Supporting Information

Quantum Mechanical Predictions of the Stereoselectivities of Proline-Catalyzed Asymmetric Intermolecular Aldol Reactions

S. Bahmanyar,† K. N. Houk,*† Harry J. Martin,‡ Benjamin List*‡

†*Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095-1569;*

‡*Department of Molecular Biology, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, CA 92037*

Synthesis of aldols syn-2a and anti-2a. (S)- or (rac)-proline (35 mg, 0.3 mmol) in 10 mL of DMSO/cyclohexanone (4:1) was treated with benzaldehyde (1 mmol) at room temperature. The mixture was stirred for 4 days and worked up in the usual manner using aq. NH_4Cl solution and ethyl acetate. Chromatography on silica using hexane/ethyl acetate (5:1) furnished known aldols *syn*-**2a** (87 mg, 0.425 mmol, ($[\alpha]_D$ = - 63°) and *anti*-**2a** (87 mg, 0.425 mmol, ($[\alpha]_D$ = + 12°). ee-Determination: *syn*-diastereomer, Chiralpak AD, 5% i-PrOH/hexanes, t_r (*syn*-**2a**) = 14.7 min, area = 132463 , t_r (ent-*syn*-**2a**) = 11.3 min, area = 18565; er = 7.1, ee = 75±5%. anti-diastereomer, Chiralpak AS, 5% i-PrOH/hexanes, t_r (*anti*-**2a**) = 13.8 min, area = 168010, t_r (ent-*anti*-**2a**) = 16.3 min, area = 13933; er = 12.1, ee = 85±5%.

To ascertain whether or not there is a potential epimerization under the reaction conditions, both diastereomers anti-**2a** and syn-**2a** were prepared and separated. Subsequently both diastereomers were exposed to the original reaction conditions (vide supra) in deutero-DMSO and the mixtures were monitored by ^{1}H-NMR spectroscopy over a period of 4 days. Within this time no interconversion of the diastereomers was detected.

Synthesis of aldol anti-2b. Similarly, (S)- or (rac)-proline (35 mg, 0.3 mmol) in 10 mL of DMSO/cyclohexanone (4:1) was treated with isobutyraldehyde (1 mmol) at room temperature. The mixture was stirred for 5 days and worked up in the usual manner using aq. NH_4Cl solution and ethyl acetate. Chromatography on silica using hexane/ethyl acetate (5:1) furnished known aldol *anti*-**2b** as a single diastereomer (116 mg, 0.68 mmol). ee-Determination: Chiralpak AD-RH, 20% H_2O (0.1% TFA)/CH_3CN, t_r (*anti*-**2b**) = 11.6 min, area = 128954, t_r (ent-*anti*-**2b**) = 7.4 min, area = 2236, er = 57.7, ee = 97±3%.

Synthesis of hydrazone 5. Aldol anti-**2b** (170 mg, 1 mmol) in EtOH (5 mL) was treated with p-toluenesulfonylhydrazide (380 mg, 2 mmol) at room temperature. The mixture was stirred for 1 h, concentrated, and chromatographed on silica using hexane/ethyl acetate (4:1) to give hydrazone **5** as a solid (314 mg, 0.93 mmol). Recrystallization from MeOH furnished crystals suitable for X-ray crystallography. The Flack parameter was 0.02(11) confirming the proposed absolute configuration.

Coordinates for transition state geometries for the reaction of proline enamine of acetone (3a-d) and cyclohexanone (4a-d) with acetaldehyde.

Transition state 3a

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	2.308552	-0.449049	-0.526562
2	1	-2.070629	2.833417	0.786070
3	1	-0.708800	-1.278818	2.483528
4	1	1.028298	-1.562852	2.730063
5	1	-1.687483	3.242704	-0.895098
6	6	-2.315998	1.154301	-0.577505
7	1	-2.089593	0.944032	-1.628893
8	1	-3.401773	1.165614	-0.462758
9	1	0.228516	-2.134002	1.254913
10	6	3.696686	0.098366	-0.848612
11	6	1.965090	0.355109	1.154277
12	1	2.182656	1.393917	0.922881
13	7	-0.340806	0.629734	0.640821
14	1	2.355427	-1.503604	-0.191153
15	6	0.265574	-1.318488	1.987862
16	6	0.605561	-0.018466	1.310400
17	8	1.368531	-0.146533	-1.370414
18	1	2.658444	-0.075624	1.873465
19	1	-2.253057	-0.074818	1.229731
20	6	-1.671720	0.067580	0.313485
21	6	-0.182269	2.007865	0.103435
22	6	-1.659862	-1.299921	-0.420517
23	1	3.642102	1.168550	-1.072339
24	1	4.065232	-0.412836	-1.746357
25	1	4.412060	-0.069350	-0.036117
26	8	-2.657427	-1.988847	-0.310051
27	8	-0.617079	-1.615783	-1.151562
28	1	0.214601	-0.924844	-1.229058
29	1	0.342341	2.624562	0.839199
30	6	-1.626205	2.452654	-0.141374
31	1	0.402650	1.965413	-0.816957

HF=-671.691581
ZPE=0.264253
Sum of electronic and thermal Enthalpies= -671.412470
Sum of electronic and thermal Free Energies= -671.467463

Transition state 3b

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	-2.307084	-0.496221	-0.817948
2	1	2.819564	-2.240991	0.636941
3	1	0.019217	0.695238	2.794836
4	1	-1.748154	0.607978	2.631861
5	1	2.741115	-2.494618	-1.115244
6	6	2.597538	-0.387604	-0.484203
7	1	2.413703	-0.108865	-1.527860
8	1	3.607292	-0.064076	-0.223684
9	1	-0.793734	1.602646	1.519106
10	1	0.483500	-2.838764	0.393660
11	6	-1.821963	-1.295421	0.804172
12	1	-1.638794	-2.308788	0.457524
13	7	0.468930	-0.725317	0.529257
14	6	-3.155195	0.730887	-0.483286
15	6	-0.809186	0.660611	2.078350
16	6	-0.677784	-0.529128	1.166299
17	8	-1.247441	-0.317217	-1.562113

18	1	-2.663282	-1.235109	1.491424
19	1	1.955943	0.502500	1.411470
20	6	1.542268	0.288878	0.421188
21	6	0.828480	-1.978863	-0.187628
22	6	1.099361	1.652809	-0.181035
23	6	2.352848	-1.889499	-0.291107
24	1	0.339674	-1.978959	-1.163479
25	1	-2.944921	-1.336972	-1.140373
26	8	1.787469	2.617685	0.103835
27	8	0.064932	1.680399	-0.980927
28	1	-0.492929	0.751583	-1.226009
29	1	-3.602257	1.094587	-1.416584
30	1	-2.548306	1.546528	-0.079830
31	1	-3.965526	0.497664	0.216256

HF=-671.6895025
ZPE=0.263854
Sum of electronic and thermal Enthalpies= -671.410930
Sum of electronic and thermal Free Energies= -671.465305

Transition state 3c

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	-0.588296	-1.816314	-0.897483
2	1	0.357745	-1.211110	-1.087551
3	8	-2.204393	-2.307601	0.570087
4	6	2.195420	-0.976167	-0.152010
5	1	1.970254	-1.943337	0.324555
6	6	3.677652	-0.654808	-0.183980
7	1	2.391256	0.375068	1.952147
8	8	1.519985	-0.692297	-1.224363
9	1	-3.533284	-0.174316	0.454684
10	1	4.163469	-0.853076	0.776514
11	6	-1.059736	1.799253	-0.741276
12	1	1.037479	3.168313	0.194869
13	6	-1.375959	-0.115732	0.747544
14	1	-2.501619	0.487576	-1.695164
15	6	-1.376553	-1.543348	0.097620
16	6	1.605973	2.233912	0.165722
17	6	0.825194	1.065510	0.694866
18	6	1.512241	0.053052	1.401320
19	6	-2.729155	0.561799	0.461019
20	7	-0.410909	0.891873	0.238587
21	1	2.529665	2.366496	0.730847
22	1	0.924704	-0.698766	1.920119
23	1	-1.208490	-0.256649	1.817523
24	1	3.853688	0.385860	-0.474363
25	6	-2.478035	1.234673	-0.895091
26	1	-2.946539	1.314166	1.229518
27	1	4.145108	-1.290752	-0.946546
28	1	1.866342	2.023251	-0.881277
29	1	-0.489070	1.809131	-1.673367
30	1	-1.082897	2.818351	-0.336045
31	1	-3.202062	2.017508	-1.136913

