Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Excited State Dynamics and Conjugation Effects of the Photoisomerization Reactions of Dihydroazulene

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1 Structures and energies

In this section, we have included the used structures of the different dihydroazulene (DHA), transition states (TS), and vinylhepatefulvene (VHF) systems given in Cartesian coordinates with units in Å. Along with the structures, we have given the electronic energy including the zero-point vibrational energy in atomic units of the given structure. The structures and associated energies are calculated in the first electronically excited singlet state using time-dependent density functional theory employing the M06-2X/6-311+G* methodology as implemented in Gaussian 16.

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Parent-DHA vacuum Energy: -802.105562

C	4.58406	-0.45003	0.18539
C	3.97816	-1.72589	0.13415
C	2.64108	-2.05693	-0.01661
C	1.55280	-1.17941	-0.18763
C	1.60515	0.24388	-0.64003
C	2.74490	1.14411	-0.44390
C	4.02642	0.81233	-0.05339
C	0.19708	-1.53410	-0.01612
C	-0.65819	-0.45753	-0.04929
C	0.20219	0.80284	-0.10433
C	-0.29629	1.85969	-0.99306
N	-0.63567	2.67470	-1.72708
H	5.64336	-0.45278	0.42105
H	4.65111	-2.56146	0.29946
H	2.38474	-3.10826	0.08508
H	1.43961	0.20448	-1.73699
H	2.55414	2.17976	-0.71676
H	-0.12319	-2.55293	0.16884
C	-2.10251	-0.44690	-0.00181
C	-2.81842	0.70139	0.38277
C	-2.82990	-1.61061	-0.31914
C	-4.20344	0.68180	0.44948
H	-2.29206	1.60908	0.65814
C	-4.21211	-1.62499	-0.24334
H	-2.30183	-2.49714	-0.65268
C	-4.90746	-0.47856	0.13980
H	-4.73552	1.57612	0.75251
H	-4.75402	-2.52908	-0.49697
H	-5.98991	-0.49001	0.19309
H	4.71710	1.64669	0.02447
C	0.39427	1.33616	1.25371
N	0.55278	1.73559	2.31862

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Parent-DHA acetonitrile Energy: -802.105005

C	-4.60356	0.47023	0.16944
C	-3.98697	1.74062	0.07998
C	-2.64965	2.05528	-0.05735
C	-1.55821	1.16227	-0.18956
C	-1.61942	-0.27883	-0.60477
C	-2.75769	-1.17059	-0.30350
C	-4.04138	-0.80977	0.02835
C	-0.21644	1.52668	-0.03828
C	0.65546	0.44933	-0.07519
C	-0.20212	-0.81829	-0.11890
C	0.28861	-1.86134	-1.02927
N	0.63575	-2.66158	-1.77544
H	-5.66995	0.48858	0.37046
H	-4.65774	2.58589	0.19552
H	-2.38556	3.10738	0.00389
H	-1.52389	-0.26905	-1.70788
H	-2.56310	-2.22867	-0.46387
H	0.09635	2.54996	0.13192
C	2.08957	0.44945	-0.01382
C	2.82511	-0.71396	0.30354
C	2.80990	1.64380	-0.24922
C	4.20894	-0.68065	0.37963
H	2.31599	-1.64665	0.52098
C	4.19093	1.66770	-0.16629
H	2.27675	2.54768	-0.52076
C	4.90162	0.50665	0.14609
H	4.75084	-1.58496	0.63163
H	4.72173	2.59367	-0.35597
H	5.98340	0.52823	0.20624
H	-4.73614	-1.63494	0.15350
C	-0.33040	-1.36275	1.24404
N	-0.44068	-1.75157	2.31899

32
Parent-DHA cyclohexane Energy: -802.113210

C	4.59257	-0.45905	0.17676
C	3.98180	-1.73264	0.11455
C	2.64407	-2.05685	-0.02914
C	1.55493	-1.17340	-0.18604
C	1.61011	0.25660	-0.62512
C	2.75024	1.15479	-0.39111
C	4.03322	0.81078	-0.02570
C	0.20403	-1.53150	-0.02203
C	-0.65743	-0.45510	-0.05725
C	0.20207	0.80799	-0.10902
C	-0.29334	1.85865	-1.00746
N	-0.63426	2.66793	-1.74694
H	5.65512	-0.46819	0.39735
H	4.65343	-2.57239	0.26256
H	2.38462	-3.10834	0.06002
H	1.47154	0.22703	-1.72517
H	2.55745	2.20065	-0.61989
H	-0.11370	-2.55169	0.15883
C	-2.09814	-0.44842	-0.00552
C	-2.82115	0.70628	0.35290
C	-2.82304	-1.62401	-0.29267
C	-4.20576	0.68205	0.42208
H	-2.30114	1.62365	0.60724
C	-4.20486	-1.64159	-0.21515
H	-2.29326	-2.51777	-0.60290
C	-4.90573	-0.48882	0.14081
H	-4.74123	1.58083	0.70534
H	-4.74292	-2.55420	-0.44533
H	-5.98800	-0.50374	0.19573
H	4.72592	1.64180	0.06791
C	0.36962	1.34869	1.25009
N	0.51039	1.74859	2.31729

32
Parent-DHA ethanol Energy: -802.125622

C	-4.60357	0.46986	0.16918
C	-3.98720	1.74032	0.08038
C	-2.64975	2.05528	-0.05643
C	-1.55837	1.16262	-0.18883
C	-1.61931	-0.27822	-0.60461
C	-2.75745	-1.17031	-0.30482
C	-4.04131	-0.80989	0.02719
C	-0.21627	1.52690	-0.03704
C	0.65538	0.44977	-0.07413
C	-0.20202	-0.81785	-0.11858
C	0.28890	-1.86034	-1.02950
N	0.63580	-2.66016	-1.77624
H	-5.66993	0.48799	0.37038
H	-4.65811	2.58544	0.19628
H	-2.38588	3.10739	0.00566
H	-1.52322	-0.26770	-1.70773
H	-2.56252	-2.22820	-0.46602
H	0.09654	2.55010	0.13367
C	2.08973	0.44969	-0.01324
C	2.82487	-0.71371	0.30434
C	2.81020	1.64361	-0.24954
C	4.20873	-0.68080	0.37997
H	2.31540	-1.64610	0.52227
C	4.19125	1.66722	-0.16704
H	2.27712	2.54739	-0.52157
C	4.90164	0.50615	0.14573
H	4.75041	-1.58518	0.63212
H	4.72229	2.59291	-0.35744
H	5.98344	0.52743	0.20552
H	-4.73595	-1.63524	0.15179
C	-0.33072	-1.36344	1.24384
N	-0.44122	-1.75377	2.31822

32
Parent-DHA toluene Energy: -802.114617

C	4.59358	-0.46040	0.17630
C	3.98217	-1.73366	0.11106
C	2.64449	-2.05674	-0.03214
C	1.55516	-1.17223	-0.18679
C	1.61099	0.25901	-0.62344
C	2.75116	1.15662	-0.38233
C	4.03402	0.81067	-0.02007
C	0.20525	-1.53099	-0.02419
C	-0.65733	-0.45448	-0.05960
C	0.20209	0.80903	-0.11014
C	-0.29281	1.85937	-1.00929
N	-0.63416	2.66817	-1.74907
H	5.65648	-0.47057	0.39519
H	4.65362	-2.57408	0.25592
H	2.38452	-3.10830	0.05420
H	1.47675	0.23154	-1.72385
H	2.55833	2.20402	-0.60388
H	-0.11196	-2.55146	0.15574
C	-2.09732	-0.44843	-0.00679
C	-2.82153	0.70719	0.34774
C	-2.82185	-1.62607	-0.28847
C	-4.20605	0.68206	0.41796
H	-2.30270	1.62623	0.59838
C	-4.20358	-1.64427	-0.21015
H	-2.29186	-2.52096	-0.59491
C	-4.90536	-0.49058	0.14166
H	-4.74207	1.58143	0.69830
H	-4.74098	-2.55830	-0.43613
H	-5.98757	-0.50623	0.19734
H	4.72697	1.64109	0.07694
C	0.36573	1.34959	1.24962
N	0.50382	1.74774	2.31783

32
Parent-TS vacuum Energy: -802.102203

C	4.47805	-0.40718	0.18917
C	3.88829	-1.69074	0.23480
C	2.56926	-2.05238	0.03519
C	1.48142	-1.20127	-0.24827
C	1.57566	0.13433	-0.90663
C	2.71911	0.97315	-0.94302
C	3.95114	0.77449	-0.31872
C	0.14547	-1.50400	0.06707
C	-0.69042	-0.39671	0.06347
C	0.14058	0.83317	0.03051
C	-0.36062	1.98434	-0.69589
N	-0.69982	2.88102	-1.33074
H	5.50386	-0.35609	0.53947
H	4.54970	-2.49322	0.54675
H	2.31104	-3.08698	0.24941
H	1.03584	0.12711	-1.85938
H	2.60556	1.88145	-1.52953
H	-0.18170	-2.50203	0.33594
C	-2.14203	-0.39821	0.04827
C	-2.87956	0.69407	0.53461
C	-2.84091	-1.52136	-0.42825
C	-4.26614	0.66303	0.53886
H	-2.36433	1.56066	0.93502
C	-4.22617	-1.55139	-0.41140
H	-2.28704	-2.35914	-0.83801
C	-4.94481	-0.45820	0.06906
H	-4.81953	1.51358	0.91963
H	-4.75011	-2.42280	-0.78739
H	-6.02849	-0.48024	0.07567
H	4.63155	1.62072	-0.34113
C	0.74155	1.19821	1.30243
N	1.23619	1.48425	2.30018

