466
H	5.77312	-2.82378	-0.13675
H	3.70307	-3.33786	-3.86293
N	5.94344	-3.92528	-2.55608
O	6.92653	-4.09752	-1.82509
O	5.86323	-4.3842	-3.70214
N	-4.04611	-1.42627	2.19128
N	-4.53785	-3.97677	0.74245
N	-1.85057	-3.18708	1.53217
C	-2.69889	-1.07546	2.64727
C	-4.6424	-2.58085	2.86237
C	-5.35662	-3.53478	1.89039
C	-3.51903	-5.01496	1.00874
H	-5.17464	-4.35812	0.04969
C	-1.69509	-2.2531	2.64221
C	-2.29759	-4.53786	1.83197
H	-1.09183	-3.12949	0.8568
H	-2.31474	-0.3088	1.97287
H	-2.7117	-0.64222	3.66716
H	-3.87377	-3.12546	3.40659
H	-5.37928	-2.27381	3.62081
H	-5.72242	-4.39958	2.46416
H	-6.22847	-3.02601	1.46772
H	-3.17921	-5.35383	0.02558
H	-3.9633	-5.88045	1.52385
H	-0.69564	-1.80341	2.61654
H	-1.75976	-2.79858	3.59198
H	-1.5029	-5.27862	1.66213
H	-2.54011	-4.6038	2.8965

H	2.07343	1.55537	-2.46261
C	1.97659	3.03641	-0.9109
H	2.44461	3.99897	-0.65818
H	2.31446	2.32266	-0.15314
C	0.45363	3.15893	-0.78805
H	0.20499	3.29377	0.27299
H	-0.00537	2.20862	-1.08397
C	-0.17801	4.30977	-1.57692
H	0.29612	5.25585	-1.27799
H	0.01822	4.19395	-2.6509
C	-1.68887	4.40256	-1.34504
H	-1.88186	4.42367	-0.26256
H	-2.16163	3.48337	-1.71603
C	-2.3518	5.63038	-1.98032
H	-1.86512	6.53191	-1.58566
H	-2.16926	5.63305	-3.06437
C	-3.86259	5.70289	-1.70853
H	-4.23135	6.71901	-1.89848
H	-4.02758	5.51689	-0.63949
C	-4.68348	4.71315	-2.54729
H	-4.1674	3.7474	-2.58759
H	-4.718	5.07338	-3.58358
C	-6.11824	4.48925	-2.04522
H	-6.63406	3.8296	-2.75567
H	-6.66477	5.44178	-2.05841
C	-6.22087	3.86865	-0.63973
H	-7.27515	3.63981	-0.4349
H	-5.91945	4.60016	0.12102
C	-5.38189	2.59916	-0.47109
H	-4.31698	2.85572	-0.52828
H	-5.57398	1.92039	-1.31473
C	-5.6276	1.83875	0.83598
H	-5.53232	2.52336	1.69013
H	-6.66075	1.46397	0.85335
C	-4.64399	0.67519	0.98214
H	-3.63089	1.0812	1.08181
H	-4.64004	0.08276	0.05911
N	2.67734	1.556	2.63712
C	3.85704	0.89363	2.84166
C	2.81556	2.9127	2.81854
C	4.9641	1.89441	3.2337
O	4.01988	-0.32171	2.73749
C	4.27	3.25901	3.13464
O	1.90443	3.73053	2.72002
H	5.25599	1.67399	4.26448
H	4.66999	3.8759	2.32591
H	4.33141	3.84416	4.05565
S	6.53137	1.67669	2.29267

C	5.97544	1.1508	0.62245
H	6.91273	0.91608	0.10685
H	5.42364	0.21664	0.7367
C	5.16296	2.16786	-0.17764
H	5.74441	3.08913	-0.30417
H	4.26458	2.43713	0.3802
C	3.99115	2.56184	-2.46696
H	4.20099	2.29216	-3.50937
H	4.37744	3.58272	-2.33671
C	4.77599	1.60035	-1.553
H	4.19716	0.67933	-1.41469
H	5.70076	1.30073	-2.0633
Ag	1.05247	0.69727	1.60751
Ag	-3.46717	-2.25698	-0.29014