HF=-671.6852618
ZPE=0.263291
Sum of electronic and thermal Enthalpies= -671.407157
Sum of electronic and thermal Free Energies= -671.462237

Transition state 3d

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0.113765	-1.845450	0.869225
2	1	-0.618680	-1.050637	1.099444
3	8	1.672655	-2.587808	-0.544575
4	6	-2.454115	-0.143443	0.373972

5	6	-3.083781	-1.454777	-0.087018
6	1	0.849929	1.785777	1.667555
7	1	-2.399633	0.933536	-1.827212
8	8	-1.597047	-0.177370	1.348756
9	1	3.342782	-0.774019	-0.553742
10	1	1.577347	2.659759	0.299648
11	6	1.371186	1.665820	0.714169
12	1	-0.376212	3.467359	-0.347255
13	6	1.228396	-0.290304	-0.748573
14	1	2.573831	0.105349	1.629157
15	6	0.977584	-1.692046	-0.091925
16	6	-1.131835	2.690458	-0.194510
17	6	-0.666209	1.338833	-0.656681
18	6	-1.603367	0.464990	-1.254267
19	6	2.701625	0.107169	-0.537466
20	7	0.512765	0.902903	-0.226175
21	1	-2.043542	2.980637	-0.719447
22	1	-1.232824	-0.454099	-1.700268
23	1	0.985075	-0.404264	-1.807592
24	1	3.531717	1.458200	1.004674
25	6	2.655703	0.832251	0.814001
26	1	3.023663	0.793769	-1.330166
27	1	-3.193508	0.672924	0.443244
28	1	-1.352946	2.637611	0.880021
29	1	-3.738752	-1.814440	0.717061
30	1	-2.317555	-2.216721	-0.256014
31	1	-3.686137	-1.329749	-0.993349

HF=-671.686075
ZPE=0.263568
Sum of electronic and thermal Enthalpies= -671.407661
Sum of electronic and thermal Free Energies= -671.462979

Transition state 3e

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	-2.340876	0.226928	-0.728952
2	1	2.700841	-2.420722	-1.404657
3	1	-0.022939	0.284317	2.760084
4	1	-4.209186	-0.847652	-1.102027
5	1	2.284331	-0.792549	-1.952608
6	6	2.777467	-0.860015	0.158114
7	1	3.662483	-0.249220	-0.019277
8	1	3.015297	-1.629054	0.902611
9	1	-1.290422	1.067907	1.759632
10	1	-2.756669	-1.417033	1.062183
11	6	-1.916028	-1.291824	0.384389
12	1	-1.825785	-2.104698	-0.331548
13	7	0.440244	-0.836350	0.375907
14	6	-3.858473	0.148710	-0.811619
15	6	-0.925575	0.110757	2.173077
16	6	-0.735696	-0.783377	0.990912
17	8	-1.852503	1.346253	-0.283054
18	1	-4.200758	0.872896	-1.561395
19	1	1.693198	0.216340	1.725454
20	6	1.615138	0.008136	0.657125
21	6	0.714549	-1.733155	-0.777853
22	6	1.610411	1.394739	-0.085310
23	1	-1.706040	-0.289290	2.824397
24	1	-1.848878	-0.186968	-1.628015
25	1	-4.305286	0.426852	0.148226
26	8	2.680651	1.978915	-0.102787
27	8	0.525400	1.839609	-0.655856
28	1	-0.501205	1.503941	-0.462187
29	1	0.516044	-2.764752	-0.465322
30	6	2.197735	-1.493866	-1.116429
31	1	0.052976	-1.496278	-1.614035

HF=-671.6822377
ZPE=0.263073
Sum of electronic and thermal Enthalpies= -671.404177
Sum of electronic and thermal Free Energies= -671.460313

Transition state 3f

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	-2.614019	0.412880	-0.295520
2	1	2.658081	-2.161641	-1.641947
3	1	-0.058803	-0.604860	2.907824
4	1	0.409343	-2.599429	-0.937175
5	1	2.287061	-0.467401	-1.980862
6	6	2.679183	-0.827638	0.120046
7	1	3.556420	-0.184378	0.056628
8	1	2.908570	-1.693042	0.753020
9	1	-1.214958	0.581181	2.214769
10	1	-2.804759	-1.754129	0.847952
11	6	-2.006910	-1.369501	0.217578
12	1	-1.909530	-1.911251	-0.718587
13	7	0.341741	-0.884325	0.274887
14	6	2.150365	-1.274302	-1.254533
15	6	-0.960019	-0.486071	2.302613
16	6	-0.816747	-1.012302	0.908167
17	8	-1.976098	1.369423	0.318641
18	1	0.029953	-1.115220	-1.825735
19	1	1.524966	0.024968	1.783381
20	6	1.486302	-0.058107	0.696114
21	6	0.645956	-1.534020	-1.027629
22	6	1.442390	1.407960	0.110397
23	1	-1.793587	-0.983942	2.802976
24	6	-2.509240	0.387773	-1.818348
25	1	-3.648152	0.269572	0.054514
26	8	2.517092	1.985164	0.066206
27	8	0.316829	1.908516	-0.305585
28	1	-0.719610	1.562683	-0.027310
29	1	-1.464807	0.449451	-2.138252
30	1	-3.014057	1.284864	-2.198670
31	1	-2.984473	-0.492023	-2.264152

HF=-671.6782541
ZPE=0.262671
Sum of electronic and thermal Enthalpies= -671.400610
Sum of electronic and thermal Free Energies= -671.456668

Transition state 3g

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	4.637649	-0.971647	-0.182752
2	1	2.335634	-0.243320	-1.203473
3	6	0.498803	1.464346	-0.037381
4	6	1.652658	1.093203	0.683488
5	7	-0.662040	0.797780	0.005548
6	6	0.570132	2.651385	-0.970102
7	1	0.048783	3.517782	-0.542702
8	1	0.116592	2.438265	-1.943547
9	1	1.611639	2.940139	-1.124639
10	6	-1.954761	1.305872	-0.505760
11	6	-3.008739	0.752092	0.487887
12	6	-2.239109	-0.221017	1.417183
13	6	-0.919511	-0.489854	0.684652
14	1	-0.079261	-0.753870	1.329511
15	1	-2.129919	0.923289	-1.516003
16	1	-1.938153	2.396017	-0.541071
17	1	-3.470897	1.563710	1.057605
18	1	-3.789895	0.224730	-0.059522

19	1	-2.793466	-1.143590	1.596647
20	1	-2.023829	0.250225	2.382355
21	6	-1.105702	-1.576548	-0.427646
22	8	-2.215325	-1.767808	-0.896285
23	8	-0.028141	-2.200472	-0.837182
24	6	2.567322	-0.471257	-0.147011
25	8	2.042603	-1.519594	0.369940
26	1	1.518012	0.579447	1.629556
27	6	4.012301	-0.167215	0.225132
28	1	0.848824	-1.938753	-0.312835
29	1	4.139539	-0.166067	1.312051
30	1	4.359104	0.785191	-0.188359
31	1	2.410467	1.870942	0.713920

HF=-671.6850158
ZPE=0.265114
Sum of electronic and thermal Enthalpies= -671.404767
Sum of electronic and thermal Free Energies= -671.461050