32
Parent-TS acetonitrile Energy: -802.119639

C	-4.48241	-0.42897	0.19704
C	-3.88142	-1.71175	0.22547
C	-2.56367	-2.05861	0.01583
C	-3.96781	0.76028	-0.30678
C	-1.47940	-1.18696	-0.24833
C	-2.74011	0.97522	-0.93560
C	-1.58870	0.14588	-0.91179
H	-5.50841	-0.39041	0.54829
H	-4.53701	-2.52413	0.52271
H	-2.29580	-3.09594	0.20089
H	-4.65957	1.59737	-0.32910
H	-2.64321	1.88574	-1.52113
C	-0.15231	-1.48810	0.07699
C	0.69361	-0.38179	0.06940
C	-0.12638	0.85482	0.03463
C	0.37877	2.00106	-0.69153
C	-0.73715	1.22162	1.29774
N	0.72540	2.89638	-1.32492
N	-1.25077	1.50248	2.28813
H	-1.04763	0.14775	-1.86254
H	0.16962	-2.48661	0.34940
C	2.14121	-0.39667	0.05420
C	2.89388	0.69843	0.51843
C	2.82830	-1.53781	-0.40427
C	4.28044	0.65401	0.51616
H	2.39200	1.57541	0.91317
C	4.21359	-1.57894	-0.39531
H	2.26674	-2.38110	-0.79078
C	4.94622	-0.48271	0.06067
H	4.84447	1.50375	0.88279
H	4.72683	-2.46270	-0.75634
H	6.02954	-0.51534	0.06238

32
Parent-TS cyclohexane Energy: -802.108864

C	-4.48072	-0.41650	0.18773
C	-3.88626	-1.69924	0.22967
C	-2.56687	-2.05482	0.03028
C	-3.95769	0.76798	-0.31794
C	-1.48029	-1.19600	-0.24505
C	-2.72642	0.97238	-0.94210
C	-1.57983	0.13755	-0.90791
H	-5.50720	-0.37017	0.53665
H	-4.54559	-2.50540	0.53609
H	-2.30523	-3.08995	0.23678
H	-4.64231	1.61078	-0.34165
H	-2.61851	1.88113	-1.52880
C	-0.14799	-1.49714	0.07630
C	0.69188	-0.39018	0.06932
C	-0.13494	0.84181	0.03402
C	0.36775	1.99066	-0.69310
C	-0.74109	1.20942	1.30154
N	0.70900	2.88633	-1.32850
N	-1.24284	1.49644	2.29570
H	-1.03829	0.13262	-1.85920
H	0.17747	-2.49453	0.34924
C	2.14198	-0.39742	0.05190
C	2.88662	0.69580	0.52795
C	2.83507	-1.52801	-0.41848
C	4.27317	0.65906	0.52740
H	2.37771	1.56691	0.92663
C	4.22033	-1.56298	-0.40687
H	2.27715	-2.36779	-0.81840
C	4.94559	-0.46867	0.06259
H	4.83154	1.50942	0.90117
H	4.73928	-2.43947	-0.77777
H	6.02915	-0.49517	0.06543

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Parent-TS ethanol Energy: -802.119209

C	-4.48258	-0.42874	0.19615
C	-3.88174	-1.71146	0.22504
C	-2.56381	-2.05849	0.01621
C	-3.96760	0.76049	-0.30728
C	-1.47946	-1.18720	-0.24800
C	-2.73965	0.97520	-0.93565
C	-1.58838	0.14570	-0.91138
H	-5.50869	-0.39003	0.54709
H	-4.53747	-2.52372	0.52236
H	-2.29614	-3.09572	0.20217
H	-4.65911	1.59778	-0.32960
H	-2.64229	1.88572	-1.52110
C	-0.15222	-1.48831	0.07735
C	0.69353	-0.38200	0.06973
C	-0.12669	0.85444	0.03485
C	0.37839	2.00071	-0.69145
C	-0.73704	1.22148	1.29820
N	0.72479	2.89596	-1.32504
N	-1.24985	1.50282	2.28885
H	-1.04730	0.14733	-1.86215
H	0.16987	-2.48677	0.34980
C	2.14121	-0.39671	0.05422
C	2.89377	0.69832	0.51858
C	2.82835	-1.53759	-0.40466
C	4.28032	0.65406	0.51612
H	2.39180	1.57519	0.91343
C	4.21363	-1.57862	-0.39583
H	2.26677	-2.38077	-0.79144
C	4.94617	-0.48245	0.06035
H	4.84429	1.50385	0.88277
H	4.72695	-2.46221	-0.75719
H	6.02949	-0.51495	0.06191

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Parent-TS toluene Energy: -802.110175

C	-4.48120	-0.41823	0.18780
C	-3.88583	-1.70085	0.22874
C	-2.56643	-2.05526	0.02904
C	-3.95899	0.76685	-0.31739
C	-1.48012	-1.19492	-0.24478
C	-2.72791	0.97249	-0.94160
C	-1.58072	0.13838	-0.90814
H	-5.50778	-0.37288	0.53653
H	-4.54473	-2.50776	0.53404
H	-2.30408	-3.09055	0.23368
H	-4.64447	1.60895	-0.34123
H	-2.62113	1.88142	-1.52819
C	-0.14849	-1.49589	0.07743
C	0.69213	-0.38900	0.07003
C	-0.13389	0.84345	0.03452
C	0.36905	1.99193	-0.69263
C	-0.74075	1.21129	1.30139
N	0.71079	2.88749	-1.32797
N	-1.24375	1.49809	2.29503
H	-1.03903	0.13405	-1.85924
H	0.17660	-2.49326	0.35081
C	2.14193	-0.39729	0.05241
C	2.88782	0.69619	0.52650
C	2.83402	-1.52933	-0.41656
C	4.27437	0.65838	0.52527
H	2.38001	1.56817	0.92468
C	4.21928	-1.56520	-0.40572
H	2.27542	-2.36955	-0.81454
C	4.94570	-0.47062	0.06163
H	4.83362	1.50873	0.89774
H	4.73734	-2.44270	-0.77544
H	6.02923	-0.49796	0.06395

32
Parent-VHF vacuum Energy: -802.123697

C	4.55280	-0.63654	0.30292
C	3.82407	-1.80025	0.45080
C	2.42049	-1.95021	0.25614
C	1.54784	-1.09876	-0.35031
C	1.91530	0.06096	-1.17633
C	3.04904	0.81659	-1.07504
C	4.18715	0.58550	-0.27880
C	0.11091	-1.28991	-0.15852
C	-0.73014	-0.23497	-0.01761
C	-0.14625	1.11193	0.15683
C	-0.61027	2.21202	-0.59579
N	-0.97924	3.09274	-1.24709
H	5.56958	-0.67508	0.68682
H	4.33515	-2.64160	0.90421
H	1.97997	-2.82932	0.72451
H	1.20522	0.32527	-1.95234
H	3.07518	1.71418	-1.68938
H	-0.28389	-2.29996	-0.09801
C	-2.20049	-0.37784	0.02984
C	-2.98341	0.51396	0.77191
C	-2.83817	-1.41318	-0.66525
C	-4.36271	0.36180	0.83333
H	-2.51005	1.32396	1.31629
C	-4.21565	-1.56802	-0.59587
H	-2.25295	-2.08112	-1.28781
C	-4.98332	-0.68113	0.15407
H	-4.95299	1.06014	1.41535
H	-4.69392	-2.37180	-1.14409
H	-6.06011	-0.79682	0.19945
H	4.92751	1.37602	-0.24769
C	0.76444	1.35149	1.20388
N	1.52945	1.49520	2.06072

32
Parent-VHF acetonitrile Energy: -802.137734

C	-4.55438	-0.58632	0.24488
C	-3.84735	-1.77817	0.41818
C	-2.47033	-1.98131	0.24292
C	-4.15171	0.60849	-0.35267
C	-1.52820	-1.10930	-0.28156
C	-2.97702	0.82329	-1.09990
C	-1.83238	0.06676	-1.11596
H	-5.57708	-0.59837	0.61152
H	-4.39789	-2.60326	0.85511
H	-2.07575	-2.90933	0.65248
H	-4.89082	1.40143	-0.38203
H	-2.97779	1.69730	-1.74657
C	-0.13729	-1.32466	-0.01478
C	0.72127	-0.24971	0.04357
C	0.11324	1.07866	0.13994
C	0.64430	2.18163	-0.57873
C	-0.81635	1.37431	1.16848
N	1.07039	3.06004	-1.19416
N	-1.58668	1.58251	2.00433
H	-1.11995	0.26571	-1.91021
H	0.23101	-2.32831	0.17646
C	2.18491	-0.38366	0.05387
C	2.99110	0.54189	0.73340
C	2.80222	-1.45568	-0.60859
C	4.37225	0.39310	0.75661
H	2.53454	1.36782	1.26889
C	4.18229	-1.60459	-0.57720
H	2.19716	-2.15921	-1.16991
C	4.97282	-0.68038	0.10355
H	4.97987	1.11308	1.29265
H	4.64396	-2.43609	-1.09727
H	6.05048	-0.79479	0.12163

