

Supporting Information for:

**Gas-Phase Chemical Dynamics Simulations on the Bifurcating Potential
Energy Surface of the Pimaradienyl Cation Rearrangement. Role of
Enzymatic Steering in Abietic Acid Biosynthesis**

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Contents:

S2 B3LYP/6-31G(d) coordinates and energies for **1-8**, **TS₁₋₇** and **TS₇₋₈**

1

E_h = -781.7181544

ZPEC = 0.491473

Coordinates

C	-1.57976489	2.69715954	0.17567345
C	-0.21224337	3.37111572	0.43690477
C	0.78702026	2.25315716	0.83863761
C	-0.33361312	0.62047497	-0.78634464
C	-1.51187872	1.61373516	-0.90949872
H	-1.95313956	2.28802134	1.12241146
H	-1.39484383	2.10438165	-1.88266964
H	-2.46009141	1.07392034	-0.95739832
H	-2.30641807	3.45775409	-0.13285137
H	-0.05003660	0.25965370	-1.78027448
C	-0.33341063	4.38926995	1.58886809
H	-1.01192494	5.20241376	1.31024841
H	-0.73186216	3.91663443	2.49430514
H	0.63819899	4.83396814	1.82833514
C	0.25400343	4.08497327	-0.81689223
C	1.37361070	3.87668536	-1.51505264
C	0.85467876	1.12608274	-0.11918783
H	1.78831049	2.64281966	1.04878361
C	2.10351278	0.35717059	-0.27051940
H	2.32845553	0.20505139	-1.33310447
H	2.95492161	0.84654953	0.20863302
H	-0.43007370	4.86343120	-1.15792801
H	1.59195645	4.45159656	-2.41003700
H	0.42695688	1.81911574	1.78958998
H	2.13933604	3.16128835	-1.22271028
C	1.86255417	-1.06896851	0.35777160
H	2.76760184	-1.64367825	0.14893568
H	1.78948094	-0.97683393	1.44587480
C	0.62245844	-1.72545360	-0.25212065
C	-0.65999793	-0.86135260	-0.03044675
C	-1.83831468	-1.48637389	-0.81021246
H	-2.76457119	-0.93532057	-0.61958049
H	-1.63917806	-1.42103255	-1.88828134
C	-2.04008547	-2.96670717	-0.43267756
C	0.48014941	-3.26359341	0.08315677
C	-0.77154059	-3.78946619	-0.66431834
H	-2.37559367	-3.05398616	0.60723965
H	-2.85799324	-3.36453596	-1.04462205
H	-0.94451152	-4.83273049	-0.37300978
H	-0.55430271	-3.80413917	-1.74214096
H	0.77731613	-1.72181729	-1.34215959
C	-1.06450195	-0.61782621	1.43076275
H	-0.22761789	-0.34743024	2.08144090
H	-1.81725119	0.17317107	1.49717326
H	-1.52055362	-1.51091751	1.85946717
C	0.40166842	-3.59230588	1.58901391
H	1.24124084	-3.16363594	2.14765533
H	-0.52314607	-3.25836916	2.06462091
H	0.45272986	-4.67847381	1.72216948
C	1.70859059	-4.00823687	-0.49045445
H	1.53212779	-5.08875295	-0.45613488
H	1.89626250	-3.73947010	-1.53716101
H	2.62153272	-3.81683435	0.08345943