Transition state 3h

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	1.335847	0.663218	1.985119
2	6	1.628734	1.118104	1.044245
3	6	0.598882	1.471044	0.145562
4	1	2.385853	1.890751	1.155711
5	7	-0.555383	0.801442	0.030423
6	6	0.805038	2.640959	-0.788280
7	1	0.231047	3.514077	-0.451334
8	1	0.492693	2.412806	-1.812389
9	1	1.858476	2.926878	-0.798821
10	6	-1.764339	1.301968	-0.662741
11	6	-2.946127	0.784954	0.198769
12	6	-2.315707	-0.166008	1.248292
13	6	-0.914918	-0.465805	0.702381
14	1	-0.166662	-0.722313	1.454629
15	1	-1.807682	0.889305	-1.675235
16	1	-1.731850	2.390201	-0.728362
17	1	-3.470853	1.616197	0.678949
18	1	-3.653752	0.246545	-0.431611
19	1	-2.899561	-1.078421	1.380180
20	1	-2.222694	0.331671	2.219712
21	6	-0.967904	-1.579842	-0.396515
22	8	-2.009355	-1.781914	-0.997084
23	8	0.150793	-2.217387	-0.650717
24	6	2.666606	-0.466840	0.495179
25	8	2.012049	-1.505489	0.864509
26	1	3.436415	0.704878	-1.185275
27	1	3.695381	-1.050426	-1.284724
28	1	2.085370	-0.395004	-1.597793
29	6	2.982774	-0.271532	-0.983725
30	1	3.504453	-0.172569	1.151311
31	1	0.949072	-1.941580	-0.025707

HF=-671.6851704
ZPE=0.265398
Sum of electronic and thermal Enthalpies= -671.404770
Sum of electronic and thermal Free Energies= -671.460447

Transition state 4a

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	1.350917	-1.248179	1.191522
2	1	-2.498020	-0.778511	-2.848188
3	1	0.191317	2.382293	-1.047972
4	6	2.108795	2.261155	-0.033011
5	1	-2.948406	-2.270007	-2.003207

6	6	-3.070600	-0.443080	-0.774822
7	1	-3.302539	-1.066983	0.095818
8	1	-3.985446	0.075566	-1.068064
9	1	0.066877	2.026267	0.661883
10	1	2.157783	3.348619	-0.156085
11	6	1.634593	-0.542602	-0.552453
12	1	1.493457	-1.472110	-1.099004
13	7	-0.706663	-0.142953	-0.794012
14	1	1.740369	-0.389989	1.770779
15	6	0.654163	1.803989	-0.234934
16	6	0.514341	0.341424	-0.598365
17	8	0.097519	-1.560579	1.378260
18	6	3.045382	0.041087	-0.693885
19	1	-2.053934	1.482456	-0.984866
20	6	-1.953850	0.559281	-0.405860
21	6	-1.000259	-1.454971	-1.430841
22	6	-2.058596	0.959856	1.095183
23	1	2.722992	1.720355	-2.036114
24	6	2.300528	-2.442865	1.220610
25	1	4.068912	1.940913	-0.917890
26	8	-2.860828	1.842206	1.354883
27	8	-1.332348	0.318127	1.966661
28	1	-0.679526	-0.554761	1.650112
29	1	-0.303818	-1.620652	-2.257911
30	6	-2.453837	-1.301552	-1.885256
31	1	-0.877894	-2.248486	-0.691354
32	6	3.050406	1.544131	-1.001264
33	1	3.592128	-0.507857	-1.469517
34	1	3.605810	-0.116786	0.238813
35	1	2.423801	2.049123	0.997124
36	1	3.322742	-2.195793	0.919332
37	1	1.914000	-3.240854	0.578592
38	1	2.329397	-2.826200	2.247630

HF=-788.4244823
ZPE=0.329355
Sum of electronic and thermal Enthalpies= -788.078249
Sum of electronic and thermal Free Energies= -788.137657

Transition state 4b

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	1.181331	-0.560621	1.845867
2	1	-2.834165	-2.172296	-1.705144
3	1	0.139425	1.235493	-2.036474
4	1	4.308188	0.227868	-1.499893
5	1	-3.369886	-2.696108	-0.098740
6	6	-3.144738	-0.514542	-0.329371
7	1	-3.340542	-0.393014	0.741923
8	1	-4.024482	-0.167837	-0.875650
9	1	0.937703	1.747078	-0.564161
10	1	3.143916	-1.821791	-1.105111
11	6	1.486848	-1.121637	0.067086
12	1	1.185501	-2.155025	0.229877
13	7	-0.779309	-0.668037	-0.530317
14	6	1.956644	0.722326	2.137376
15	6	0.901642	0.940776	-1.309309
16	6	0.504244	-0.348133	-0.629537
17	8	-0.107194	-0.537993	2.087443
18	6	3.336696	0.324512	-1.000629
19	1	-1.945802	0.609070	-1.765031
20	6	-1.890317	0.297454	-0.717783
21	6	-1.291046	-2.023571	-0.182370
22	6	-1.769703	1.592305	0.134851
23	1	2.193066	0.087923	-2.826766
24	1	3.459612	1.086254	-0.222251
25	1	1.698098	-1.434290	2.277691

26	8	-2.314207	2.589552	-0.310030
27	8	-1.143568	1.519615	1.277617
28	1	-0.692574	0.537537	1.638036
29	1	-0.702100	-2.777764	-0.712813
30	6	-2.753133	-1.966268	-0.630989
31	1	-1.195554	-2.175363	0.893753
32	1	3.600009	-1.245612	0.483588
33	6	2.948870	-1.024648	-0.372631
34	1	2.554124	1.765520	-2.430259
35	6	2.273288	0.800368	-1.993906
36	1	3.019235	0.642308	1.891016
37	1	1.875311	0.908355	3.215431
38	1	1.522072	1.588625	1.631026

HF=-788.4239176
ZPE=0.332505
Sum of electronic and thermal Enthalpies= -783.777762
Sum of electronic and thermal Free Energies= -783.835591

Transition state 4c

Center No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	1.228810	1.805739	0.269788
2	1	-3.049918	-0.495726	2.923997
3	1	0.038450	-1.490428	-1.763058
4	6	2.076795	-2.090648	-1.231102
5	1	-2.951503	0.851059	1.780955
6	6	-3.002691	-1.078800	0.792356
7	1	-3.986954	-0.868195	0.374592
8	1	-2.959280	-2.134407	1.086446
9	1	1.184970	-0.151713	-1.730797
10	1	1.688965	-3.115469	-1.223394
11	6	1.631258	0.001900	0.859648
12	1	1.520363	0.104786	1.937588
13	7	-0.708218	-0.565294	0.590654
14	6	2.452042	2.610005	0.685027
15	6	0.890342	-1.084228	-1.217613
16	6	0.550680	-0.619953	0.163438
17	8	0.914379	1.841138	-0.990162
18	6	3.027933	-0.411041	0.396767
19	1	-1.761843	-1.629629	-0.910843
20	6	-1.909671	-0.778266	-0.242734
21	6	-1.085346	-0.238629	1.992073
22	6	-2.311758	0.435345	-1.157159
23	1	2.742948	-2.510768	0.798401
24	1	0.388959	1.946505	0.974359
25	1	4.057041	-2.193343	-0.330711
26	8	-3.448809	0.396906	-1.597744
27	8	-1.465726	1.390090	-1.429567
28	1	-0.406861	1.480594	-1.165423
29	1	-0.713781	-1.040871	2.642403
30	6	-2.618520	-0.175045	1.971786
31	1	-0.629355	0.698022	2.315594
32	6	3.044253	-1.881297	-0.049444
33	1	3.751146	-0.238778	1.200433
34	1	3.346793	0.213801	-0.449363
35	1	2.607767	-1.964942	-2.181186
36	1	3.308385	2.384920	0.043413
37	1	2.725866	2.443899	1.732673
38	1	2.211860	3.672177	0.552124

HF=-788.4118021
Zero-point correction= 0.329351
Sum of electronic and thermal Enthalpies= -788.065450
Sum of electronic and thermal Free Energies= -788.125765