32
Parent-VHF cyclohexane Energy: -802.130068

C	-4.55792	-0.61234	0.28210
C	-3.83202	-1.77364	0.47966
C	-2.43512	-1.94457	0.29155
C	-4.18238	0.58589	-0.34245
C	-1.54313	-1.10606	-0.31927
C	-3.02842	0.79885	-1.11703
C	-1.88397	0.04689	-1.16640
H	-5.57841	-0.63445	0.65607
H	-4.35167	-2.59614	0.95720
H	-2.00737	-2.82521	0.76804
H	-4.92784	1.37232	-0.35948
H	-3.04377	1.67775	-1.75765
C	-0.11835	-1.30657	-0.10490
C	0.72496	-0.24267	0.00399
C	0.13297	1.09804	0.14399
C	0.65373	2.20283	-0.57067
C	-0.80759	1.36373	1.16349
N	1.07207	3.08768	-1.18381
N	-1.58959	1.54233	1.99669
H	-1.16794	0.27939	-1.94737
H	0.27211	-2.31475	-0.00059
C	2.19394	-0.38071	0.03792
C	2.98072	0.49481	0.79665
C	2.82631	-1.40202	-0.68307
C	4.36031	0.34107	0.84654
H	2.50987	1.28925	1.36619
C	4.20496	-1.55651	-0.62717
H	2.23485	-2.05885	-1.31167
C	4.97675	-0.68580	0.13790
H	4.95442	1.02374	1.44303
H	4.68018	-2.34802	-1.19543
H	6.05377	-0.80233	0.17456

32
Parent-VHF ethanol Energy: -802.137302

C	-4.55421	-0.58733	0.24557
C	-3.84714	-1.77901	0.41741
C	-2.46979	-1.98169	0.24157
C	-4.15186	0.60852	-0.35050
C	-1.52834	-1.10961	-0.28286
C	-2.97743	0.82448	-1.09748
C	-1.83281	0.06779	-1.11550
H	-5.57688	-0.59999	0.61233
H	-4.39732	-2.60453	0.85401
H	-2.07483	-2.90964	0.65096
H	-4.89097	1.40149	-0.37830
H	-2.97811	1.69985	-1.74233
C	-0.13689	-1.32501	-0.01701
C	0.72129	-0.25030	0.04210
C	0.11276	1.07810	0.13934
C	0.64154	2.18107	-0.58105
C	-0.81419	1.37371	1.17030
N	1.06528	3.05952	-1.19800
N	-1.58216	1.58191	2.00827
H	-1.12110	0.26750	-1.91024
H	0.23179	-2.32884	0.17254
C	2.18507	-0.38368	0.05333
C	2.99045	0.54213	0.73330
C	2.80326	-1.45530	-0.60886
C	4.37163	0.39391	0.75739
H	2.53332	1.36807	1.26829
C	4.18334	-1.60370	-0.57659
H	2.19891	-2.15895	-1.17081
C	4.97306	-0.67927	0.10473
H	4.97857	1.11427	1.29366
H	4.64566	-2.43491	-1.09656
H	6.05076	-0.79318	0.12338

32
Parent-VHF toluene Energy: -802.130589

C	-4.55703	-0.61226	0.27881
C	-3.83374	-1.78019	0.46292
C	-2.44066	-1.95503	0.27398
C	-4.17825	0.58992	-0.33259
C	-1.54081	-1.10586	-0.31700
C	-3.02157	0.80941	-1.10225
C	-1.87691	0.05737	-1.15310
H	-5.57717	-0.63559	0.65335
H	-4.35774	-2.60625	0.92949
H	-2.01774	-2.84741	0.73257
H	-4.92283	1.37741	-0.34477
H	-3.03584	1.69181	-1.73797
C	-0.12163	-1.30977	-0.09623
C	0.72437	-0.24463	0.00505
C	0.12875	1.09439	0.13980
C	0.64395	2.19809	-0.58193
C	-0.79972	1.36546	1.17023
N	1.05696	3.08097	-1.20117
N	-1.57133	1.54889	2.01166
H	-1.16450	0.28772	-1.93821
H	0.26480	-2.31798	0.02189
C	2.19245	-0.38110	0.03832
C	2.98077	0.50552	0.78308
C	2.82416	-1.41279	-0.66907
C	4.36059	0.35320	0.83208
H	2.51114	1.30727	1.34333
C	4.20293	-1.56582	-0.61362
H	2.23197	-2.07931	-1.28665
C	4.97609	-0.68362	0.13707
H	4.95552	1.04449	1.41773
H	4.67727	-2.36557	-1.17094
H	6.05321	-0.79931	0.17335

34

34-DHA vacuum Energy: -878.318632

C	4.65420	0.60686	0.14929
C	3.91698	1.80357	-0.02602
C	2.54917	1.98591	-0.15557
C	4.21800	-0.72138	0.12337
C	1.54903	0.99756	-0.20513
C	2.95629	-1.22233	-0.13745
C	1.75580	-0.45051	-0.48758
H	5.71578	0.74468	0.32782
H	4.50817	2.71353	0.00366
H	2.20444	3.01564	-0.17526
H	2.84290	-2.30153	-0.20878
C	-0.58927	0.05397	-0.10362
C	0.38219	-1.11996	-0.07170
H	1.74374	-0.49515	-1.60356
C	0.05609	-2.21604	-0.99533
C	0.47912	-1.64348	1.30206
N	-0.15914	-3.05737	-1.74622
N	0.55792	-2.03137	2.37964
H	4.98575	-1.46883	0.29972
C	-1.99270	0.01819	-0.03528
C	-2.66912	1.27774	-0.01222
C	-2.76198	-1.17521	0.04210
C	-4.12909	-1.11452	0.11275
H	-2.26781	-2.14005	0.04877
C	-4.79835	0.12944	0.11534
H	-4.70384	-2.03189	0.16981
H	-5.88036	0.15749	0.17017
C	0.14337	1.24026	-0.12957
C	-0.54802	2.48622	-0.08168
C	-1.91021	2.48646	-0.03526
H	-2.45057	3.42749	-0.00740
H	0.00117	3.42025	-0.09034
C	-4.07876	1.29774	0.05807
H	-4.58725	2.25659	0.07201

34
34-DHA acetonitrile Energy: -878.337341

C	4.65251	0.60225	0.17305
C	3.91718	1.80117	-0.02299
C	2.55614	1.98101	-0.17069
C	4.21378	-0.72780	0.15539
C	1.55088	0.98823	-0.21953
C	2.96012	-1.23108	-0.11883
C	1.75972	-0.46440	-0.51026
H	5.71223	0.74005	0.36184
H	4.50898	2.71027	0.00605
H	2.21116	3.00976	-0.20673
H	2.85363	-2.31169	-0.17429
C	-0.58657	0.05049	-0.11704
C	0.38227	-1.12710	-0.09113
H	1.75337	-0.51726	-1.62098
C	0.03794	-2.22065	-1.01036
C	0.47195	-1.64802	1.28454
N	-0.20396	-3.05852	-1.75660
N	0.54080	-2.01929	2.36875
H	4.97963	-1.47236	0.35071
C	-1.98640	0.01955	-0.03516
C	-2.65966	1.28415	-0.01143
C	-2.76216	-1.17103	0.05698
C	-4.12951	-1.10376	0.13683
H	-2.27469	-2.13937	0.07163
C	-4.79382	0.14411	0.13386
H	-4.70840	-2.01742	0.20732
H	-5.87515	0.17727	0.19453
C	0.15656	1.23723	-0.14167
C	-0.53365	2.48843	-0.09017
C	-1.89482	2.49252	-0.04032
H	-2.43153	3.43522	-0.01320
H	0.01658	3.42156	-0.10278
C	-4.06784	1.31081	0.06605
H	-4.57147	2.27195	0.07809

34
34-DHA cyclohexane Energy: -878.325623

C	4.65349	0.60448	0.16119
C	3.91659	1.80285	-0.01571
C	2.55148	1.98437	-0.15442
C	4.21686	-0.72449	0.13098
C	1.54967	0.99468	-0.21157
C	2.95843	-1.22542	-0.13707
C	1.75722	-0.45472	-0.49957
H	5.71407	0.74162	0.34548
H	4.50732	2.71249	0.02232
H	2.20619	3.01364	-0.17372
H	2.84824	-2.30487	-0.20660
C	-0.58823	0.05362	-0.11026
C	0.38275	-1.12148	-0.08016
H	1.74439	-0.50121	-1.61333
C	0.04842	-2.21747	-1.00057
C	0.47803	-1.64389	1.29425
N	-0.17731	-3.05871	-1.74838
N	0.55288	-2.02730	2.37376
H	4.98394	-1.47130	0.31194
C	-1.99019	0.01890	-0.03558
C	-2.66630	1.27990	-0.01440
C	-2.76059	-1.17384	0.05241
C	-4.12759	-1.11174	0.12854
H	-2.26818	-2.13956	0.06506
C	-4.79626	0.13337	0.12553
H	-4.70299	-2.02784	0.19583
H	-5.87794	0.16246	0.18389
C	0.14791	1.24007	-0.13713
C	-0.54395	2.48782	-0.09023
C	-1.90577	2.48876	-0.04258
H	-2.44495	3.43033	-0.01671
H	0.00475	3.42204	-0.10251
C	-4.07548	1.30144	0.05970
H	-4.58272	2.26084	0.07047

34

34-DHA ethanol Energy: -878.336799

C	4.65259	0.60238	0.17256
C	3.91716	1.80127	-0.02261
C	2.55595	1.98118	-0.16987
C	4.21394	-0.72764	0.15449
C	1.55084	0.98853	-0.21912
C	2.96008	-1.23083	-0.11939
C	1.75966	-0.46399	-0.50978
H	5.71236	0.74016	0.36108
H	4.50890	2.71041	0.00688
H	2.21095	3.00995	-0.20506
H	2.85344	-2.31141	-0.17525
C	-0.58664	0.05064	-0.11678
C	0.38230	-1.12685	-0.09073
H	1.75310	-0.51658	-1.62060
C	0.03842	-2.22041	-1.01013
C	0.47208	-1.64806	1.28481
N	-0.20277	-3.05835	-1.75653
N	0.54101	-2.02015	2.36874
H	4.97985	-1.47228	0.34925
C	-1.98655	0.01954	-0.03519
C	-2.65992	1.28400	-0.01155
C	-2.76210	-1.17112	0.05678
C	-4.12943	-1.10406	0.13653
H	-2.27446	-2.13937	0.07133
C	-4.79392	0.14370	0.13361
H	-4.70818	-2.01782	0.20692
H	-5.87525	0.17670	0.19425
C	0.15623	1.23737	-0.14148
C	-0.53406	2.48843	-0.09021
C	-1.89526	2.49239	-0.04044
H	-2.43207	3.43505	-0.01336
H	0.01609	3.42161	-0.10280
C	-4.06813	1.31045	0.06583
H	-4.57191	2.27152	0.07786