2⁺

E_h = -781.6639772

ZPEC = 0.486547

Coordinates

C	1.53375490	-2.56940887	0.34350442
C	0.20917855	-3.36483907	0.45538073
C	-0.98754927	-2.42099625	0.27269417
C	0.35981621	-0.52354828	-0.74935013
C	1.52530079	-1.54561540	-0.80005006
H	1.68636457	-2.06720945	1.30378851
H	1.47303253	-2.07898616	-1.75859180
H	2.48401371	-1.02254189	-0.81484446
H	2.37277104	-3.26470533	0.21755441
H	0.13323399	-0.24068561	-1.78834297
C	0.15363477	-4.12559210	1.81054190
H	0.98407374	-4.83393833	1.89299669
H	0.23817080	-3.41020169	2.63350596
H	-0.78402244	-4.67900851	1.92291051
C	0.10797939	-4.36077392	-0.67273805
C	-1.06688378	-4.45631004	-1.38671954
C	-0.90656093	-1.12873128	-0.20646966
H	-1.21412811	-3.07207631	-1.12189498
C	-2.13302202	-0.26876351	-0.26125052
H	-2.39841007	-0.11474679	-1.31777244
H	-2.98310181	-0.76393166	0.22015739
H	1.01376948	-4.86507443	-1.01153804
H	-1.07700349	-4.96220040	-2.34971624
H	-1.92140491	-2.71471184	0.75442554
H	-2.03690411	-4.48388157	-0.88117872
C	-1.86443445	1.11925321	0.36583295
H	-2.75410491	1.73153983	0.19774374
H	-1.75802103	1.01631203	1.45108386
C	-0.62077558	1.77186347	-0.25940212
C	0.65631958	0.87985170	-0.03684180
C	1.85339052	1.54853523	-0.75826082
H	2.77795943	0.99450240	-0.55862494
H	1.68673436	1.50281488	-1.84484541
C	2.04789626	3.01701102	-0.35604469
C	-0.48766674	3.31027165	0.04919102
C	0.79129621	3.84032177	-0.64617828
H	2.32278897	3.08927934	0.70338471
H	2.89707608	3.42823283	-0.91443922
H	0.94756457	4.88672763	-0.35565715
H	0.62243143	3.84600979	-1.73320338
H	-0.77978031	1.74609538	-1.35050622
C	1.01287140	0.63807735	1.44473696
H	0.22291206	0.11472732	1.99442363
H	1.92630429	0.03909239	1.52488961
H	1.20838893	1.57057541	1.97284774
C	-0.47299723	3.67363538	1.55090626
H	-1.31177700	3.22212088	2.09218621
H	0.44912793	3.38633990	2.06206450
H	-0.56909050	4.75972618	1.66059644
C	-1.69120570	4.04699762	-0.58576650
H	-1.52174900	5.12902568	-0.55303134
H	-1.82909204	3.76729063	-1.63750745
H	-2.63021027	3.85615543	-0.05514308

3⁺

E_h = -781.6963881

ZPEC = 0.48972

Coordinates

C	1.49819309	-2.57277789	0.36113627
C	0.08519056	-3.32871139	0.54585807
C	-1.05150379	-2.34890240	0.38624087
C	0.31097749	-0.53184135	-0.74627955
C	1.47450253	-1.55676062	-0.77966755
H	1.63664398	-2.09666009	1.33690587
H	1.44623910	-2.09442251	-1.73596278
H	2.43953580	-1.04060098	-0.76661788
H	2.31481365	-3.29241434	0.23512413
H	0.09593446	-0.28356824	-1.79608387
C	0.12587357	-4.02239400	1.95603359
H	1.00351421	-4.66848906	2.05899858
H	0.17103722	-3.23827392	2.71607595
H	-0.77560357	-4.61878642	2.12521546
C	0.12451956	-4.38842224	-0.43291225
C	-0.75329114	-4.54702266	-1.57652773
C	-0.96460854	-1.13228210	-0.18181221
H	-1.31312336	-3.64254318	-1.82192856
C	-2.17812405	-0.24349984	-0.29085575
H	-2.44267686	-0.14966095	-1.35537142
H	-3.03806703	-0.70143723	0.21100662
H	0.85989997	-5.17984646	-0.26069367
H	-0.27273602	-5.02592822	-2.43684482
H	-2.01360905	-2.69068218	0.76815889
H	-1.48993500	-5.30172082	-1.21338151
C	-1.91116412	1.16558597	0.26996256
H	-2.77758966	1.79145027	0.03762213
H	-1.85024453	1.11339131	1.36267416
C	-0.63195710	1.78756010	-0.31923790
C	0.62470502	0.86960253	-0.06377698
C	1.84193835	1.52602592	-0.76302180
H	2.75548600	0.94810966	-0.57525135
H	1.68028071	1.51300507	-1.85184848
C	2.06845354	2.97726255	-0.31784344
C	-0.47573017	3.32126439	0.00978641
C	0.84261649	3.84296805	-0.61693857
H	2.31448335	3.01007553	0.75075435
H	2.94377352	3.38365041	-0.83855609
H	1.01474290	4.87258919	-0.27781015
H	0.71590020	3.89795085	-1.70815992
H	-0.75714374	1.76807755	-1.41553296
C	0.94738651	0.63348459	1.42632612
H	0.14627276	0.09801760	1.94526730
H	1.86719086	0.04371467	1.52575182
H	1.12126901	1.56163183	1.96807461
C	-0.52054759	3.66161412	1.51724158
H	-1.38837532	3.21416533	2.01351625
H	0.37365457	3.34986360	2.06249472
H	-0.60420170	4.74695846	1.64279235
C	-1.63237501	4.10036887	-0.66131122
H	-1.44631722	5.17766880	-0.58156249
H	-1.71982719	3.85953238	-1.72790019
H	-2.60094858	3.90908914	-0.18746878