Transition state 4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		1.277752	2.008049	0.074493
2	1		-2.902556	-0.952922	2.822604
3	1		0.414512	-1.523528	-1.740397
4	6		2.496674	-1.811962	-1.123954
5	1		-2.982503	0.412956	1.700728
6	6		-2.719182	-1.483125	0.684008
7	1		-3.715051	-1.416376	0.246748
8	1		-2.519139	-2.525333	0.960827
9	1		1.362850	-0.036920	-1.748648
10	1		2.250729	-2.879810	-1.129739
11	6		1.701631	0.292428	0.848425
12	1		1.517462	0.445898	1.909473
13	7		-0.524416	-0.624690	0.546932
14	1		2.310522	2.388787	0.157708
15	6		1.183971	-0.976007	-1.196540
16	6		0.738165	-0.502786	0.150993
17	8		0.841500	1.899523	-1.149544
18	6		3.165402	-0.003561	0.502112
19	1		-1.377573	-1.792514	-1.006808
20	6		-1.664295	-0.995183	-0.318064
21	6		-0.978600	-0.387272	1.944902
22	6		-2.226217	0.178722	-1.203901
23	1		3.052217	-2.107987	0.958546
24	6		0.344258	2.706876	1.062365
25	1		4.407277	-1.697778	-0.089641
26	8		-3.353438	0.005408	-1.637938
27	8		-1.514360	1.243449	-1.449062
28	1		-0.452341	1.445648	-1.232254
29	1		-0.506460	-1.143125	2.584839
30	6		-2.502637	-0.554477	1.886137
31	1		-0.676377	0.596532	2.301448
32	6		3.352415	-1.476403	0.111481
33	1		3.804162	0.259245	1.352392
34	1		3.492963	0.626343	-0.337658
35	1		3.066574	-1.617819	-2.039406
36	1		0.700604	2.659431	2.097288
37	1		-0.673033	2.311255	0.994495
38	1		0.290430	3.762010	0.766544

HF=-788.4082285
Zero-point correction= 0.329534
Sum of electronic and thermal Enthalpies= -788.061872
Sum of electronic and thermal Free Energies= -788.121767

Coordinates for transition state geometries for the reaction of proline enamine of cyclohexanone with benzaldehyde (5a-d) and Isobutyraldehyde. Those geometries marked with a prime (') indicate different conformation of cyclohexanone ring which leads to a higher energy transition state.

Transition state 5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		0.989496	-0.183294	0.740706
2	1		-3.368334	-1.286850	-2.733077
3	1		-2.307714	2.441306	-0.512028
4	6		-0.406512	3.216950	0.196411
5	1		-2.870411	-2.921192	-2.260290
6	6		-3.598110	-1.663433	-0.599567
7	1		-3.329672	-2.465873	0.096882
8	1		-4.687032	-1.638435	-0.672070
9	1		-1.836875	1.830564	1.062129
10	1		-0.930441	4.162889	0.372375

11	6	0.474241	0.728673	-0.916567
12	1	0.727076	-0.101443	-1.570001
13	7	-1.735090	-0.183118	-0.769513
14	1	0.862252	0.657069	1.439590
15	6	-1.445118	2.090307	0.073052
16	6	-0.913569	0.848546	-0.610634
17	8	0.193504	-1.210662	0.907951
18	6	1.287142	1.995045	-1.196163
19	1	-3.694888	0.509278	-0.365849
20	6	-3.040542	-0.319359	-0.078570
21	6	-1.480205	-1.338102	-1.668461
22	6	-2.969050	-0.320190	1.482131
23	1	-0.171252	3.426834	-1.938369
24	6	2.432457	-0.503320	0.485743
25	1	1.141003	4.152526	-1.013777
26	8	-4.036742	-0.131756	2.048237
27	8	-1.824886	-0.542248	2.046886
28	1	-0.842604	-0.894211	1.431539
29	1	-0.960761	-0.994780	-2.567291
30	6	-2.887123	-1.874674	-1.942101
31	1	-0.855259	-2.071914	-1.154568
32	6	0.469160	3.287422	-1.055423
33	1	1.712968	1.929661	-2.204830
34	1	2.149454	2.038834	-0.519504
35	1	0.227507	3.045577	1.076416
36	6	5.134305	-1.130696	0.049495
37	6	3.445339	0.344137	0.952832
38	6	2.789450	-1.681259	-0.186568
39	6	4.129207	-1.990340	-0.405800
40	6	4.789514	0.034178	0.734615
41	1	3.182038	1.238682	1.512582
42	1	2.005359	-2.357793	-0.512458
43	1	4.393889	-2.907742	-0.925161
44	1	5.564358	0.697912	1.108844
45	1	6.179466	-1.375292	-0.119859

HF=-980.1617752
Zero-point correction= 0.381626
Sum of electronic and thermal Enthalpies= -979.759866
Sum of electronic and thermal Free Energies= -979.828378
Total free energy in sol.(with non electrost.terms) (a.u.) = -980.173941

Transition state 5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0.769305	0.155401	-1.576398
2	1	-4.612836	1.487720	-0.489060
3	1	-1.190212	0.398994	2.384311
4	1	2.370227	2.818002	1.969493
5	1	-4.596046	0.734945	-2.093500
6	6	-3.953124	-0.586331	-0.447773
7	1	-3.688345	-1.353369	-1.184373
8	1	-4.861157	-0.909975	0.065422
9	1	0.244629	-0.308575	1.664763
10	1	0.897893	3.585011	0.234711
11	6	0.146036	1.716604	-0.486660
12	1	-0.318399	2.212500	-1.336351
13	7	-1.960470	0.659794	-0.079761
14	6	2.017070	-0.389678	-0.945166
15	6	-0.326701	0.625316	1.753306
16	6	-0.772301	1.047372	0.373136
17	8	-0.263004	-0.614269	-1.818211
18	6	1.743001	2.050642	1.499921
19	1	-3.155224	-0.068456	1.516749

20	6	-2.784762	-0.405937	0.544153
21	6	-2.616013	1.209822	-1.295442
22	6	-2.035756	-1.751623	0.774950
23	1	-0.042612	2.601716	2.603444
24	1	2.370402	1.161797	1.374075
25	1	1.017803	0.812426	-2.419279
26	8	-2.445488	-2.446711	1.693632
27	8	-1.081642	-2.052227	-0.051722
28	1	-0.680241	-1.300292	-0.938802
29	1	-2.483513	2.295504	-1.321701
30	6	-4.075969	0.780046	-1.132230
31	1	-2.157098	0.768768	-2.183120
32	1	2.111045	2.607633	-0.564234
33	6	1.264124	2.552122	0.129776
34	1	0.907060	1.335476	3.376374
35	6	0.558248	1.703111	2.404750
36	6	4.424974	-1.361986	0.137205
37	6	2.016595	-1.519835	-0.109523
38	6	3.244485	0.219169	-1.255227
39	6	4.438655	-0.255975	-0.714879
40	6	3.213642	-1.994242	0.427544
41	1	1.086870	-2.037987	0.103766
42	1	3.265011	1.061618	-1.943150
43	1	5.378052	0.228116	-0.968668
44	1	3.198605	-2.870194	1.070673
45	1	5.353390	-1.738273	0.558535

HF=-980.1615863
Zero-point correction= 0.382514
Sum of electronic and thermal Enthalpies= -979.759241
Sum of electronic and thermal Free Energies= -979.825437
Total free energy in sol.
(with non electrost.terms) (a.u.) = -980.172836