34

34-DHA toluene Energy: -878.327045

C	4.65342	0.60436	0.16251
C	3.91654	1.80282	-0.01579
C	2.55187	1.98409	-0.15546
C	4.21664	-0.72477	0.13332
C	1.54975	0.99404	-0.21242
C	2.95878	-1.22595	-0.13536
C	1.75753	-0.45570	-0.50096
H	5.71392	0.74160	0.34721
H	4.50729	2.71244	0.02193
H	2.20650	3.01329	-0.17578
H	2.84911	-2.30555	-0.20339
C	-0.58810	0.05328	-0.11114
C	0.38276	-1.12201	-0.08140
H	1.74514	-0.50286	-1.61434
C	0.04744	-2.21787	-1.00158
C	0.47741	-1.64437	1.29312
N	-0.17988	-3.05890	-1.74912
N	0.55141	-2.02678	2.37304
H	4.98366	-1.47133	0.31556
C	-1.98981	0.01894	-0.03564
C	-2.66563	1.28033	-0.01429
C	-2.76081	-1.17355	0.05307
C	-4.12783	-1.11088	0.12979
H	-2.26900	-2.13958	0.06605
C	-4.79603	0.13453	0.12670
H	-4.70359	-2.02671	0.19771
H	-5.87766	0.16407	0.18549
C	0.14882	1.23979	-0.13783
C	-0.54291	2.48791	-0.09067
C	-1.90465	2.48915	-0.04278
H	-2.44358	3.43084	-0.01691
H	0.00590	3.42204	-0.10317
C	-4.07468	1.30244	0.06033
H	-4.58154	2.26202	0.07118

34

34-TS vacuum Energy: -878.310900

C	-4.50845	-0.56041	0.24375
C	-3.78850	-1.77649	0.15517
C	-2.45027	-1.97808	-0.12731
C	-4.13167	0.70154	-0.18733
C	-1.46938	-1.00574	-0.39466
C	-2.95418	1.07031	-0.85084
C	-1.73862	0.35639	-0.91541
H	-5.51218	-0.64523	0.64767
H	-4.34715	-2.66677	0.42635
H	-2.08975	-2.99653	-0.00723
H	-2.96173	2.02164	-1.37612
C	0.62816	0.00588	-0.04025
C	-0.32684	1.13168	0.09874
H	-1.19815	0.52980	-1.85156
C	-0.02772	2.40645	-0.51138
C	-0.93946	1.25931	1.40515
N	0.15230	3.40348	-1.05668
N	-1.45297	1.35434	2.42989
H	-4.88984	1.47497	-0.10697
C	2.04772	0.05284	-0.00650
C	2.73752	-1.19501	-0.05746
C	2.80632	1.24262	0.13349
C	4.17845	1.19553	0.17397
H	2.30690	2.20020	0.20905
C	4.85921	-0.03491	0.09534
H	4.74195	2.11599	0.27423
H	5.94217	-0.05639	0.13001
C	-0.07298	-1.20409	-0.18170
C	0.63887	-2.44028	-0.16069
C	1.99706	-2.41993	-0.11821
H	2.55491	-3.35067	-0.13852
H	0.10625	-3.38128	-0.23281
C	4.14637	-1.20600	-0.00963
H	4.66177	-2.16019	-0.05193

34
34-TS acetonitrile Energy: -878.295826

C	-4.67751	0.46042	-0.17402
C	-3.92588	1.66701	0.11475
C	-2.56740	1.94511	0.14990
C	-4.22753	-0.69195	-0.76461
C	-1.53099	0.99695	0.10570
C	-2.81797	-0.82440	-1.02543
C	-1.99218	-0.43105	0.06773
H	-5.75181	0.56217	-0.04784
H	-4.56352	2.52942	0.28616
H	-2.29450	2.98890	0.27074
H	-2.44909	-0.78537	-2.05022
C	0.60363	-0.00378	0.09155
C	-0.26805	-1.21112	0.27163
H	-2.50085	-0.65048	1.01218
C	-0.33379	-1.67446	1.64053
C	-0.12286	-2.28502	-0.68513
N	-0.41166	-2.00861	2.73995
N	-0.08739	-3.10430	-1.49166
H	-4.95295	-1.43135	-1.09923
C	2.01485	0.00080	-0.04405
C	2.66364	1.27079	-0.13570
C	2.81902	-1.17112	-0.05308
C	4.18028	-1.08568	-0.20785
H	2.36389	-2.14427	0.07905
C	4.81254	0.16900	-0.33860
H	4.77664	-1.99055	-0.21599
H	5.88829	0.22076	-0.45797
C	-0.13006	1.18962	0.15075
C	0.54569	2.44887	0.12081
C	1.89488	2.47519	-0.03663
H	2.41968	3.42351	-0.08558
H	-0.02002	3.37005	0.19220
C	4.06500	1.32242	-0.29089
H	4.54579	2.29210	-0.36560

34
34-TS cyclohexane Energy: -878.317246
C -4.50939 -0.56724 0.25171
C -3.78776 -1.78317 0.15032
C -2.45108 -1.98060 -0.13639
C -4.13693 0.69733 -0.17448
C -1.47107 -1.00163 -0.39229
C -2.96305 1.07031 -0.84317
C -1.74617 0.35939 -0.91475
H -5.51142 -0.65673 0.65870
H -4.34559 -2.67634 0.41316
H -2.09005 -3.00023 -0.03076
H -2.97725 2.02136 -1.36866
C 0.62911 0.00887 -0.04086
C -0.32017 1.13944 0.09491
H -1.20998 0.53317 -1.85293
C -0.01937 2.41010 -0.52096
C -0.93058 1.27502 1.40043
N 0.16032 3.40530 -1.06994
N -1.44324 1.37649 2.42525
H -4.89693 1.46845 -0.08923
C 2.04818 0.05097 -0.00585
C 2.73452 -1.19925 -0.05701
C 2.81046 1.23869 0.13576
C 4.18274 1.18795 0.17504
H 2.31407 2.19748 0.21635
C 4.85978 -0.04478 0.09395
H 4.74915 2.10637 0.27717
H 5.94266 -0.06935 0.12770
C -0.07681 -1.20027 -0.17772
C 0.63198 -2.43936 -0.15280
C 1.99017 -2.42272 -0.11404
H 2.54498 -3.35515 -0.13305
H 0.09721 -3.37940 -0.21932
C 4.14335 -1.21444 -0.01069
H 4.65616 -2.16991 -0.05298

34

34-TS ethanol Energy: -878.327025

C	-4.50935	-0.57693	0.26742
C	-3.78571	-1.79296	0.14349
C	-2.45269	-1.98411	-0.15396
C	-4.14425	0.69156	-0.15246
C	-1.47370	-0.99450	-0.39113
C	-2.97652	1.07180	-0.82970
C	-1.75764	0.36540	-0.91401
H	-5.50860	-0.67400	0.67936
H	-4.34272	-2.69070	0.39138
H	-2.09148	-3.00583	-0.07649
H	-3.00145	2.02243	-1.35526
C	0.63025	0.01392	-0.04341
C	-0.30988	1.15260	0.08797
H	-1.22875	0.54118	-1.85538
C	-0.00594	2.41733	-0.53528
C	-0.91648	1.29764	1.39210
N	0.17571	3.41081	-1.08703
N	-1.43025	1.40224	2.41664
H	-4.90792	1.45839	-0.06038
C	2.04832	0.04814	-0.00494
C	2.72914	-1.20601	-0.05565
C	2.81666	1.23266	0.13923
C	4.18909	1.17564	0.17786
H	2.32501	2.19339	0.22636
C	4.86020	-0.06098	0.09414
H	4.76051	2.09057	0.28293
H	5.94288	-0.09063	0.12724
C	-0.08296	-1.19380	-0.17440
C	0.62072	-2.43753	-0.14302
C	1.97886	-2.42712	-0.10818
H	2.52912	-3.36203	-0.12525
H	0.08223	-3.37559	-0.20257
C	4.13800	-1.22818	-0.01045
H	4.64614	-2.18596	-0.05296

34
34-TS toluene Energy: -878.318502

C	-4.50954	-0.56853	0.25337
C	-3.78748	-1.78442	0.14968
C	-2.45115	-1.98102	-0.13798
C	-4.13791	0.69656	-0.17188
C	-1.47134	-1.00082	-0.39208
C	-2.96468	1.07045	-0.84144
C	-1.74759	0.36007	-0.91455
H	-5.51128	-0.65898	0.66081
H	-4.34509	-2.67813	0.41106
H	-2.08996	-3.00084	-0.03521
H	-2.98012	2.02153	-1.36680
C	0.62929	0.00946	-0.04121
C	-0.31908	1.14087	0.09411
H	-1.21232	0.53410	-1.85315
C	-0.01823	2.41079	-0.52292
C	-0.92869	1.27767	1.39965
N	0.16122	3.40561	-1.07268
N	-1.44098	1.37969	2.42467
H	-4.89830	1.46720	-0.08573
C	2.04824	0.05071	-0.00576
C	2.73398	-1.19993	-0.05704
C	2.81118	1.23805	0.13638
C	4.18348	1.18665	0.17557
H	2.31533	2.19705	0.21793
C	4.85988	-0.04649	0.09397
H	4.75042	2.10468	0.27819
H	5.94274	-0.07162	0.12768
C	-0.07746	-1.19952	-0.17739
C	0.63079	-2.43913	-0.15187
C	1.98897	-2.42315	-0.11367
H	2.54327	-3.35586	-0.13253
H	0.09563	-3.37898	-0.21751
C	4.14281	-1.21588	-0.01084
H	4.65515	-2.17158	-0.05321