4

E_h = -781.7629426

ZPEC = 0.492378

Coordinates

C	1.44104960	-2.71074239	-0.80245803
C	0.13875134	-3.22932792	-0.28446919
C	-0.89749031	-2.33473602	-0.04098547
C	0.54794789	-0.32839769	-0.61340784
C	1.73105003	-1.27849007	-0.34722648
H	2.25567875	-3.39055759	-0.52864686
H	2.62626208	-0.91040610	-0.85359695
H	1.95676924	-1.30019407	0.72378435
H	1.37571253	-2.76928620	-1.90414405
H	0.52123919	-0.10130110	-1.69518261
C	0.57637810	-5.04137399	1.31946233
H	-0.03525231	-4.59455660	2.10937520
H	0.56356502	-6.12807431	1.44635776
H	1.60855812	-4.69826180	1.43760181
C	-0.00524261	-4.70702679	-0.09138852
C	-1.42701757	-5.26773841	-0.24339458
C	-0.77236068	-0.97248002	-0.32998963
H	-1.39024065	-6.35962847	-0.18767975
C	-2.00250408	-0.14254243	-0.46453686
H	-2.18856172	-0.09984116	-1.55355215
H	-2.86752264	-0.65812033	-0.03366911
H	0.65311538	-5.19166530	-0.82552877
H	-2.09246604	-4.92546561	0.55636415
H	-1.87445946	-2.71343646	0.24234533
H	-1.87059423	-4.99658992	-1.20694931
C	-1.87504526	1.30930129	0.04712188
H	-2.73278320	1.86821675	-0.33485875
H	-1.96409462	1.31180061	1.13778547
C	-0.55373748	1.95162714	-0.40107013
C	0.66363530	1.09554781	0.09773783
C	1.98397104	1.75238415	-0.37143275
H	2.84253679	1.21134447	0.04371511
H	2.05615541	1.66741806	-1.46639766
C	2.07454285	3.23703900	0.00438360
C	-0.49076613	3.50655741	-0.15009621
C	0.90258177	4.02064619	-0.59146892
H	2.10793019	3.35407691	1.09454125
H	3.02162526	3.64192981	-0.37076731
H	0.98642639	5.08371360	-0.33414129
H	0.96806650	3.96440704	-1.68818232
H	-0.52036553	1.86850048	-1.50026067
C	0.68733160	0.88724295	1.62923073
H	1.58508614	0.34432671	1.94075120
H	0.69937949	1.83733221	2.16193091
H	-0.17789904	0.32249214	1.99510290
C	-0.78272137	3.94501976	1.30255555
H	0.00965903	3.68119424	2.00749606
H	-0.88264208	5.03569737	1.33507255
H	-1.72215278	3.52729942	1.68046616
C	-1.54390680	4.18997989	-1.05401658
H	-1.40269070	5.27620023	-1.03202498
H	-1.45224553	3.86733925	-2.09844371
H	-2.57053890	3.99583338	-0.72491531