Transition state 5b' (higher energy transition state than 5b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0.811538	0.148866	-1.616920
2	1	-4.561557	1.526765	-0.309514
3	1	-1.099889	0.969700	2.429880
4	6	1.035587	1.289321	2.173036
5	1	-4.696466	0.757222	-1.900633
6	6	-3.978435	-0.571445	-0.291623
7	1	-3.817236	-1.356230	-1.039541
8	1	-4.851297	-0.849553	0.302572
9	1	-0.247709	-0.434227	1.829950
10	1	1.081376	1.301172	3.267789
11	6	0.132928	1.752331	-0.521057
12	1	-0.350675	2.177194	-1.395898
13	7	-1.927595	0.620704	-0.079394
14	6	2.023624	-0.406158	-0.943898
15	6	-0.300557	0.656921	1.742871
16	6	-0.738990	1.044945	0.347733
17	8	-0.235277	-0.591104	-1.888947
18	6	1.231576	2.636298	0.064386
19	1	-2.979876	-0.120149	1.603520
20	6	-2.717863	-0.439607	0.590262
21	6	-2.644729	1.167089	-1.259148
22	6	-1.989404	-1.816401	0.714195
23	1	0.346232	3.325273	1.924914
24	1	2.102037	3.173039	1.978418
25	1	1.078395	0.817928	-2.440844
26	8	-2.395498	-2.548074	1.608968
27	8	-1.073393	-2.083275	-0.155988
28	1	-0.631769	-1.264399	-1.069747
29	1	-2.479496	2.246663	-1.320331

30	6	-4.102937	0.792021	-0.982264
31	1	-2.266222	0.697061	-2.170192
32	6	1.189380	2.699086	1.598854
33	1	1.139881	3.645688	-0.355863
34	1	2.219560	2.268333	-0.239858
35	1	1.868065	0.665636	1.829147
36	6	4.386247	-1.400173	0.212007
37	6	3.266334	0.191831	-1.216063
38	6	1.983440	-1.532307	-0.103011
39	6	3.158983	-2.017809	0.468556
40	6	4.438783	-0.295894	-0.639531
41	1	3.316744	1.031067	-1.906407
42	1	1.040493	-2.036546	0.086438
43	1	3.115408	-2.891722	1.113028
44	1	5.390364	0.178032	-0.864946
45	1	5.297124	-1.786740	0.661305

HF=-980.1586241
Zero-point correction= 0.382621
Sum of electronic and thermal Enthalpies= -979.756077
Sum of electronic and thermal Free Energies= -979.822990
Total free energy in sol.(with non electrost.terms) (a.u.) = -980.169312

Transition state 5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	-2.060362	-2.181809	-0.390469
2	1	-1.025135	-1.606081	-0.856537
3	8	-3.462322	-2.237173	1.370075
4	6	0.713370	-1.153755	-0.035051
5	1	1.831492	0.368625	2.389376
6	1	-1.969100	0.967015	-2.282499
7	6	1.125949	1.093670	1.968602
8	8	-0.007492	-1.180296	-1.131771
9	1	-4.988970	-0.375844	0.348431
10	1	-2.699479	2.302462	-1.360686
11	6	-2.579476	1.213288	-1.410391
12	6	4.068511	-0.342325	-1.598840
13	6	-2.851705	-0.087297	0.64877
14	1	-3.872750	-0.466922	-1.864406
15	6	-2.762638	-1.653155	0.549586
16	6	4.444072	-1.171369	0.640543
17	6	-0.685875	1.079970	0.195120
18	6	0.037600	0.362572	1.189232
19	6	-4.222184	0.361614	0.107608
20	7	-1.911522	0.726862	-0.174379
21	1	6.019263	-0.558098	-0.699452
22	1	-0.573802	-0.273468	1.826353
23	1	-2.715867	0.179337	1.698503
24	1	-4.703392	1.102185	-1.922433
25	6	-3.945593	0.517914	-1.392898
26	1	-4.512846	1.324602	0.547011
27	6	2.176676	-0.964257	-0.209662
28	1	2.682694	-1.739684	1.739911
29	1	0.653720	1.584282	2.834180
30	1	2.004983	-0.279461	-2.237943
31	1	0.451147	-1.895017	0.727746
32	1	4.457938	0.019703	-2.546767
33	6	0.046084	2.140397	-0.590284
34	1	5.123199	-1.454891	1.440005
35	6	1.889672	2.143507	1.148988
36	6	4.947281	-0.671872	-0.562703
37	6	3.068530	-1.322363	0.812838
38	6	2.693985	-0.492858	-1.427325
39	1	0.668748	1.626279	-1.337616
40	6	0.932833	3.007383	0.323547

41	1	-0.651235	2.772727	-1.144909
42	1	2.595683	1.646794	0.475563
43	1	0.290229	3.599758	0.989576
44	1	1.489583	3.722040	-0.293823
45	1	2.483403	2.773454	1.822297

HF=-980.1568069
Zero-point correction= 0.382765
Sum of electronic and thermal Enthalpies= -979.754132
Sum of electronic and thermal Free Energies= -979.821804
Total free energy in sol.(with non electrost.terms) (a.u.) = -980.169629

Transition state 5c' (higher energy transition state than 5c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		-1.991379	-2.174591	-0.468292
2	1		-0.912373	-1.552840	-0.931409
3	8		-3.392259	-2.364188	1.288227
4	6		0.763141	-1.101766	-0.044763
5	1		2.082022	0.730158	1.869450
6	1		-2.105538	0.920950	-2.264334
7	6		1.109348	1.234331	1.914925
8	8		0.075166	-1.125828	-1.169111
9	1		-4.972850	-0.471760	0.487489
10	1		-2.770890	2.264234	-1.311764
11	6		-2.669466	1.172998	-1.362293
12	1		-0.771898	2.977442	-0.798309
13	6		-2.829421	-0.164241	0.679539
14	1		-3.999839	-0.485271	-1.785025
15	6		-2.708040	-1.723405	0.495284
16	6		-0.070275	2.138344	-0.699961
17	6		-0.717654	1.079843	0.161717
18	6		0.052066	0.421739	1.164240
19	6		-4.230326	0.283915	0.227967
20	7		-1.943948	0.688870	-0.160525
21	6		1.277365	2.646536	-0.156278
22	1		-0.521337	-0.234459	1.813760
23	1		-2.643079	0.061809	1.731037
24	1		-4.822045	1.087952	-1.748329
25	6		-4.038337	0.485183	-1.280957
26	1		-4.507940	1.229936	0.710717
27	6		2.230938	-0.934746	-0.174980
28	1		0.049776	1.722756	-1.710548
29	1		0.836803	1.269239	2.977436
30	1		2.189016	3.111953	1.761645
31	1		0.464888	-1.842835	0.702368
32	1		0.436446	3.293289	1.726369
33	1		1.470033	3.645543	-0.563643
34	1		2.090143	2.000636	-0.504793
35	6		1.266836	2.664316	1.373760
36	6		5.018307	-0.719988	-0.444558
37	6		3.081013	-1.291306	0.883204
38	6		2.797539	-0.488835	-1.379794
39	6		4.180316	-0.378944	-1.510534
40	6		4.465494	-1.182525	0.750933
41	1		2.654459	-1.673642	1.807813
42	1		2.140674	-0.262342	-2.213120
43	1		4.608004	-0.039726	-2.450319
44	1		5.111231	-1.467925	1.576868
45	1		6.096657	-0.639017	-0.550982

HF=-980.15 42104
Zero-point correction= 0.383288
Sum of electronic and thermal Enthalpies= -979.750907
Sum of electronic and thermal Free Energies= -979.819154