34

34-VHF vacuum Energy: -878.342487

C	4.70516	-0.36397	-0.68592
C	3.60417	-0.74871	-1.54217
C	2.29745	-0.93564	-1.20291
C	4.70989	-0.19548	0.65486
C	1.64978	-0.78739	0.05293
C	3.60941	-0.33370	1.58030
C	2.29662	-0.58497	1.29549
H	5.64983	-0.20679	-1.19656
H	3.85584	-0.89449	-2.58620
H	1.63772	-1.20644	-2.02389
H	3.85745	-0.19969	2.62661
C	-0.71342	0.19749	-0.04647
C	-0.21030	1.53919	-0.03464
H	1.63402	-0.60875	2.15783
C	-0.96741	2.64759	0.42986
C	1.11051	1.91746	-0.37683
N	-1.52986	3.57311	0.82922
N	2.14841	2.32425	-0.67779
H	5.65795	0.08171	1.10469
C	-2.14979	-0.05326	-0.09756
C	-2.63393	-1.36547	0.14960
C	-3.09910	0.92910	-0.46208
C	-4.44561	0.64779	-0.48434
H	-2.78217	1.91688	-0.76094
C	-4.92136	-0.63369	-0.15664
H	-5.14395	1.42555	-0.77015
H	-5.98529	-0.83878	-0.16738
C	0.16213	-0.90662	0.06306
C	-0.36608	-2.19761	0.26083
C	-1.71245	-2.42512	0.34588
H	-2.09299	-3.42371	0.53305
H	0.33332	-3.01707	0.37766
C	-4.02381	-1.62615	0.13915
H	-4.36277	-2.63480	0.35096

34

34-VHF acetonitrile Energy: -878.341682

C	-4.60593	-0.59559	0.31070
C	-3.76069	-1.66449	0.64873
C	-2.37946	-1.75592	0.42322
C	-4.35896	0.50668	-0.48379
C	-1.55388	-0.91954	-0.30028
C	-3.20527	0.73431	-1.29219
C	-1.99826	0.11413	-1.23666
H	-5.60436	-0.64867	0.73653
H	-4.19776	-2.45066	1.25198
H	-1.87991	-2.56126	0.95840
H	-3.30677	1.51109	-2.04496
C	0.68268	0.10277	0.05798
C	-0.00744	1.36658	0.27673
H	-1.26592	0.40147	-1.98478
C	0.38862	2.57156	-0.35078
C	-1.08847	1.46903	1.17711
N	0.69039	3.54869	-0.88682
N	-1.96295	1.55696	1.92931
H	-5.17173	1.21349	-0.60250
C	2.11849	0.01435	0.07360
C	2.72330	-1.25557	-0.14276
C	2.96636	1.11342	0.36287
C	4.33283	0.96834	0.36531
H	2.54657	2.08085	0.60428
C	4.92802	-0.28143	0.10000
H	4.95913	1.82509	0.58486
H	6.00702	-0.37871	0.10415
C	-0.09769	-1.05004	-0.15123
C	0.53882	-2.30342	-0.31294
C	1.90145	-2.40123	-0.32369
H	2.37733	-3.36278	-0.48406
H	-0.07263	-3.17986	-0.49432
C	4.13291	-1.37386	-0.13759
H	4.57231	-2.35005	-0.31301

34
34-VHF cyclohexane Energy: -878.342559

C	4.69757	-0.39972	-0.69289
C	3.59445	-0.78029	-1.54671
C	2.28191	-0.93616	-1.20963
C	4.69935	-0.19845	0.64371
C	1.63718	-0.77701	0.04535
C	3.59425	-0.31049	1.57109
C	2.28297	-0.55835	1.29388
H	5.64623	-0.26600	-1.20278
H	3.84599	-0.94285	-2.58813
H	1.61836	-1.19742	-2.03074
H	3.84448	-0.15988	2.61481
C	-0.71389	0.19191	-0.05319
C	-0.19323	1.52446	-0.03431
H	1.61845	-0.56718	2.15481
C	-0.94726	2.64108	0.42138
C	1.13314	1.90092	-0.36146
N	-1.50111	3.57277	0.81688
N	2.16794	2.32881	-0.64606
H	5.64804	0.07959	1.09103
C	-2.15063	-0.04983	-0.10279
C	-2.63834	-1.35684	0.16188
C	-3.09268	0.93240	-0.48338
C	-4.44110	0.65612	-0.50583
H	-2.76874	1.91335	-0.79851
C	-4.92147	-0.61893	-0.16184
H	-5.13612	1.43162	-0.80524
H	-5.98596	-0.82048	-0.17341
C	0.15836	-0.91531	0.06448
C	-0.37270	-2.20258	0.28645
C	-1.71999	-2.41921	0.37572
H	-2.10637	-3.41268	0.57682
H	0.32362	-3.02300	0.41380
C	-4.02838	-1.61210	0.15086
H	-4.37284	-2.61597	0.37535

34

34-VHF ethanol Energy: -878.341552

C	-4.60589	-0.59547	0.31279
C	-3.76006	-1.66164	0.65507
C	-2.37794	-1.75231	0.42939
C	-4.36008	0.50453	-0.48594
C	-1.55452	-0.92001	-0.29955
C	-3.20700	0.73010	-1.29543
C	-1.99987	0.11019	-1.23938
H	-5.60436	-0.64782	0.73866
H	-4.19579	-2.44544	1.26232
H	-1.87692	-2.55361	0.96928
H	-3.30900	1.50507	-2.05001
C	0.68271	0.10276	0.05829
C	-0.00688	1.36721	0.27656
H	-1.26771	0.39620	-1.98816
C	0.39019	2.57145	-0.35156
C	-1.08928	1.47046	1.17497
N	0.69288	3.54808	-0.88804
N	-1.96493	1.55915	1.92575
H	-5.17340	1.21030	-0.60664
C	2.11852	0.01414	0.07437
C	2.72341	-1.25549	-0.14342
C	2.96634	1.11289	0.36514
C	4.33271	0.96779	0.36793
H	2.54647	2.08008	0.60731
C	4.92805	-0.28174	0.10142
H	4.95893	1.82429	0.58862
H	6.00706	-0.37898	0.10588
C	-0.09732	-1.04962	-0.15193
C	0.53901	-2.30254	-0.31609
C	1.90174	-2.40065	-0.32650
H	2.37755	-3.36204	-0.48804
H	-0.07279	-3.17851	-0.49862
C	4.13314	-1.37378	-0.13782
H	4.57258	-2.34976	-0.31433

34

34-VHF toluene Energy: -878.343354

C	4.69501	-0.40160	-0.69359
C	3.59247	-0.78466	-1.54694
C	2.27964	-0.93915	-1.21036
C	4.69625	-0.19651	0.64252
C	1.63475	-0.77755	0.04444
C	3.59099	-0.30776	1.57013
C	2.28015	-0.55698	1.29387
H	5.64382	-0.26900	-1.20345
H	3.84465	-0.95031	-2.58772
H	1.61620	-1.20185	-2.03112
H	3.84140	-0.15570	2.61363
C	-0.71375	0.19095	-0.05388
C	-0.18959	1.52146	-0.03438
H	1.61542	-0.56545	2.15461
C	-0.94192	2.64064	0.41883
C	1.13820	1.89564	-0.35879
N	-1.49319	3.57436	0.81288
N	2.17327	2.32490	-0.64092
H	5.64458	0.08322	1.08946
C	-2.15083	-0.04859	-0.10314
C	-2.63984	-1.35461	0.16354
C	-3.09121	0.93434	-0.48551
C	-4.44018	0.65970	-0.50776
H	-2.76570	1.91411	-0.80293
C	-4.92196	-0.61416	-0.16176
H	-5.13427	1.43537	-0.80881
H	-5.98665	-0.81454	-0.17329
C	0.15725	-0.91763	0.06426
C	-0.37509	-2.20420	0.28860
C	-1.72260	-2.41830	0.37876
H	-2.11051	-3.41086	0.58122
H	0.32014	-3.02542	0.41668
C	-4.03003	-1.60820	0.15274
H	-4.37589	-2.61123	0.37865

38
56-DHA vacuum Energy: -955.676573
C 2.79650 1.59718 -0.19494
C 1.47856 1.74043 -0.51280
C 3.62100 0.44455 -0.03564
C 0.47240 0.69119 -0.72764
H 0.27282 0.67036 -1.81541
C 0.67541 -0.73422 -0.32704
C 3.20208 -0.95307 -0.12186
C 1.89094 -1.42769 -0.23292
H 1.78546 -2.50855 -0.16155
C -0.59266 -1.31241 -0.11825
C -0.96692 0.99864 -0.10868
C -1.61515 -0.38360 -0.08058
H -0.73688 -2.37412 0.04563
C -0.79960 1.50078 1.26542
C -1.66484 1.99998 -0.92589
N -2.15842 2.78245 -1.60577
N -0.65670 1.87725 2.34083
C -5.79128 -1.11120 0.23155
C -4.92856 -2.11720 -0.20365
C -3.57142 -1.87296 -0.31727
C -3.03370 -0.61040 0.01074
C -3.91919 0.39415 0.45009
C -5.27760 0.14247 0.55585
H -6.85475 -1.30305 0.31505
H -5.32190 -3.09239 -0.46812
H -2.91546 -2.65157 -0.69090
H -3.54148 1.36948 0.73790
H -5.94003 0.92784 0.90140
H 3.33962 2.53425 -0.10473
H 1.12261 2.75099 -0.70168
C 4.99702 0.70284 0.19214
H 5.30945 1.73913 0.26823
C 4.22497 -1.95427 -0.00188
H 3.91920 -2.99310 -0.07013
C 5.53674 -1.64813 0.20136
H 6.27394 -2.43770 0.28982
C 5.93490 -0.28884 0.30737
H 6.97565 -0.03866 0.47626