5

$E_h = -781.7456302$

$ZPEC = 0.493627$

Coordinates

C	-1.69879311	2.59884214	0.17969112
C	0.75962613	3.33051865	0.53726343
C	1.43830574	2.20469362	0.07812100
C	-0.35694811	0.56536026	-0.88653765
C	-1.50641759	1.58866783	-0.95554976
H	-1.76165210	2.09733017	1.14952406
H	-1.38367331	2.13797086	-1.89689952
H	-2.43787167	1.03152801	-1.08047500
H	-2.67173764	3.08273926	0.03269340
H	-0.31937214	0.11266198	-1.88531520
C	1.54626618	4.31247799	1.34903222
H	2.62657948	4.17288074	1.27355600
H	1.28826569	5.34630328	1.09506734
H	1.26026993	4.18215497	2.40516623
C	-0.66015968	3.72837070	0.27073890
C	-0.66060285	4.64231406	-0.99577383
C	1.01515040	1.05296896	-0.60844075
H	-0.33396284	4.10127709	-1.88753866
C	2.08863141	0.09600930	-1.02228545
H	1.99922893	-0.06824284	-2.10508079
H	3.08638124	0.49810922	-0.82696231
H	-0.96086067	4.37787925	1.10379924
H	-1.67992782	5.00531474	-1.16005754
H	2.50750487	2.22172876	0.27887202
H	-0.00976859	5.51210963	-0.87051589
C	1.91420991	-1.28371977	-0.31710872
H	2.63836957	-1.96520475	-0.77022964
H	2.19542041	-1.18131292	0.73587760
C	0.48403757	-1.81464856	-0.46726956
C	-0.56411924	-0.77042627	0.05842010
C	-1.98936837	-1.31024665	-0.19940091
H	-2.73640953	-0.63757239	0.23693665
H	-2.17626814	-1.33746800	-1.28251902
C	-2.19025478	-2.72742906	0.36429920
C	0.30732409	-3.30461667	0.02021496
C	-1.16974334	-3.71016125	-0.21272567
H	-2.14155551	-2.71431581	1.45961312
H	-3.20535163	-3.05799400	0.11468163
H	-1.33361294	-4.71127936	0.20498271
H	-1.34218888	-3.79748150	-1.29547061
H	0.28882149	-1.88075656	-1.54924767
C	-0.40252616	-0.40916158	1.54765164
H	-0.64316223	-1.25962472	2.18507756
H	0.60908500	-0.08500155	1.80884753
H	-1.08813830	0.39339869	1.83157824
C	0.71771186	-3.56747844	1.48556022
H	0.04586212	-3.11529319	2.21855682
H	0.70956527	-4.64707532	1.67251034
H	1.73285377	-3.21513451	1.69906463
C	1.18282909	-4.21825196	-0.87012138
H	0.92826338	-5.26771745	-0.68540812
H	1.02004085	-4.02318106	-1.93716775
H	2.25228820	-4.10836268	-0.66085242

6

E_h = -781.7416459

ZPEC = 0.492674

Coordinates

C	1.60927864	-2.51985416	0.67664250
C	0.34610780	-3.35926919	0.53859473
C	-0.89831883	-2.50388088	0.00090898
C	0.57387255	-0.51617550	-0.63683621
C	1.78985347	-1.46147184	-0.42187949
H	1.59503634	-2.04947832	1.66516556
H	2.03290109	-1.95390305	-1.36942940
H	2.67408618	-0.86886323	-0.18275325
H	2.47232653	-3.19760378	0.66525171
H	0.53348772	-0.27279775	-1.71169070
C	0.01932307	-4.23409593	1.73510877
H	0.01390042	-3.63962919	2.65362684
H	-0.94507929	-4.73950270	1.64845720
H	0.79314404	-5.00441792	1.83729949
C	-0.10793589	-3.69178181	-0.80012483
C	-0.96136943	-4.87655739	-1.18259303
C	-0.74742825	-1.16236339	-0.35086034
H	-1.56789132	-4.65108314	-2.06479003
C	-1.98241259	-0.32922780	-0.47256139
H	-2.15991118	-0.24471691	-1.55945270
H	-2.84849831	-0.85859118	-0.06259036
H	0.47458484	-3.29144283	-1.62399850
H	-0.29625927	-5.71035455	-1.44130231
H	-1.88256551	-2.83627379	0.31567819
H	-1.62177104	-5.21208438	-0.38038460
C	-1.85629148	1.09628636	0.09789459
H	-2.73427053	1.65906634	-0.22805081
H	-1.90355057	1.05417462	1.19076548
C	-0.56159708	1.76591339	-0.37996548
C	0.68995226	0.92750056	0.06339472
C	1.96508116	1.62013696	-0.48287211
H	2.86548320	1.10979922	-0.12395453
H	1.97343471	1.53927564	-1.58007028
C	2.04776498	3.10490032	-0.10418978
C	-0.52301445	3.31900774	-0.11307433
C	0.83050717	3.87260373	-0.62157508
H	2.14636380	3.21731874	0.98245431
H	2.96382355	3.52720270	-0.53338648
H	0.90611581	4.93298605	-0.35089822
H	0.83617151	3.83543412	-1.72096849
H	-0.56298582	1.69589490	-1.48085313
C	0.81283706	0.72606315	1.58860968
H	-0.03898434	0.18633407	2.01747553
H	1.71813473	0.15958809	1.82939849
H	0.89082571	1.67574392	2.11690114
C	-0.74999622	3.72940638	1.35913226
H	0.08636679	3.48109329	2.01707846
H	-0.88238804	4.81569966	1.41351192
H	-1.65429081	3.27635342	1.77983792
C	-1.63803962	3.98830139	-0.95149886
H	-1.51616283	5.07677052	-0.92607301
H	-1.59708488	3.67742798	-2.00269629
H	-2.64150799	3.77215754	-0.56924745