Path 5

IM1:

	x	y	z
C	4.85702	-1.49325	0.06571
H	4.60753	-0.43298	-0.01106
H	4.76306	-1.76007	1.12252
C	6.29482	-1.73984	-0.40494
H	6.63701	-2.71446	-0.04182
H	6.34067	-1.77994	-1.49952
C	7.2403	-0.62969	0.0864
H	7.14502	-0.52131	1.17557
H	8.27603	-0.9359	-0.10211
C	6.97763	0.72061	-0.58917
H	5.94107	1.02682	-0.40825
H	7.06829	0.6021	-1.67776
C	7.90468	1.85316	-0.13408
H	8.92979	1.63102	-0.45597
H	7.92807	1.89421	0.96397
C	7.45827	3.21578	-0.68908
H	8.287	3.93306	-0.64599
H	7.22022	3.09302	-1.75342
C	6.2517	3.80859	0.05855
H	5.5501	3.00961	0.32615
H	6.60123	4.22244	1.01278
C	1.55712	2.6066	-0.49249
H	1.24255	2.13566	-1.43521
H	2.10358	1.84186	0.07719
C	0.31705	3.0389	0.30532
H	-0.123	2.16372	0.79237

H	0.63755	3.69974	1.12154
C	-0.75856	3.75741	-0.52412
H	-1.54666	4.10258	0.15427
H	-0.33817	4.66247	-0.97984
C	-1.40832	2.90266	-1.62555
H	-0.71049	2.75875	-2.46049
H	-2.25462	3.46476	-2.04016
C	-1.89337	1.5255	-1.1541
H	-1.03278	0.87944	-0.95258
H	-2.40876	1.61894	-0.19111
C	-2.82591	0.82569	-2.16103
H	-2.76315	-0.25385	-2.01837
H	-2.50187	1.02586	-3.18862
C	-4.2764	1.27144	-1.96692
H	-4.38805	2.34327	-2.15814
P	-0.96125	-0.77013	2.52221
O	-1.29476	-1.35159	1.12825
O	0.15518	0.24256	2.49783
O	-0.68289	-1.97466	3.54987
C	0.30461	-2.97798	3.20456
H	0.18115	-3.76818	3.94622
H	0.07054	-3.38961	2.21989
C	1.74506	-2.46937	3.26827
H	2.39119	-3.3215	3.04183
C	2.11468	-1.85217	4.60731
H	3.16025	-1.5378	4.59832
H	1.48453	-0.98489	4.81979
H	1.97514	-2.58428	5.40702
O	2.03017	-1.49065	2.21858
H	-4.58965	1.09823	-0.93647
S	-5.54154	0.52072	-3.06726
C	-5.62425	-1.25599	-2.54839
C	-4.67729	-2.21028	-3.29296
H	-6.67528	-1.51722	-2.68284
H	-4.15219	-1.74654	-4.12944
H	-5.20313	-3.09109	-3.67481
C	-5.24589	-1.43392	-1.06897
C	-3.67838	-2.64879	-2.23421
O	-5.82314	-0.93862	-0.11303
O	-2.64065	-3.27051	-2.4218
N	-4.10398	-2.21051	-0.99131
N	3.78238	-2.21733	-0.66937
C	3.89447	-3.6924	-0.57596
C	3.61082	-1.73202	-2.06728
Zn	1.93353	-1.86767	0.27321
C	2.59721	-4.40694	-1.03229
H	4.09001	-3.91744	0.47612
H	4.737	-4.07576	-1.16165

C	2.62536	-0.55969	-2.15885
H	3.27018	-2.56186	-2.68306
H	4.56684	-1.41214	-2.48852
N	1.35498	-3.5998	-0.80713
N	1.37319	-0.80333	-1.39745
H	2.515	-5.34196	-0.47611
H	2.65759	-4.67261	-2.08933
H	2.40746	-0.35747	-3.21263
H	3.07819	0.33829	-1.73433
C	0.67924	-3.13035	-2.06169
H	0.69536	-4.16184	-0.28
C	0.33207	-1.63349	-2.05018
H	0.9656	0.09652	-1.15947
H	-0.25109	-3.68009	-2.21171
H	1.33072	-3.35692	-2.9058
H	-0.5842	-1.47012	-1.48394
H	0.15506	-1.30281	-3.07933
O	-2.32079	-0.21114	3.21634
C	-2.92017	0.93999	2.71119
C	-4.16296	0.81341	2.09019
C	-2.28784	2.17731	2.85272
C	-4.77191	1.94423	1.55746
H	-4.63158	-0.15724	1.98803
C	-2.89643	3.30834	2.32251
H	-1.3272	2.23894	3.34662
C	-4.11922	3.17145	1.66452
H	-5.72207	1.87386	1.04589
H	-2.43239	4.2817	2.40309
N	-4.71431	4.34526	1.0317
O	-5.80705	4.21416	0.47676
O	-4.08462	5.40529	1.07037
C	5.49758	4.89852	-0.71823
H	4.78814	5.38947	-0.04137
H	6.20679	5.67811	-1.02682
C	4.74617	4.39818	-1.96613
H	5.46784	4.01938	-2.69975
H	4.25401	5.25546	-2.44408
C	3.6973	3.30606	-1.70308
H	4.18475	2.43362	-1.24802
H	3.30114	2.95787	-2.66611
C	2.52701	3.748	-0.81855
H	1.98967	4.56488	-1.31783
H	2.90234	4.16038	0.12621
Zn	-2.83486	-2.11856	0.42228
H	1.45721	-0.6734	2.37734