38
56-DHA acetonitrile Energy: -955.699449

C	2.79627	1.61139	-0.00311
C	1.48626	1.77244	-0.28516
C	3.64226	0.44286	0.03166
C	0.49228	0.73515	-0.65918
H	0.40214	0.75108	-1.75793
C	0.68484	-0.70474	-0.27570
C	3.21937	-0.94120	-0.11395
C	1.90935	-1.40883	-0.21436
H	1.79786	-2.49047	-0.19260
C	-0.56080	-1.29429	-0.09270
C	-0.98180	1.02150	-0.14579
C	-1.61508	-0.37161	-0.10158
H	-0.69039	-2.35517	0.08271
C	-0.93624	1.57302	1.22108
C	-1.65511	1.97081	-1.04298
N	-2.14294	2.70426	-1.77914
N	-0.88859	1.96473	2.29980
C	-5.77146	-1.16997	0.23101
C	-4.87038	-2.19730	-0.06398
C	-3.51877	-1.93435	-0.17963
C	-3.01259	-0.61867	-0.00123
C	-3.94419	0.40788	0.30170
C	-5.29509	0.13034	0.41346
H	-6.83075	-1.38071	0.31898
H	-5.23215	-3.20850	-0.21197
H	-2.83955	-2.73950	-0.43449
H	-3.60596	1.42280	0.47928
H	-5.98510	0.93109	0.65377
H	3.33571	2.53599	0.18388
H	1.11689	2.79458	-0.32765
C	5.01580	0.69390	0.21829
H	5.33346	1.72418	0.33992
C	4.24514	-1.95287	-0.08022
H	3.93494	-2.98639	-0.19108
C	5.56617	-1.65517	0.08630
H	6.30589	-2.44686	0.10343
C	5.96491	-0.30629	0.24380
H	7.01075	-0.05906	0.38281

38
56-DHA cyclohexane Energy: -955.685108

C	2.79825	1.60487	-0.10266
C	1.48438	1.75875	-0.40544
C	3.63136	0.44346	-0.00017
C	0.48266	0.71329	-0.69365
H	0.33602	0.70951	-1.78867
C	0.68114	-0.71919	-0.30377
C	3.21102	-0.94788	-0.12004
C	1.89995	-1.41832	-0.22784
H	1.79168	-2.49990	-0.18172
C	-0.57800	-1.30272	-0.10778
C	-0.97481	1.00981	-0.12670
C	-1.61473	-0.37847	-0.09117
H	-0.71449	-2.36413	0.06175
C	-0.86849	1.53785	1.24453
C	-1.66029	1.98642	-0.98406
N	-2.14775	2.74745	-1.69208
N	-0.77368	1.92708	2.32085
C	-5.78190	-1.14121	0.23389
C	-4.90067	-2.16079	-0.13069
C	-3.54634	-1.90711	-0.24787
C	-3.02460	-0.61608	0.00409
C	-3.93174	0.40189	0.37481
C	-5.28665	0.13815	0.48469
H	-6.84325	-1.34224	0.32117
H	-5.27867	-3.15625	-0.33481
H	-2.87925	-2.70156	-0.56289
H	-3.57305	1.39880	0.60650
H	-5.96230	0.93388	0.77665
H	3.34047	2.53687	0.03222
H	1.12362	2.77762	-0.52778
C	5.00679	0.69666	0.21234
H	5.32118	1.73006	0.31439
C	4.23553	-1.95492	-0.04417
H	3.92795	-2.99097	-0.13852
C	5.55093	-1.65427	0.14542
H	6.28953	-2.44559	0.19667
C	5.94927	-0.29949	0.28334
H	6.99233	-0.05195	0.44113

38

56-DHA ethanol Energy: -955.699017

C	2.79646	1.61118	-0.00443
C	1.48626	1.77213	-0.28651
C	3.64220	0.44286	0.03112
C	0.49222	0.73463	-0.65907
H	0.40144	0.75016	-1.75784
C	0.68487	-0.70511	-0.27555
C	3.21930	-0.94136	-0.11383
C	1.90915	-1.40904	-0.21398
H	1.79778	-2.49069	-0.19142
C	-0.56128	-1.29448	-0.09251
C	-0.98167	1.02117	-0.14515
C	-1.61505	-0.37184	-0.10103
H	-0.69112	-2.35536	0.08287
C	-0.93552	1.57272	1.22164
C	-1.65487	1.97093	-1.04204
N	-2.14228	2.70491	-1.77794
N	-0.88747	1.96512	2.30008
C	-5.77177	-1.16942	0.23042
C	-4.87104	-2.19670	-0.06553
C	-3.51936	-1.93393	-0.18093
C	-3.01295	-0.61873	-0.00116
C	-3.94405	0.40771	0.30267
C	-5.29507	0.13051	0.41406
H	-6.83113	-1.37993	0.31814
H	-5.23312	-3.20765	-0.21454
H	-2.84029	-2.73895	-0.43666
H	-3.60543	1.42232	0.48121
H	-5.98482	0.93128	0.65503
H	3.33593	2.53593	0.18176
H	1.11688	2.79424	-0.32998
C	5.01590	0.69390	0.21767
H	5.33358	1.72423	0.33882
C	4.24502	-1.95292	-0.07959
H	3.93480	-2.98650	-0.18990
C	5.56599	-1.65521	0.08682
H	6.30565	-2.44695	0.10439
C	5.96484	-0.30620	0.24369
H	7.01069	-0.05901	0.38262

38

56-DHA toluene Energy: -955.686856

C	2.79858	1.60600	-0.08728
C	1.48511	1.76131	-0.38612
C	3.63345	0.44331	0.00480
C	0.48435	0.71682	-0.68721
H	0.34689	0.71584	-1.78313
C	0.68195	-0.71678	-0.29845
C	3.21247	-0.94694	-0.11859
C	1.90138	-1.41671	-0.22472
H	1.79253	-2.49832	-0.18174
C	-0.57551	-1.30115	-0.10475
C	-0.97609	1.01176	-0.12946
C	-1.61471	-0.37739	-0.09224
H	-0.71103	-2.36246	0.06587
C	-0.88029	1.54479	1.24079
C	-1.65948	1.98347	-0.99420
N	-2.14643	2.73993	-1.70743
N	-0.79385	1.93624	2.31703
C	-5.78021	-1.14634	0.23318
C	-4.89577	-2.16721	-0.12074
C	-3.54190	-1.91179	-0.23762
C	-3.02293	-0.61674	0.00330
C	-3.93389	0.40262	0.36349
C	-5.28816	0.13656	0.47350
H	-6.84124	-1.34905	0.32052
H	-5.27111	-3.16538	-0.31636
H	-2.87267	-2.70795	-0.54352
H	-3.57847	1.40254	0.58697
H	-5.96617	0.93318	0.75745
H	3.34057	2.53703	0.05496
H	1.12309	2.78114	-0.49602
C	5.00887	0.69584	0.21274
H	5.32396	1.72876	0.31748
C	4.23708	-1.95493	-0.04934
H	3.92883	-2.99056	-0.14592
C	5.55340	-1.65502	0.13612
H	6.29208	-2.44659	0.18201
C	5.95212	-0.30107	0.27665
H	6.99576	-0.05387	0.43115

38
56-TS vacuum Energy: -955.670210

C	2.75085	1.52747	-0.57489
C	1.46976	1.58404	-1.09266
C	3.53561	0.41898	-0.18435
C	0.46103	0.59430	-1.04740
H	-0.16845	0.57096	-1.93957
C	0.60464	-0.76182	-0.45120
C	3.12242	-0.97524	-0.17834
C	1.81003	-1.45423	-0.29285
H	1.69388	-2.52031	-0.10310
C	-0.64268	-1.28230	-0.05905
C	-1.01879	1.02105	0.08736
C	-1.63835	-0.31718	0.05967
H	-0.79354	-2.33164	0.16889
C	-0.32442	1.37505	1.30983
C	-1.72866	2.13674	-0.50034
N	-2.23490	3.02266	-1.03144
N	0.24555	1.65804	2.26802
C	-5.82554	-1.07201	0.16095
C	-4.95850	-1.99199	-0.42556
C	-3.59757	-1.73489	-0.47218
C	-3.07068	-0.55346	0.07970
C	-3.95650	0.36135	0.67412
C	-5.31873	0.10451	0.70724
H	-6.89055	-1.27127	0.19155
H	-5.34887	-2.90513	-0.86039
H	-2.93131	-2.43603	-0.96328
H	-3.57198	1.26470	1.13511
H	-5.98737	0.82027	1.17129
H	3.29458	2.46800	-0.59611
H	1.18718	2.50927	-1.58857
C	4.89290	0.69973	0.15134
H	5.20123	1.73952	0.16848
C	4.12315	-1.96464	0.09720
H	3.81765	-3.00562	0.08644
C	5.41460	-1.64271	0.38863
H	6.13802	-2.42165	0.59846
C	5.80504	-0.27800	0.42961
H	6.82749	-0.01443	0.67373