7

E_h = -781.6998235

ZPEC = 0.487865

Coordinates

C	-0.82458643	2.97299245	-1.54209643
C	-0.70697022	3.34975863	-0.04264593
C	-0.20968147	2.10693928	0.73155922
C	1.22181788	1.53102072	-1.23400060
C	0.51561937	2.51265627	-2.12954891
H	-1.56693103	2.16716017	-1.64087148
H	1.17487675	3.37985709	-2.28335550
H	0.36506178	2.07454248	-3.12514971
H	-1.21270116	3.82551647	-2.11242622
H	2.06425978	0.98859856	-1.66534894
C	-2.09413516	3.76334999	0.49470635
H	-2.46099265	4.66221863	-0.01315874
H	-2.83150740	2.96620614	0.33359325
H	-2.05185621	3.98197591	1.56772533
C	0.22118406	4.54573806	0.09147105
C	1.36901983	4.63642516	0.76396281
C	0.91912853	1.34510728	0.06147256
H	0.09171208	2.39951685	1.74725632
C	1.69236066	0.36508092	0.91876964
H	2.53432711	-0.03814272	0.34637876
H	2.12537462	0.88494069	1.78487813
H	-0.13601214	5.43094102	-0.43861965
H	1.93070840	5.56590124	0.78920849
H	-1.07116223	1.43127790	0.87529142
H	1.80193395	3.80472007	1.31318213
C	0.83257008	-0.79739375	1.47930587
H	1.46350281	-1.45377015	2.08687919
H	0.09215888	-0.37373929	2.16570938
C	0.11390658	-1.58697998	0.36218737
C	-1.27319833	-1.94716497	0.56800918
C	-2.05845095	-2.34084680	-0.61286034
H	-3.12451507	-2.44853188	-0.39786267
H	-1.91143422	-1.63439803	-1.43664131
C	-1.45435142	-3.73190347	-1.06597538
C	0.81506389	-3.07328950	-0.03064866
C	0.05479038	-3.61556752	-1.25822149
H	-1.71200047	-4.49673590	-0.32649323
H	-1.95902464	-4.00408114	-1.99776993
H	0.46135382	-4.60687746	-1.49597973
H	0.26652391	-2.97698722	-2.12513856
H	0.20417955	-1.04580375	-0.58926934
C	-1.88294609	-2.07568893	1.90710079
H	-2.67507131	-2.83089594	1.92968813
H	-1.16034936	-2.23153711	2.71018478
H	-2.38055621	-1.10816277	2.10777329
C	0.77347435	-4.05082087	1.15326556
H	1.22618475	-3.62277767	2.05288003
H	-0.23636323	-4.38553129	1.41031153
H	1.35606581	-4.94268430	0.89783228
C	2.27365684	-2.77381030	-0.40512739
H	2.74260821	-3.70675573	-0.73997995
H	2.34667791	-2.04796388	-1.22060970
H	2.85284119	-2.40738429	0.44613833