IM2:

	x	y	z
C	4.56787	-1.57048	0.27575
H	4.33071	-0.50375	0.26769
H	4.34559	-1.918	1.28689
C	6.05057	-1.78562	-0.06819
H	6.39806	-2.7235	0.37815
H	6.18055	-1.89508	-1.15182
C	6.92686	-0.61506	0.40992
H	6.75153	-0.43546	1.47972
H	7.9828	-0.89632	0.31506
C	6.67701	0.67857	-0.37444
H	5.6318	0.98726	-0.25538
H	6.81066	0.47962	-1.44708
C	7.58333	1.84826	0.02625
H	8.62057	1.60069	-0.23235
H	7.5608	1.97732	1.11752
C	7.17005	3.16426	-0.65368
H	8.00763	3.87297	-0.64602
H	6.95872	2.95734	-1.71077
C	5.95528	3.83362	0.00778
H	5.1989	3.0773	0.24925
H	6.27123	4.25103	0.97238
C	1.35294	2.74241	-0.75899
H	1.08725	2.20467	-1.68012
H	1.88918	2.02786	-0.11957
C	0.0756	3.19465	-0.0357
H	-0.33351	2.35305	0.52961
H	0.34464	3.9469	0.7175
C	-1.01414	3.7722	-0.95175
H	-1.82338	4.16295	-0.3242
H	-0.61928	4.63378	-1.505
C	-1.61502	2.77027	-1.95287
H	-0.89765	2.55475	-2.7554
H	-2.47567	3.24396	-2.44238
C	-2.05589	1.44245	-1.3243
H	-1.17606	0.87605	-1.00237
H	-2.6167	1.63571	-0.40258
C	-2.91033	0.56753	-2.26309
H	-2.72315	-0.48517	-2.04928
H	-2.61962	0.72257	-3.30827
C	-4.40371	0.85284	-2.0863
H	-4.66198	1.84849	-2.46006
P	-0.53202	-0.34899	2.59872
O	-0.76909	-0.92975	1.15893
O	0.40498	0.80047	2.7045
O	-0.37162	-1.55014	3.64934
C	0.16758	-2.8484	3.29601

H	-0.06065	-3.49092	4.14923
H	-0.3538	-3.23764	2.41621
C	1.67096	-2.77124	3.02263
H	1.96186	-3.78463	2.68561
C	2.45732	-2.4445	4.29438
H	3.52533	-2.39365	4.06482
H	2.14335	-1.47401	4.68997
H	2.30298	-3.2048	5.06778
O	1.93626	-1.79423	2.05856
H	-4.67619	0.827	-1.02957
S	-5.56686	-0.24957	-2.98827
C	-5.42926	-1.89166	-2.13184
C	-4.43998	-2.88727	-2.75872
H	-6.45311	-2.26873	-2.12126
H	-4.01513	-2.54909	-3.70539
H	-4.89712	-3.86705	-2.92865
C	-4.93463	-1.73577	-0.68567
C	-3.33731	-3.02291	-1.72095
O	-5.50868	-1.13455	0.20841
O	-2.26914	-3.60777	-1.85683
N	-3.7027	-2.35649	-0.56669
N	3.58507	-2.21269	-0.63047
C	3.66244	-3.68383	-0.63178
C	3.56319	-1.59026	-1.9702
Zn	1.58748	-1.94414	0.23707
C	2.41203	-4.35225	-1.26103
H	3.74158	-3.98038	0.41826
H	4.55657	-4.05729	-1.14711
C	2.60319	-0.39506	-2.00473
H	3.27736	-2.33699	-2.70831
H	4.55646	-1.23874	-2.26731
N	1.16589	-3.53494	-1.14532
N	1.2753	-0.7143	-1.42911
H	2.25277	-5.30624	-0.75535
H	2.59043	-4.57991	-2.31457
H	2.50678	-0.0334	-3.03475
H	3.01569	0.41911	-1.40713
C	0.70636	-2.93781	-2.43736
H	0.41698	-4.12044	-0.78889
C	0.35045	-1.45125	-2.31769
H	0.83024	0.15351	-1.14463
H	-0.1791	-3.46576	-2.79094
H	1.49068	-3.07785	-3.18023
H	-0.64684	-1.35265	-1.8924
H	0.32808	-1.00579	-3.31913
O	-2.05855	0.08355	3.12368
C	-2.70911	1.18685	2.61879
C	-3.9924	0.99282	2.09186