Transition state 5d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0.750660	-2.266789	0.694119	
2	1	0.357907	-1.280061	1.183614	
3	8	1.544560	-3.171138	-1.196242	
4	6	-0.997063	0.393357	0.997148	
5	1	-1.985163	1.832337	-1.403423	
6	1	2.871530	0.504071	1.931471	
7	6	-0.928964	2.113131	-1.329959	
8	8	-0.122787	-0.267919	1.706429	
9	1	3.882189	-2.240985	-1.106408	
10	1	3.818798	1.281176	0.639771	
11	6	3.223956	0.398746	0.902175	
12	1	-3.601362	-3.271902	-0.346755	
13	6	2.161170	-0.930115	-0.855757	
14	1	3.675461	-1.687339	1.302990	
15	6	1.404106	-2.232533	-0.425483	
16	6	-3.553081	-2.204550	-0.148009	
17	6	1.131593	1.237395	-0.140054	
18	6	-0.149506	0.964767	-0.696882	
19	6	3.675558	-1.211399	-0.813459	
20	7	2.055071	0.289943	-0.008962	
21	1	-3.384651	1.581834	0.626328	
22	1	-0.226730	0.033999	-1.256082	
23	1	1.813981	-0.686100	-1.861874	
24	1	5.092749	-0.737696	0.818584	
25	6	4.023288	-0.884875	0.644474	
26	1	4.207432	-0.536929	-1.496360	
27	1	-1.199663	1.403691	1.381780	
28	6	-4.696093	-1.414185	-0.296384	
29	1	-0.582588	2.249229	-2.365703	
30	6	-2.346677	-1.638855	0.261320	
31	6	-2.266466	-0.261412	0.522583	
32	1	-5.633792	-1.863072	-0.613306	
33	6	1.342574	2.572794	0.535138	
34	1	-1.469944	-2.265239	0.388797	
35	6	-0.777433	3.439611	-0.572101	
36	1	-5.517592	0.573445	-0.116276	
37	6	-3.423801	0.521390	0.385802	
38	6	-4.630372	-0.047461	-0.022720	
39	1	0.905606	2.505977	1.543499	
40	6	0.692690	3.725795	-0.253142	
41	1	2.406793	2.777110	0.676338	
42	1	-1.349673	3.407482	0.364494	
43	1	1.249196	3.875701	-1.188660	
44	1	0.793550	4.652902	0.323218	
45	1	-1.201863	4.257920	-1.165894	

HF=-980.1582048
Zero-point correction= 0.382074
Sum of electronic and thermal Enthalpies= -979.756153
Sum of electronic and thermal Free Energies= -979.823818
Total free energy in sol.
(with non electrost.terms) (a.u.) = -980.169627

transition state 5d' (higher energy transition state than 5d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		-0.714187	-2.259829	-0.695411
2	1		-0.299018	-1.245880	-1.204011
3	8		-1.656497	-3.218748	1.098424
4	6		1.027260	0.400169	-1.003200
5	1		1.950983	2.146858	0.968356
6	1		-2.871958	0.470833	-1.942889
7	6		0.927073	2.109400	1.360010
8	8		0.156907	-0.266798	-1.716140
9	1		-3.902844	-2.189716	1.141690
10	1		-3.754061	1.334895	-0.663806
11	6		-3.210099	0.413974	-0.904220
12	1		-2.329368	2.933538	-0.238196
13	6		-2.153288	-0.936327	0.836994
14	1		-3.783603	-1.649433	-1.266935
15	6		-1.437512	-2.255048	0.375719
16	6		-1.350626	2.553788	-0.562212
17	6		-1.108722	1.227347	0.123213
18	6		0.162018	0.961260	0.701059
19	6		-3.675022	-1.165947	0.844738
20	7		-2.033500	0.281424	-0.009345
21	6		-0.267113	3.609017	-0.272103
22	1		0.241949	0.016188	1.232352
23	1		-1.766665	-0.705485	1.832262
24	1		-5.129237	-0.627379	-0.733771
25	6		-4.062265	-0.826418	-0.600624
26	1		-4.161895	-0.476412	1.545940
27	1		1.224909	1.409597	-1.388073
28	1		-1.437437	2.376359	-1.642889
29	1		1.032315	1.899951	2.431744
30	1		0.948848	4.281920	1.401072
31	6		2.293575	-0.250419	-0.519893
32	1		-0.597321	3.574599	1.859425
33	1		-0.685066	4.605898	-0.451868
34	1		0.569408	3.493679	-0.972079
35	6		0.247638	3.473898	1.163091
36	6		4.717634	-1.400880	0.316429
37	6		3.464912	0.519261	-0.441210
38	6		2.356664	-1.615449	-0.193986
39	6		3.560591	-2.179655	0.223224
40	6		4.668867	-0.048714	-0.023210
41	1		3.440009	1.565725	-0.737361
42	1		1.468856	-2.233697	-0.280990
43	1		3.596222	-3.237096	0.471339
44	1		5.566973	0.561469	0.025523
45	1		5.653219	-1.848914	0.640679

HF= -980.1557048
Zero-point correction= 0.381761
Sum of electronic and thermal Enthalpies= -979.753801
Sum of electronic and thermal Free Energies= -979.822087

Transition state 6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		1.542332	-0.538754	0.592892
2	1		-2.891192	-0.749604	-2.827437
3	1		-1.355904	2.662233	-0.306924
4	6		0.621754	3.139977	0.457761
5	1		-2.559290	-2.452542	-2.465948

6	6	-3.140668	-1.237688	-0.720316
7	1	-2.940664	-2.101707	-0.076634
8	1	-4.222759	-1.103037	-0.773638
9	1	-0.973578	1.876648	1.210153
10	1	0.214660	4.136253	0.662407
11	6	1.186693	0.621327	-0.855543
12	1	1.307239	-0.097574	-1.661797
13	7	-1.127496	0.034461	-0.800610
14	1	1.660117	0.235684	1.375987
15	6	-0.545912	2.161547	0.243178
16	6	-0.175394	0.924527	-0.546202
17	8	0.570662	-1.395589	0.768694
18	6	2.201183	1.770250	-0.910235
19	1	-3.007917	0.919478	-0.382186
20	6	-2.450124	0.012300	-0.130055
21	6	-1.007618	-1.063589	-1.795968
22	6	-2.414583	-0.070886	1.423949
23	6	2.907379	-1.180960	0.255616
24	1	0.993332	3.417455	-1.656124
25	1	2.336592	3.917053	-0.628429
26	8	-3.433052	0.278064	1.998269
27	8	-1.342367	-0.534219	2.003577
28	1	-0.477145	-0.925285	1.391228
29	1	-0.473275	-0.697324	-2.677336
30	6	-2.464944	-1.432495	-2.082577
31	1	-0.448380	-1.890252	-1.354153
32	6	1.558727	3.154228	-0.750472
33	1	2.762353	1.717536	-1.850499
34	1	2.944769	1.646699	-0.109581
35	1	1.191255	2.846813	1.349362
36	6	3.499911	-1.728482	1.568831
37	1	3.587083	-0.406683	-0.122521
38	6	2.789400	-2.299265	-0.785514
39	1	2.097621	-3.070207	-0.434224
40	1	3.766872	-2.762567	-0.961675
41	1	2.423985	-1.932045	-1.752391
42	1	2.836744	-2.488139	1.995470
43	1	3.627987	-0.934395	2.313968
44	1	4.481214	-2.183993	1.390791

HF=-867.0519234
Zero-point correction= 0.386134
Sum of electronic and thermal Enthalpies= -866.646100
Sum of electronic and thermal Free Energies= -866.711924
Total free energy in sol.(with non electrost.terms) (a.u.) = -867.059742

Transition state 6a' (higher energy transition state than 6a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		-1.495879	-0.744097	-0.534753
2	1		2.833696	-0.503832	2.961715
3	1		1.355719	2.632987	0.092041
4	6		-0.614935	3.066072	-0.713419
5	1		2.558760	-2.236593	2.710984
6	6		3.176046	-1.131951	0.905485
7	1		3.021463	-2.043430	0.317116
8	1		4.251708	-0.964888	0.987360
9	1		0.966190	1.728887	-1.356642
10	6		-2.684037	-1.601296	-0.032187
11	6		-1.203058	0.617837	0.764004
12	1		-1.329652	-0.002647	1.649309
13	7		1.128000	0.085172	0.818894