8

E_h = -781.6781584

ZPEC = 0.482995

Coordinates

c	2.33662549	-2.14076271	-0.21690882
c	-2.31568912	-1.20088361	-0.63893658
c	2.62575137	-2.59904646	1.15901669
c	0.97691208	-2.12072350	-0.72957540
c	0.23365839	-3.49245087	-0.59896903
c	-1.22499830	-3.37052999	-1.10643270
c	-2.61561993	-3.07758010	1.02720616
c	-3.06722533	-0.13291357	0.10939211
h	0.25062292	-0.02102071	2.04526764
c	-2.21535474	0.58254115	1.20595620
c	0.26986753	0.69699765	1.22386659
c	1.61359523	1.21037607	0.79370636
c	-0.94564458	2.20178764	-0.35639740
c	1.54959723	2.00756101	-0.51604810
c	0.36227947	3.00596876	-0.53440919
c	0.33108666	3.73738237	-1.89390657
c	0.58186314	4.04528041	0.55279829
c	-0.19116005	4.32062677	1.60399312
h	0.07402511	5.10984040	2.30176977
h	-1.11418539	3.78840518	1.81671850
h	1.49320477	4.63116691	0.41565872
h	-0.52934318	4.41256475	-1.95361866
h	1.23592749	4.33825141	-2.03991183
h	0.26344031	3.02325859	-2.72426583
h	2.49285836	2.54343462	-0.67824082
h	1.42687851	1.31833722	-1.36583408
h	-1.19427316	1.72540534	-1.31787829
h	-1.78003624	2.88728073	-0.15718270
h	2.04289595	1.82712369	1.59706869
h	2.31847237	0.36423559	0.68375023
c	-0.90048475	1.13574473	0.71878198
h	-2.83004901	1.39786618	1.61305174
h	-2.03357058	-0.12051551	2.02687341
h	-3.95365372	-0.54736581	0.60234341
h	-3.43265873	0.61267122	-0.60502298
h	-3.19307664	-2.36941911	1.62481881
c	-2.08221669	-2.47042091	-0.24790311
h	-3.26526249	-3.93309691	0.79979985
h	-1.80841606	-3.46486427	1.66401480
h	-1.21007232	-3.01643543	-2.14367980
h	-1.63619955	-4.38886117	-1.12377009
h	0.76921071	-4.24247325	-1.19212667
h	0.24428137	-3.83054588	0.44195513
h	3.56449192	-2.58363701	-1.85539685
h	0.94615061	-1.77197348	-1.76662056
h	0.38845174	-1.38495401	-0.11662236
h	4.41817640	-1.66843861	-0.58581163
h	3.23125766	-0.87788740	-1.68481408
h	3.40345840	-1.98216664	1.62395022
h	3.06210013	-3.61206980	1.09083798
h	1.74233942	-2.65363292	1.79745196
h	-1.89670238	-0.89370921	-1.59818521
c	3.46411096	-1.77985517	-1.10405226

TS₁₋₇
E_h = -781.6993368
ZPEC = 0.487809

Coordinates

c	-0.77350022	-1.54558097	-1.45930444
c	1.15049478	1.81834731	0.40207122
c	-0.26910994	1.67128840	0.14917971
c	-1.11551346	0.85498181	1.15241779
h	-0.49223062	0.47511464	1.96737272
c	-1.81529969	-0.34100563	0.45687898
c	-0.86366161	-1.35895404	-0.13306981
c	-0.02374426	-2.16520078	0.84263567
c	0.63102101	-3.43219716	0.24517575
c	1.77223879	-3.90174027	1.17340235
c	1.21192781	-3.06980702	-1.14577598
c	0.13227479	-2.55766154	-2.10771740
c	-0.34321702	-4.58779336	0.08398847
c	-1.64203975	-4.62824284	0.38269129
c	-0.77616603	3.26516243	-0.06940093
c	0.09452252	3.86256095	-1.19524077
h	2.16577031	4.07907888	-1.84190656
c	1.59843276	3.74596890	-0.96750247
c	-0.68096262	4.07410030	1.23167005
c	-2.23872548	3.18290033	-0.53385692
c	1.74552779	1.73687840	1.75104047
h	2.65572296	2.33716197	1.84158822
h	1.04289028	1.95402411	2.55816214
h	2.05557173	0.68256943	1.87945151
h	1.93068227	4.35306224	-0.11921537
h	0.34779788	4.26033365	1.55591792
h	-1.21225426	3.58606834	2.05476457
h	-1.15500784	5.05007401	1.08035502
h	-0.16954041	4.92269596	-1.29942320
h	-0.16779588	3.38302572	-2.14679569
h	-2.90151412	2.77944870	0.23572823
h	-2.58725187	4.19709062	-0.76210977
h	-2.34550975	2.57866214	-1.44027403
h	-1.87339204	1.48486630	1.62626625
h	-0.39722384	1.26948306	-0.86173377
h	1.76520589	1.67334695	-1.63407808
h	-2.45645718	-0.81933304	1.21025487
h	-2.48437923	0.04062300	-0.32414717
h	-1.42942400	-0.97801107	-2.12137365
h	-2.18458382	-3.77727620	0.78551589
h	-2.22302333	-5.53349548	0.23086105
h	-0.48207895	-3.39782524	-2.46393844
h	0.11950445	-5.48877903	-0.32389194
h	1.71895032	-3.94096382	-1.57795722
h	1.98231299	-2.29618913	-1.00985418
h	1.39838293	-4.11209860	2.18176499
h	2.55705792	-3.13778138	1.24911506
h	2.23715342	-4.81824726	0.79338046
h	0.78114466	-1.53012320	1.25110094
h	-0.63276747	-2.44074519	1.71480717
c	2.00072146	2.23142565	-0.72276746
h	3.06859506	2.16161137	-0.50196155
h	0.59560770	-2.12872998	-3.00650175