C	-2.13075	2.46218	2.65784
C	-4.68538	2.06893	1.5533
H	-4.42146	-0.00128	2.05912
C	-2.82222	3.53899	2.11927
H	-1.14065	2.58482	3.07439
C	-4.08331	3.32778	1.55879
H	-5.66379	1.93654	1.11129
H	-2.39396	4.53224	2.1202
N	-4.77382	4.44524	0.93207
O	-5.92112	4.2638	0.51536
O	-4.17301	5.52041	0.83538
C	5.30829	4.94587	-0.83185
H	4.57853	5.47775	-0.20971
H	6.07302	5.68787	-1.09775
C	4.62077	4.46617	-2.12428
H	5.37525	4.06542	-2.81186
H	4.18394	5.33663	-2.63145
C	3.53008	3.40338	-1.92111
H	3.96928	2.52602	-1.4291
H	3.18647	3.05101	-2.90243
C	2.3178	3.87942	-1.11286
H	1.79071	4.65924	-1.67843
H	2.64814	4.3496	-0.17843
Zn	-2.31353	-1.84409	0.62984

IM3:

	x	y	z
C	3.48848	-1.58732	0.26729
H	3.46731	-0.65816	-0.3056
H	3.0535	-1.37163	1.24589
C	4.927	-2.0847	0.44429
H	4.94092	-2.91292	1.16015
H	5.31299	-2.48075	-0.50257
C	5.87588	-0.97564	0.9281
H	5.54409	-0.59985	1.90511
H	6.86607	-1.41924	1.08891
C	5.99351	0.18882	-0.06073
H	5.05331	0.75024	-0.07122
H	6.11794	-0.2131	-1.07665
C	7.14647	1.15791	0.22258
H	8.09553	0.61165	0.15031
H	7.07942	1.52592	1.256
C	7.14917	2.34687	-0.75253
H	8.13106	2.83569	-0.75124
H	7.0083	1.9565	-1.76852
C	6.06899	3.39419	-0.43488

H	5.16805	2.89301	-0.06291
H	6.41842	4.02068	0.39539
C	1.76671	2.23036	-1.05175
H	1.41924	1.53866	-1.83105
H	2.32933	1.61706	-0.33476
C	0.56353	2.85408	-0.33243
H	0.05814	2.08595	0.26154
H	0.92598	3.59181	0.39476
C	-0.46285	3.53438	-1.25427
H	-1.27133	3.9261	-0.62742
H	-0.00755	4.40185	-1.74689
C	-1.07189	2.61248	-2.32492
H	-0.32873	2.38184	-3.09959
H	-1.88228	3.14936	-2.83338
C	-1.60477	1.30458	-1.7354
H	-0.76932	0.73802	-1.31273
H	-2.25599	1.54298	-0.88568
C	-2.37139	0.3991	-2.70921
H	-2.43335	-0.59575	-2.26478
H	-1.82783	0.28474	-3.6554
C	-3.79182	0.90781	-2.98967
H	-3.80673	1.64155	-3.79987
P	0.21194	-1.05364	2.58753
O	-0.52731	-1.26486	1.19229
O	0.8533	0.26577	2.80335
O	-0.81545	-1.55426	3.74195
C	-0.6966	-2.99249	3.87644
H	-1.05159	-3.26157	4.87085
H	-1.31623	-3.47628	3.11569
C	0.79637	-3.30053	3.67401
H	0.92977	-4.28697	3.22513
C	1.63536	-3.14988	4.92957
H	2.697	-3.23415	4.68604
H	1.45698	-2.17731	5.39749
H	1.37762	-3.93564	5.6457
O	1.23678	-2.32408	2.68071
H	-4.20854	1.39059	-2.10331
S	-4.99731	-0.36492	-3.54344
C	-5.17639	-1.49262	-2.07872
C	-4.33624	-2.77719	-2.11264
H	-6.24684	-1.70135	-2.03511
H	-3.73619	-2.88062	-3.01944
H	-4.94671	-3.67998	-2.0198
C	-4.75837	-0.817	-0.76493
C	-3.4204	-2.66387	-0.90097
O	-5.26135	0.19302	-0.29508
O	-2.55493	-3.47615	-0.58726
N	-3.70127	-1.51308	-0.20255