14	1	-1.783203	-0.082968	-1.376050
15	6	0.541814	2.097287	-0.417130
16	6	0.164794	0.925551	0.465171
17	8	-0.417880	-1.469461	-0.697082
18	6	-2.222933	1.765286	0.679635
19	1	3.001320	0.992692	0.422765
20	6	2.479285	0.055589	0.205248
21	6	0.999953	-0.943060	1.885963
22	6	2.523963	-0.126375	-1.341308
23	1	-2.321199	-2.116490	0.868529
24	6	-2.954870	-2.674148	-1.106255
25	6	-3.988431	-0.871542	0.309961
26	8	3.578208	0.175881	-1.876083
27	8	1.477330	-0.608866	-1.949836
28	1	0.590691	-0.975459	-1.347226
29	1	0.420950	-0.532601	2.718178
30	6	2.454111	-1.249141	2.252270
31	1	0.483488	-1.814383	1.479419
32	6	-1.581041	3.141524	0.467419
33	1	-2.836861	1.774570	1.587184
34	1	-2.916320	1.586462	-0.152099
35	1	-1.163388	2.728264	-1.602314
36	1	-0.199173	4.049390	-0.959084
37	1	-1.041164	3.454975	1.372908
38	1	-2.359648	3.891620	0.285135
39	1	-4.767237	-1.604879	0.549810
40	1	-4.353552	-0.279924	-0.538970
41	1	-3.895090	-0.206591	1.172982
42	1	-3.730346	-3.370621	-0.765384
43	1	-2.044278	-3.233693	-1.328850
44	1	-3.308824	-2.212696	-2.037689

HF=-867.0463083
Zero-point correction= 0.386168
Sum of electronic and thermal Enthalpies= -866.640618
Sum of electronic and thermal Free Energies= -866.706193

Transition state 6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	-1.286350	0.778947	-1.234413
2	1	3.651353	-2.054720	-1.028326
3	1	0.393702	-1.949474	1.936032
4	6	-1.742587	-1.591577	1.796669
5	1	3.958062	-0.828562	-2.271458
6	6	3.541428	-0.019135	-0.261345
7	1	3.559409	0.990655	-0.686822
8	1	4.452258	-0.151039	0.326409
9	1	-0.035721	-0.258357	2.035701
10	1	-1.808522	-1.990143	2.815220
11	6	-0.991954	-1.173112	-0.935808
12	1	-0.623371	-1.287111	-1.951655
13	7	1.281609	-0.772578	-0.312934
14	6	-2.102854	1.495256	-0.136323
15	6	-0.284479	-1.191676	1.516632
16	6	0.036513	-1.079050	0.042721
17	8	-0.094941	1.253299	-1.500042
18	6	-2.213723	-2.052729	-0.654607
19	1	2.465323	-0.871520	1.444074
20	6	2.278996	-0.185013	0.612923
21	6	1.863066	-1.001070	-1.662008
22	6	1.846258	1.182492	1.228198
23	1	-1.587452	-3.507922	0.826042
24	1	-3.247022	-2.962227	1.030075
25	1	-1.888993	0.580584	-2.132703

26	8	2.361477	1.473939	2.299418
27	8	1.026754	1.913543	0.540943
28	1	0.502735	1.548702	-0.513769
29	1	1.463389	-1.931094	-2.076370
30	6	3.366793	-1.055458	-1.379421
31	1	1.598007	-0.174182	-2.323831
32	6	-2.236408	-2.621753	0.776489
33	1	-2.214283	-2.885499	-1.369980
34	1	-3.136000	-1.499412	-0.857204
35	1	-2.384140	-0.704795	1.769605
36	6	-3.589126	1.106415	-0.118935
37	6	-1.979432	3.017631	-0.375828
38	1	-1.653822	1.291334	0.842310
39	1	-4.032577	1.208974	-1.118162
40	1	-4.141379	1.774693	0.551129
41	1	-3.770181	0.085454	0.223666
42	1	-2.356933	3.291781	-1.368912
43	1	-0.943566	3.348788	-0.293409
44	1	-2.574699	3.555892	0.370651

HF=-867.0412505
Zero-point correction= 0.386253
Sum of electronic and thermal Enthalpies= -866.635391
Sum of electronic and thermal Free Energies= -866.700720
Total free energy in sol.(with non electrost.terms) (a.u.) = -867.050269

Transition state 6b' (higher energy transition state than 5b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		1.353061	-0.811114	-1.160133
2	1		-3.611016	1.854938	-1.465858
3	1		-0.691892	1.840958	1.887628
4	6		1.482601	1.838017	1.911573
5	1		-3.736966	0.526879	-2.632616
6	6		-3.507853	-0.110271	-0.533340
7	1		-3.440811	-1.148935	-0.876638
8	1		-4.479823	0.021404	-0.053740
9	1		0.000849	0.240573	2.012216
10	1		1.360914	2.373800	2.859406
11	6		1.030786	1.126574	-0.877860
12	1		0.733706	1.289051	-1.910378
13	7		-1.277306	0.716126	-0.414424
14	6		2.388658	-1.329576	-0.124156
15	6		0.128311	1.211011	1.518400
16	6		-0.067908	1.051634	0.026154
17	8		0.189902	-1.399993	-1.272620
18	6		2.252659	1.959142	-0.469577
19	1		-2.650407	0.934689	1.185828
20	6		-2.353917	0.179863	0.450899
21	6		-1.727243	0.837520	-1.826249
22	6		-1.974091	-1.105992	1.246525
23	1		1.823505	-0.635115	-2.137402
24	1		1.287130	3.568507	0.625162
25	1		2.943983	3.245655	1.138173
26	8		-2.659945	-1.342647	2.230825
27	8		-1.004967	-1.835142	0.788265
28	1		-0.415767	-1.590797	-0.250755
29	1		-1.322467	1.756957	-2.259315
30	6		-3.253417	0.846015	-1.704724
31	1		-1.364013	-0.019033	-2.397892
32	6		2.012894	2.764781	0.815871
33	1		2.517688	2.633435	-1.292675
34	1		3.128324	1.320400	-0.311530
35	1		2.221523	1.048694	2.096898

36	6	2.047332	-2.752892	0.353381
37	1	2.394869	-0.677287	0.757394
38	6	3.795634	-1.314933	-0.748587
39	1	3.847152	-2.020020	-1.588001
40	1	4.548928	-1.619881	-0.013406
41	1	4.081058	-0.329425	-1.132425
42	1	1.086356	-2.793928	0.869049
43	1	2.824760	-3.102111	1.043321
44	1	2.008594	-3.448701	-0.492306

HF=-867.040877

Transition state 6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		-1.664582	-2.090334	-0.230765
2	1		-0.620597	-1.635453	-0.728898
3	8		-2.999839	-1.923356	1.571820
4	6		2.693588	-1.343169	-0.181515
5	1		2.508711	0.330726	2.276987
6	1		-1.381279	0.955297	-2.312983
7	6		1.851947	1.090605	1.835126
8	8		0.446808	-1.311219	-1.047389
9	1		-4.411882	-0.025939	0.466494
10	1		-1.999023	2.381171	-1.446772
11	6		-1.949331	1.285459	-1.439884
12	1		0.025477	2.817084	-1.208222
13	6		-2.250302	0.122944	0.696991
14	1		-3.362870	-0.327327	-1.763347
15	6		-2.286105	-1.445876	0.697554
16	6		0.720636	2.131618	-0.716295
17	6		-0.027720	1.128341	0.130464
18	6		0.680826	0.412801	1.132142
19	6		-3.601235	0.637686	0.162908
20	7		-1.279471	0.819810	-0.197482
21	1		2.314251	3.583884	-0.554951
22	1		0.046382	-0.133235	1.827352
23	1		-2.066507	0.441835	1.724710
24	1		-4.088641	1.288695	-1.896138
25	6		-3.357026	0.686143	-1.350525
26	1		-3.809257	1.643272	0.550851
27	6		2.660094	2.033604	0.933670
28	1		1.228728	1.580151	-1.519263
29	1		1.459737	1.665500	2.688348
30	1		3.335356	2.642344	1.546982
31	6		1.180578	-1.252114	0.032465
32	6		1.734116	2.939736	0.116099
33	1		3.294385	1.455961	0.252181
34	1		0.839938	-1.883788	0.862913
35	1		1.183268	3.608018	0.792432
36	1		3.211150	-0.822392	0.631752
37	6		3.152449	-0.779199	-1.532030
38	6		3.073074	-2.838136	-0.077084
39	1		2.556632	-3.421560	-0.847292
40	1		2.806109	-3.256089	0.900107
41	1		4.152802	-2.966781	-0.215438
42	1		2.964024	0.294315	-1.624493
43	1		2.627549	-1.279489	-2.350640
44	1		4.229211	-0.938251	-1.660142