38

56-TS acetonitrile Energy: -955.688623

C	2.76719	1.53255	-0.57100
C	1.48530	1.60099	-1.07936
C	3.54699	0.41443	-0.18248
C	0.47109	0.61418	-1.04380
H	-0.15588	0.59250	-1.93705
C	0.60501	-0.73888	-0.43650
C	3.12282	-0.97591	-0.17679
C	1.80981	-1.44642	-0.29379
H	1.68543	-2.51436	-0.12453
C	-0.63170	-1.25981	-0.03479
C	-1.04029	1.04473	0.09541
C	-1.64306	-0.30068	0.07204
H	-0.77231	-2.30813	0.20277
C	-0.34198	1.41077	1.30846
C	-1.75718	2.15138	-0.49484
N	-2.27321	3.03271	-1.02506
N	0.23867	1.70096	2.25902
C	-5.81899	-1.11437	0.13834
C	-4.92901	-2.03372	-0.41760
C	-3.57084	-1.75928	-0.44965
C	-3.06756	-0.55624	0.08480
C	-3.97745	0.35695	0.65181
C	-5.33637	0.08028	0.67132
H	-6.88108	-1.32926	0.15896
H	-5.29924	-2.96166	-0.83810
H	-2.88950	-2.46419	-0.91319
H	-3.61482	1.27097	1.10948
H	-6.02163	0.79188	1.11721
H	3.32222	2.46617	-0.60320
H	1.21087	2.53006	-1.57238
C	4.90717	0.68543	0.14325
H	5.22734	1.72171	0.15344
C	4.11674	-1.97701	0.09476
H	3.80230	-3.01505	0.08404
C	5.41202	-1.66416	0.38172
H	6.13085	-2.44796	0.58830
C	5.81323	-0.30215	0.41890
H	6.83954	-0.04681	0.65526

38
56-TS cyclohexane Energy: -955.677323

C	2.75825	1.52925	-0.57358
C	1.47648	1.59081	-1.08662
C	3.54106	0.41683	-0.18438
C	0.46522	0.60261	-1.04464
H	-0.16281	0.57961	-1.93760
C	0.60506	-0.75225	-0.44354
C	3.12298	-0.97557	-0.17678
C	1.80986	-1.45051	-0.29024
H	1.68990	-2.51681	-0.10535
C	-0.63829	-1.27285	-0.04768
C	-1.02725	1.03053	0.09090
C	-1.64036	-0.31028	0.06527
H	-0.78501	-2.32163	0.18502
C	-0.33345	1.39057	1.31076
C	-1.73955	2.14251	-0.49878
N	-2.24809	3.02690	-1.03055
N	0.23655	1.67867	2.26771
C	-5.82285	-1.09016	0.15006
C	-4.94593	-2.00967	-0.42375
C	-3.58623	-1.74497	-0.46389
C	-3.06962	-0.55463	0.08133
C	-3.96574	0.35925	0.66412
C	-5.32657	0.09397	0.69103
H	-6.88668	-1.29607	0.17599
H	-5.32768	-2.92892	-0.85321
H	-2.91329	-2.44721	-0.94396
H	-3.59068	1.26722	1.12383
H	-6.00237	0.80814	1.14707
H	3.30641	2.46705	-0.59936
H	1.19725	2.51770	-1.58122
C	4.89994	0.69335	0.14564
H	5.21328	1.73167	0.15960
C	4.12058	-1.96984	0.09748
H	3.81083	-3.00949	0.08891
C	5.41405	-1.65194	0.38515
H	6.13540	-2.43292	0.59420
C	5.80943	-0.28847	0.42267
H	6.83375	-0.02851	0.66275

38
56-TS ethanol Energy: -955.688206

C	2.76705	1.53246	-0.57091
C	1.48510	1.60077	-1.07925
C	3.54694	0.41447	-0.18255
C	0.47095	0.61395	-1.04351
H	-0.15598	0.59226	-1.93681
C	0.60505	-0.73920	-0.43646
C	3.12288	-0.97590	-0.17672
C	1.80981	-1.44645	-0.29340
H	1.68551	-2.51431	-0.12347
C	-0.63191	-1.26011	-0.03500
C	-1.03992	1.04434	0.09537
C	-1.64300	-0.30092	0.07192
H	-0.77269	-2.30845	0.20243
C	-0.34208	1.41036	1.30879
C	-1.75656	2.15113	-0.49506
N	-2.27213	3.03257	-1.02552
N	0.23771	1.70079	2.25977
C	-5.81909	-1.11389	0.13848
C	-4.92937	-2.03331	-0.41767
C	-3.57118	-1.75903	-0.44991
C	-3.06765	-0.55620	0.08463
C	-3.97728	0.35707	0.65176
C	-5.33623	0.08064	0.67141
H	-6.88122	-1.32860	0.15923
H	-5.29982	-2.96112	-0.83826
H	-2.88998	-2.46389	-0.91374
H	-3.61440	1.27107	1.10929
H	-6.02131	0.79239	1.11732
H	3.32187	2.46620	-0.60288
H	1.21051	2.52983	-1.57220
C	4.90715	0.68555	0.14308
H	5.22716	1.72188	0.15342
C	4.11687	-1.97684	0.09478
H	3.80248	-3.01491	0.08428
C	5.41219	-1.66393	0.38146
H	6.13107	-2.44769	0.58805
C	5.81330	-0.30191	0.41856
H	6.83961	-0.04650	0.65486

38

56-TS toluene Energy: -955.678671

C	2.75965	1.52968	-0.57305
C	1.47780	1.59224	-1.08531
C	3.54207	0.41646	-0.18418
C	0.46609	0.60429	-1.04420
H	-0.16163	0.58147	-1.93734
C	0.60515	-0.75038	-0.44234
C	3.12306	-0.97561	-0.17658
C	1.80985	-1.44982	-0.29015
H	1.68921	-2.51624	-0.10669
C	-0.63744	-1.27105	-0.04589
C	-1.02893	1.03237	0.09145
C	-1.64074	-0.30899	0.06609
H	-0.78336	-2.31976	0.18750
C	-0.33517	1.39343	1.31076
C	-1.74171	2.14364	-0.49856
N	-2.25082	3.02770	-1.03039
N	0.23517	1.68230	2.26735
C	-5.82233	-1.09360	0.14834
C	-4.94362	-2.01307	-0.42304
C	-3.58414	-1.74696	-0.46215
C	-3.06940	-0.55487	0.08159
C	-3.96740	0.35890	0.66217
C	-5.32796	0.09202	0.68812
H	-6.88592	-1.30077	0.17357
H	-5.32378	-2.93353	-0.85129
H	-2.91003	-2.44950	-0.94006
H	-3.59407	1.26778	1.12150
H	-6.00505	0.80591	1.14267
H	3.30869	2.46695	-0.59959
H	1.19921	2.51950	-1.57956
C	4.90121	0.69215	0.14496
H	5.21551	1.73017	0.15844
C	4.12009	-1.97084	0.09731
H	3.80955	-3.01024	0.08885
C	5.41390	-1.65373	0.38449
H	6.13486	-2.43512	0.59327
C	5.81020	-0.29049	0.42167
H	6.83484	-0.03124	0.66108

38

56-VHF vacuum Energy: -955.722400

C	-3.53085	-0.39860	1.80599
C	-2.34341	-0.62564	2.42996
C	-3.86260	-0.32048	0.39086
C	-1.05636	-0.84361	1.88494
H	-0.25496	-0.99531	2.59753
C	-0.70874	-0.84550	0.52623
C	-2.94623	-0.46829	-0.68745
C	-1.51821	-0.71114	-0.57410
H	-1.01598	-0.76721	-1.53450
C	0.74923	-0.99839	0.24308
C	1.40024	1.38897	0.27850
C	1.68126	-0.00334	0.13205
H	1.11552	-2.01264	0.11222
C	2.44753	2.34778	0.27208
C	0.11315	1.94451	0.47967
N	-0.90680	2.45649	0.64817
N	3.28031	3.14659	0.27101
C	5.71045	-1.20755	-0.69296
C	5.04028	-1.72032	0.41230
C	3.73637	-1.32060	0.68248
C	3.09347	-0.40217	-0.14818
C	3.77321	0.11159	-1.25371
C	5.07422	-0.29218	-1.52560
H	6.72763	-1.51727	-0.90343
H	5.53386	-2.42676	1.06967
H	3.21756	-1.70840	1.55308
H	3.28123	0.82417	-1.90733
H	5.59159	0.11037	-2.38861
H	-2.38405	-0.63383	3.51537
C	-5.20957	-0.08043	0.08886
H	-5.90742	0.03600	0.91112
C	-5.67586	0.01535	-1.21484
H	-6.72618	0.20328	-1.40332
C	-4.78217	-0.12973	-2.26817
H	-5.12188	-0.05780	-3.29456
C	-3.44238	-0.36543	-1.99580
H	-2.74637	-0.47374	-2.82048
H	-4.38331	-0.25133	2.46181

38
56-VHF acetonitrile Energy: -955.722720

C	-3.32297	1.11889	1.42183
C	-2.05378	1.31784	1.87193
C	-3.86086	0.14057	0.48451
C	-0.85170	0.66318	1.51540
H	0.04894	0.99825	2.01467
C	-0.71078	-0.39537	0.58844
C	-3.11596	-0.85955	-0.19946
C	-1.67950	-1.06844	-0.11303
H	-1.32008	-1.87553	-0.74502
C	0.67167	-0.83334	0.33453
C	1.51172	1.34074	-0.45027
C	1.71280	0.00674	-0.02177
H	0.89938	-1.88834	0.44871
C	2.59371	2.26418	-0.52377
C	0.27943	1.85569	-0.93225
N	-0.68333	2.30831	-1.38051
N	3.44474	3.04065	-0.56929
C	5.68269	-1.58363	0.11852
C	4.82424	-1.74771	1.20213
C	3.53647	-1.22509	1.15540
C	3.10002	-0.52694	0.02608
C	3.96679	-0.36646	-1.05923
C	5.25089	-0.89560	-1.01299
H	6.68577	-1.99282	0.15416
H	5.15722	-2.27929	2.08589
H	2.87054	-1.34173	2.00397
H	3.62873	0.15343	-1.94953
H	5.91250	-0.77557	-1.86288
H	-1.93873	2.11380	2.60195
C	-5.24399	0.20305	0.26275
H	-5.81596	0.96343	0.78345
C	-5.90087	-0.67199	-0.59374
H	-6.97161	-0.58714	-0.73662
C	-5.17342	-1.65071	-1.26050
H	-5.66496	-2.34333	-1.93308
C	-3.80193	-1.73216	-1.05955
H	-3.23408	-2.49289	-1.58424
H	-4.07562	1.78165	1.83735