N	2.55953	-2.52458	-0.43707
C	2.52797	-3.86546	0.20049
C	2.86766	-2.60985	-1.89354
Zn	0.49208	-1.90723	-0.36363
C	1.32056	-4.72902	-0.26262
H	2.46089	-3.68468	1.27207
H	3.45417	-4.41471	0.00385
C	2.08369	-1.58689	-2.71983
H	2.65155	-3.61973	-2.23648
H	3.93395	-2.45065	-2.07273
N	0.19694	-3.93709	-0.82966
N	0.63126	-1.59992	-2.41096
H	0.9509	-5.28255	0.60231
H	1.64348	-5.47093	-0.99648
H	2.25547	-1.77981	-3.78421
H	2.44063	-0.57817	-2.49957
C	0.0339	-4.05035	-2.30843
H	-0.68749	-4.19017	-0.39793
C	-0.17288	-2.69656	-3.00912
H	0.23337	-0.71653	-2.71645
H	-0.82913	-4.68014	-2.53436
H	0.91079	-4.55231	-2.71675
H	-1.21518	-2.39108	-2.90978
H	0.04889	-2.80544	-4.07608
O	-2.34863	0.62345	2.44345
C	-2.41267	1.92037	2.19977
C	-3.42071	2.49312	1.38084
C	-1.45499	2.77934	2.79804
C	-3.46411	3.85819	1.1661
H	-4.14848	1.83559	0.91537
C	-1.49712	4.14322	2.58214
H	-0.6691	2.32782	3.3918
C	-2.50266	4.6834	1.76643
H	-4.22579	4.30131	0.53707
H	-0.75973	4.80319	3.02105
N	-2.53496	6.10006	1.52531
O	-3.41037	6.55623	0.77274
O	-1.68508	6.81738	2.07627
C	5.68042	4.29579	-1.6161
H	4.99701	5.07121	-1.24981
H	6.56943	4.82774	-1.98
C	5.02606	3.56245	-2.80502
H	5.78849	2.99324	-3.3505
H	4.65097	4.31451	-3.51153
C	3.88648	2.60334	-2.42651
H	4.29325	1.78616	-1.81945
H	3.50109	2.12895	-3.3387
C	2.72217	3.25466	-1.67208

H	2.17716	3.92	-2.35373
H	3.10446	3.89344	-0.86646
Zn	-2.55002	-0.73219	1.14353

TS:

	x	y	z
C	4.86792	-1.05088	1.03606
H	4.54685	-0.0272	0.83111
H	4.66158	-1.21483	2.09535
C	6.37764	-1.19102	0.74072
H	6.86337	-1.73102	1.55964
H	6.54084	-1.79991	-0.15558
C	7.05933	0.17666	0.54525
H	6.91394	0.78369	1.44956
H	8.14151	0.02794	0.4462
C	6.53626	0.95641	-0.66764
H	5.45604	1.10381	-0.56259
H	6.67385	0.35724	-1.57839
C	7.18657	2.33091	-0.87098
H	8.22297	2.19334	-1.20302
H	7.24033	2.85674	0.09255
C	6.42063	3.20567	-1.88017
H	7.07476	4.00423	-2.25264
H	6.16089	2.59298	-2.75346
C	5.15747	3.84813	-1.28613
H	4.55647	3.08561	-0.77561
H	5.46761	4.55009	-0.50127
C	0.27602	2.54475	-1.47814
H	0.1833	1.59822	-2.02838
H	0.7859	2.31492	-0.53385
C	-1.13135	3.05293	-1.1383
H	-1.52495	2.43701	-0.32476
H	-1.0594	4.06889	-0.72887
C	-2.13994	3.04997	-2.3007
H	-3.11686	3.34776	-1.89778
H	-1.86773	3.81461	-3.0389
C	-2.28674	1.69846	-3.02362
H	-1.40012	1.51162	-3.64413
H	-3.13235	1.75829	-3.72043
C	-2.47327	0.50682	-2.07919
H	-1.59801	0.44292	-1.42493
H	-3.3243	0.68506	-1.41036
C	-2.65358	-0.8479	-2.78368
H	-2.32956	-1.63871	-2.10663
H	-1.99473	-0.91757	-3.65722
C	-4.10201	-1.12915	-3.20573