TS₇₋₈

E_h = -781.6692554

ZPEC = 0.482955

Coordinates

h	-1.65190963	4.24205040	-1.93449314
c	-1.04179632	3.70680226	-1.19500261
c	0.48321992	4.12625138	-1.49296731
h	0.48690679	4.55127399	-2.50003288
c	-1.62597235	5.59378664	0.40171872
c	-1.43664976	4.15651499	0.13327011
c	-1.68144090	3.19324332	1.21794988
h	-1.73019964	3.64279419	2.21179824
h	-0.96784714	2.36383234	1.17364102
h	-0.96278187	5.90164880	1.22538220
h	-2.64143539	5.74216800	0.80484042
h	-1.47233433	6.23631346	-0.46618579
h	0.80281772	4.92436981	-0.81601287
h	-1.15010672	2.62722464	-1.31870744
c	1.44374258	2.92531491	-1.42408783
c	1.62697754	2.28533971	-0.06220717
c	2.33286427	3.13329142	0.97188639
c	1.25003212	1.00499585	0.12325136
c	1.39849927	0.14647476	1.34944735
c	0.14250402	-0.71753526	1.64650492
c	-0.20674569	-1.71782613	0.56586083
c	-1.35004835	-1.63180245	-0.13050633
c	-1.76499123	-2.60987341	-1.19712355
c	-0.58973653	-3.47066686	-1.67887675
c	0.79835466	-2.82661938	0.30954791
c	0.25064499	-4.02459687	-0.49956530
c	1.43416062	-4.84672707	-1.05494770
c	-0.61855009	-4.95928361	0.32499484
c	-0.95254713	-4.86478250	1.61260644
h	2.41256652	3.30871405	-1.78094874
h	1.12103272	2.17464107	-2.15409411
h	1.87769142	4.12818310	1.08001967
h	3.37547831	3.30926364	0.67434640
h	2.35029886	2.67013745	1.96048644
h	0.80358375	0.48601659	-0.72673224
h	1.63745004	0.74452762	2.23530230
h	2.25635137	-0.52596543	1.20205476
h	-0.71799379	-0.05823766	1.82826579
h	0.32838294	-1.24855624	2.59089783
h	-2.05708619	-0.83467928	0.10814597
h	-2.56219568	-3.25410917	-0.79641355
h	-2.21339148	-2.07529908	-2.04602628
h	0.06901864	-2.86771690	-2.31981937
h	-0.95830085	-4.29853326	-2.29733330
h	2.04581098	-4.24166905	-1.73576280
h	1.07949745	-5.72159561	-1.61194371
h	2.07743471	-5.20640002	-0.24394217
h	-0.99293139	-5.81467694	-0.24166113
h	-1.57337708	-5.61963933	2.08732113
h	-0.62876467	-4.04510645	2.24821605
h	1.20778713	-3.18256518	1.26534709
h	1.66180552	-2.41298787	-0.23417964
h	-2.66838771	2.74078285	0.99768800