HF=-867.0399787
Zero-point correction= 0.386671
Sum of electronic and thermal Enthalpies= -866.633744
Sum of electronic and thermal Free Energies= -866.699525
Total free energy in sol.(with non electrost.terms) (a.u.) = -867.051265

Transition state 6c' (higher energy transition state than 6c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		1.576109	-2.200280	-0.296956
2	1		0.549892	-1.822743	0.358245
3	8		3.475600	-1.691311	-1.376635
4	6		-1.288968	-1.267850	-0.140533
5	1		-2.663142	0.420197	-1.994315
6	1		1.217233	0.724566	2.420014
7	6		-1.754167	1.034820	-1.955847
8	8		-0.436005	-1.529277	0.823665
9	1		4.420131	0.204065	-0.276003
10	1		1.706678	2.262057	1.673459
11	6		1.780190	1.170480	1.595234
12	1		-0.170603	2.970150	0.773767
13	6		2.277890	0.166499	-0.588994
14	1		3.350557	-0.297903	1.901661
15	6		2.459546	-1.392928	-0.755174
16	6		-0.792827	2.065123	0.718970
17	6		-0.026521	1.038855	-0.085168
18	6		-0.668070	0.331031	-1.139467
19	6		3.546287	0.779397	0.028760
20	7		1.205145	0.721953	0.302255
21	6		-2.162341	2.425839	0.114702
22	1		0.023270	-0.239765	-1.754685
23	1		2.092243	0.547448	-1.596864
24	1		3.890766	1.374465	2.132479
25	6		3.245578	0.727630	1.531256
26	1		3.673758	1.819581	-0.298115
27	6		-2.755306	-1.183877	0.307135
28	1		-0.901607	1.718843	1.754738
29	1		-1.416926	1.119398	-2.996253
30	1		-3.049036	2.778548	-1.838568
31	1		-1.172205	-1.877383	-1.047396
32	1		-1.331237	3.150885	-1.739296
33	1		-2.470157	3.405024	0.498791
34	1		-2.922011	1.709907	0.445335
35	6		-2.098743	2.433346	-1.415389
36	1		-3.287857	-0.443448	-0.300399
37	6		-2.908292	-0.823379	1.790626
38	6		-3.408139	-2.554126	0.024373
39	1		-2.464478	0.145447	2.036409
40	1		-2.418602	-1.573506	2.417440
41	1		-3.970046	-0.783427	2.059751
42	1		-3.379439	-2.803182	-1.042534
43	1		-4.457258	-2.552051	0.341954
44	1		-2.888259	-3.349072	0.571119

HF=-867.0370081
Zero-point correction= 0.386775
Sum of electronic and thermal Enthalpies= -866.630596
Sum of electronic and thermal Free Energies= -866.697308

Transition state 6d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		-1.474838	1.832959	0.752180
2	1		-0.616043	1.239053	1.163964
3	8		-2.504153	2.269197	-1.189911

4	6	1.425731	0.750437	0.696089
5	1	3.122156	-0.424800	-1.426919
6	1	-1.833835	-1.472163	1.933462
7	1	2.194258	-1.670264	-2.233785
8	8	0.484141	0.665044	1.589308
9	1	-4.024303	0.233328	-1.228700
10	1	-2.190012	-2.690009	0.687655
11	6	-2.152480	-1.615344	0.898020
12	1	-0.224420	-3.170235	0.941873
13	6	-1.880119	0.016308	-0.893017
14	1	-3.655242	-0.075919	1.199624
15	6	-1.936210	1.508244	-0.422978
16	6	0.581190	-2.461407	0.735874
17	6	0.095783	-1.321777	-0.128766
18	6	1.058335	-0.519043	-0.801373
19	6	-3.320861	-0.529876	-0.894661
20	7	-1.181692	-0.961396	-0.021342
21	6	1.783345	-3.206578	0.136394
22	1	0.652199	0.176135	-1.534273
23	1	-1.430733	0.002110	-1.887468
24	1	-4.333739	-1.643985	0.726262
25	6	-3.498574	-0.956047	0.568363
26	1	-3.396003	-1.396836	-1.563023
27	1	2.377686	0.274597	0.987719
28	1	0.850259	-2.006636	1.702413
29	6	2.357739	-1.187970	-1.257356
30	1	3.731046	-2.773971	-0.719067
31	6	1.640786	2.128086	0.029701
32	1	3.280506	-1.737325	0.628914
33	1	2.150279	-3.937196	0.866764
34	6	2.889638	-2.233550	-0.269120
35	1	1.453638	-3.778564	-0.742119
36	6	2.773390	2.184670	-1.002286
37	6	1.899468	3.141396	1.164788
38	1	0.705347	2.423287	-0.458619
39	1	2.946631	3.222662	-1.307905
40	1	2.548759	1.616138	-1.910100
41	1	3.716599	1.806589	-0.586074
42	1	1.065760	3.151596	1.869751
43	1	2.022561	4.148631	0.750436
44	1	2.814323	2.890652	1.717962

HF=-867.0448584
Zero-point correction= 0.386605
Sum of electronic and thermal Enthalpies= -866.638776
Sum of electronic and thermal Free Energies= -866.704566
Total free energy in sol.(with non electrost.terms) (a.u.) = -867.055007

Transition state 6d' (higher energy transition state than 6d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8		1.386763	1.938637	-0.661423
2	1		0.533341	1.316051	-1.116118
3	8		2.565648	2.288052	1.211747
4	6		-1.459208	0.717054	-0.706181
5	1		-3.199202	-0.735218	0.870191
6	1		1.876836	-1.313441	-1.987307
7	6		-2.310338	-1.245396	1.262387
8	8		-0.488358	0.720135	-1.577138
9	1		4.027393	0.263502	1.247635
10	1		2.189417	-2.604283	-0.808293
11	6		2.177699	-1.518574	-0.956238
12	1		0.156929	-3.294514	-0.608836
13	6		1.890942	0.055810	0.882530
14	1		3.717763	-0.002836	-1.185179

15	6	1.938094	1.563973	0.453011
16	6	-0.497456	-2.435496	-0.810989
17	6	-0.065769	-1.288708	0.073676
18	6	-1.041612	-0.530823	0.777022
19	6	3.328927	-0.493775	0.891099
20	7	1.203110	-0.901828	-0.019453
21	6	-1.965202	-2.851757	-0.625615
22	1	-0.638771	0.180428	1.494471
23	1	1.428402	0.014421	1.870605
24	1	4.354809	-1.592307	-0.731880
25	6	3.528388	-0.893184	-0.577093
26	1	3.394771	-1.373076	1.544166
27	1	-2.365120	0.183015	-1.038040
28	1	-0.309203	-2.140450	-1.851611
29	1	-2.376938	-1.164860	2.354584
30	1	-3.385720	-3.112365	1.002636
31	6	-1.785041	2.060935	-0.019864
32	1	-1.697679	-3.321964	1.465584
33	1	-2.094189	-3.878084	-0.987269
34	1	-2.614903	-2.219279	-1.243149
35	6	-2.374809	-2.720255	0.842040
36	6	-2.934745	2.013490	0.993009
37	6	-2.097269	3.078802	-1.136772
38	1	-0.876295	2.406422	0.486501
39	1	-1.257191	3.161298	-1.829450
40	1	-2.293893	4.065819	-0.702657
41	1	-2.986069	2.779533	-1.707953
42	1	-2.706162	1.397990	1.868372
43	1	-3.854656	1.625610	0.535998
44	1	-3.153463	3.024220	1.355548

HF=-867.0437068
Zero-point correction= 0.385901
Sum of electronic and thermal Enthalpies= -866.638157
Sum of electronic and thermal Free Energies= -866.704478