H	-4.33675	-0.69632	-4.18215
P	-0.43213	0.38303	2.21024
O	-0.28308	-0.77692	1.15869
O	0.03936	1.76067	1.93562
O	-0.35389	-0.19576	3.70378
C	0.5073	-1.33029	3.9957
H	0.31618	-1.57536	5.04144
H	0.20109	-2.16936	3.36312
C	1.96573	-0.94445	3.72479
H	2.55194	-1.87944	3.76174
C	2.50619	0.01424	4.78607
H	3.53506	0.29298	4.54212
H	1.90027	0.92511	4.81398
H	2.49586	-0.44401	5.78089
O	2.02577	-0.32977	2.46479
H	-4.80777	-0.71799	-2.48239
S	-4.50175	-2.9135	-3.43031
C	-4.55503	-3.63486	-1.70633
C	-3.46986	-4.69626	-1.4632
H	-5.56671	-4.02149	-1.58041
H	-2.95104	-5.02054	-2.36618
H	-3.87941	-5.58525	-0.97204
C	-4.27964	-2.58645	-0.62488
C	-2.49356	-4.02101	-0.5077
O	-5.00516	-1.64655	-0.33282
O	-1.3884	-4.44085	-0.18022
N	-3.05164	-2.84612	-0.04652
N	3.94114	-1.93392	0.28166
C	3.92908	-3.33723	0.73512
C	4.04989	-1.78613	-1.1853
Zn	1.91126	-1.30072	0.83696
C	2.66924	-4.10621	0.24654
H	3.93154	-3.30533	1.82813
H	4.82473	-3.88799	0.41945
C	3.1858	-0.636	-1.71492
H	3.76191	-2.72538	-1.65229
H	5.08248	-1.60553	-1.4967
N	1.47962	-3.23427	0.01327
N	1.81516	-0.65093	-1.16334
H	2.41607	-4.84688	1.00749
H	2.893	-4.6597	-0.66881
H	3.17347	-0.67138	-2.81058
H	3.63111	0.31605	-1.4244
C	1.13379	-3.04474	-1.4298
H	0.66174	-3.65249	0.45319
C	0.8602	-1.58205	-1.79739
H	1.43032	0.28792	-1.21339
H	0.2456	-3.6334	-1.6636

H	1.94673	-3.43743	-2.03974
H	-0.12653	-1.28938	-1.44223
H	0.8682	-1.48089	-2.8893
O	-2.17697	0.35931	2.12411
C	-2.98336	1.45868	1.92419
C	-4.16727	1.27303	1.19711
C	-2.65685	2.71519	2.45314
C	-4.99968	2.35707	0.95325
H	-4.43905	0.2964	0.81355
C	-3.48855	3.79841	2.20504
H	-1.74673	2.84656	3.01955
C	-4.64612	3.61214	1.4489
H	-5.91003	2.23967	0.38049
H	-3.24956	4.78091	2.58991
N	-5.50769	4.75254	1.17513
O	-6.52961	4.56494	0.50786
O	-5.17594	5.8552	1.62079
C	4.27941	4.59881	-2.30212
H	3.54207	5.2003	-1.75582
H	4.90626	5.31471	-2.8501
C	3.54689	3.70245	-3.31685
H	4.28071	3.08114	-3.84413
H	3.08207	4.33533	-4.08411
C	2.47375	2.79156	-2.70196
H	2.89196	2.29925	-1.81489
H	2.23557	1.98527	-3.40812
C	1.16493	3.48467	-2.29947
H	0.63899	3.81942	-3.20312
H	1.3742	4.38649	-1.70999
Zn	-2.01639	-1.5581	0.89928