38
56-VHF cyclohexane Energy: -955.719597

C	-3.49012	0.09494	1.84448
C	-2.30532	0.01361	2.50443
C	-3.83282	-0.19647	0.45752
C	-1.02292	-0.36268	2.02910
H	-0.21525	-0.33253	2.75046
C	-0.69336	-0.73487	0.71841
C	-2.93310	-0.64975	-0.54561
C	-1.50822	-0.88446	-0.37825
H	-1.01308	-1.20223	-1.29046
C	0.75548	-0.95874	0.47156
C	1.35733	1.37691	-0.05362
C	1.67424	0.00487	0.12833
H	1.13084	-1.97264	0.57588
C	2.38422	2.33953	-0.26581
C	0.05570	1.93871	-0.01575
N	-0.97018	2.46642	-0.00205
N	3.19357	3.14361	-0.43238
C	5.72779	-1.27191	-0.40530
C	5.06291	-1.53825	0.78729
C	3.74964	-1.11579	0.96157
C	3.09403	-0.41817	-0.05405
C	3.76714	-0.15184	-1.24782
C	5.07737	-0.58010	-1.42277
H	6.75150	-1.60110	-0.54125
H	5.56752	-2.07016	1.58549
H	3.23412	-1.31208	1.89602
H	3.26204	0.38184	-2.04620
H	5.58976	-0.37305	-2.35498
H	-2.33697	0.29208	3.55377
C	-5.17698	-0.00982	0.10751
H	-5.86340	0.33905	0.87153
C	-5.65418	-0.25207	-1.17329
H	-6.70152	-0.09320	-1.40103
C	-4.77554	-0.69633	-2.15377
H	-5.12456	-0.89131	-3.16084
C	-3.43921	-0.88642	-1.83331
H	-2.75438	-1.22885	-2.60158
H	-4.33478	0.42855	2.43917

38

56-VHF ethanol Energy: -955.723044

C	-3.32750	1.10407	1.43718
C	-2.06130	1.30147	1.89524
C	-3.85861	0.13419	0.48693
C	-0.85599	0.65153	1.53908
H	0.04240	0.98685	2.04233
C	-0.70941	-0.40012	0.60651
C	-3.10867	-0.85885	-0.20155
C	-1.67269	-1.06848	-0.10659
H	-1.30870	-1.87067	-0.74218
C	0.67626	-0.83397	0.35649
C	1.50280	1.33616	-0.45442
C	1.71090	0.00637	-0.01532
H	0.91100	-1.88544	0.48801
C	2.58281	2.25993	-0.54896
C	0.26409	1.84726	-0.92343
N	-0.70467	2.29771	-1.36082
N	3.43245	3.03670	-0.61196
C	5.68778	-1.56794	0.11377
C	4.83916	-1.71961	1.20684
C	3.54917	-1.20218	1.16366
C	3.10068	-0.52171	0.02838
C	3.95758	-0.37351	-1.06631
C	5.24394	-0.89747	-1.02354
H	6.69262	-1.97299	0.14668
H	5.18154	-2.23738	2.09520
H	2.89089	-1.30901	2.01946
H	3.61028	0.13309	-1.96071
H	5.89795	-0.78693	-1.88056
H	-1.95108	2.09205	2.63180
C	-5.24018	0.19831	0.25637
H	-5.81595	0.95347	0.78048
C	-5.89081	-0.66841	-0.61315
H	-6.96058	-0.58257	-0.76257
C	-5.15834	-1.64020	-1.28448
H	-5.64494	-2.32635	-1.96721
C	-3.78830	-1.72320	-1.07480
H	-3.21655	-2.47862	-1.60291
H	-4.08355	1.76192	1.85431

38

56-VHF toluene Energy: -955.720904

C	-3.48055	0.25860	1.82852
C	-2.29344	0.23035	2.48877
C	-3.83031	-0.15307	0.47426
C	-1.01426	-0.19023	2.04239
H	-0.20305	-0.10095	2.75493
C	-0.69155	-0.67577	0.76755
C	-2.93649	-0.69481	-0.48945
C	-1.51133	-0.91654	-0.30934
H	-1.02050	-1.31254	-1.19294
C	0.75495	-0.92342	0.53563
C	1.35596	1.36534	-0.16576
C	1.67409	0.01233	0.12097
H	1.12832	-1.92747	0.71488
C	2.38267	2.31098	-0.44678
C	0.05363	1.92694	-0.17813
N	-0.97246	2.45370	-0.21185
N	3.19168	3.10131	-0.67057
C	5.72990	-1.29921	-0.29757
C	5.05889	-1.47658	0.90824
C	3.74481	-1.04267	1.04402
C	3.09451	-0.42227	-0.02392
C	3.77356	-0.24507	-1.23091
C	5.08469	-0.68489	-1.36689
H	6.75420	-1.63742	-0.40366
H	5.55915	-1.94794	1.74623
H	3.22436	-1.16938	1.98773
H	3.27251	0.22711	-2.06953
H	5.60171	-0.54797	-2.30943
H	-2.31957	0.59911	3.51000
C	-5.17613	0.00520	0.11545
H	-5.85832	0.42177	0.84872
C	-5.65982	-0.34802	-1.13661
H	-6.70797	-0.20759	-1.37257
C	-4.78678	-0.87930	-2.07849
H	-5.14120	-1.16186	-3.06264
C	-3.44931	-1.04324	-1.74910
H	-2.76884	-1.45380	-2.48725
H	-4.32156	0.64592	2.39517

38
67-DHA vacuum Energy: -955.636237

C	-3.61400	0.91680	-0.01656
C	-2.83166	2.11249	-0.00421
C	-1.46494	2.32696	-0.02524
C	-0.44330	1.39207	-0.17559
C	-0.60669	-0.02368	-0.61376
C	-1.80421	-0.83547	-0.37047
C	0.94338	1.64229	-0.01652
C	1.70806	0.51050	-0.06187
C	0.75526	-0.68773	-0.14749
C	1.16750	-1.73058	-1.09686
N	1.44392	-2.53171	-1.87144
H	-3.42521	3.01553	0.10800
H	-1.14445	3.35475	0.12489
H	-0.49853	0.02372	-1.72054
H	-1.64222	-1.90354	-0.50491
H	1.34092	2.63341	0.17012
C	3.15041	0.38141	0.01966
C	3.76179	-0.83249	0.37428
C	3.97512	1.49010	-0.24412
C	5.14311	-0.92824	0.46962
H	3.16016	-1.70638	0.59986
C	5.35248	1.39016	-0.14168
H	3.52849	2.42762	-0.55644
C	5.94495	0.17973	0.21545
H	5.59385	-1.87359	0.74875
H	5.97039	2.25533	-0.35397
H	7.02339	0.10123	0.28925
C	0.57894	-1.27938	1.19076
N	0.43302	-1.72187	2.24028
C	-3.11806	-0.44324	-0.13923
C	-4.08031	-1.49847	-0.04956
C	-5.42469	-1.27156	0.12440
C	-5.90163	0.04584	0.21466
C	-5.00474	1.09582	0.14303
H	-3.71791	-2.51791	-0.12987
H	-6.11079	-2.10824	0.18504
H	-5.37799	2.11172	0.22277
H	-6.95938	0.24142	0.34311

38
67-DHA acetonitrile Energy: -955.657096

C	-3.62243	0.91682	-0.03270
C	-2.83363	2.11751	-0.03793
C	-1.47236	2.32435	-0.04190
C	-0.44777	1.37848	-0.16725
C	-0.61868	-0.04398	-0.59993
C	-1.81295	-0.85105	-0.28624
C	0.92804	1.63473	-0.01479
C	1.70497	0.50342	-0.07667
C	0.75610	-0.69975	-0.17018
C	1.16963	-1.72060	-1.14316
N	1.46488	-2.49896	-1.93355
H	-3.42755	3.02332	0.04243
H	-1.14659	3.35306	0.08691
H	-0.56036	-0.00695	-1.70765
H	-1.65169	-1.92572	-0.34836
H	1.31942	2.62761	0.17352
C	3.14236	0.38288	0.01594
C	3.76985	-0.84362	0.30766
C	3.96005	1.51660	-0.17244
C	5.15193	-0.92837	0.41167
H	3.18244	-1.73945	0.47824
C	5.33758	1.42526	-0.06296
H	3.50830	2.46871	-0.42658
C	5.94397	0.20222	0.22875
H	5.61118	-1.88271	0.64248
H	5.94562	2.30959	-0.21609
H	7.02242	0.13260	0.30912
C	0.62069	-1.31374	1.16443
N	0.51107	-1.75387	2.21945
C	-3.12533	-0.44829	-0.09007
C	-4.09230	-1.50341	0.03377
C	-5.43813	-1.26653	0.16945
C	-5.91282	0.05531	0.18922
C	-5.01166	1.10398	0.09149
H	-3.72987	-2.52550	0.00404
H	-6.12838	-2.09760	0.25372
H	-5.38685	2.12145	0.12319
H	-6.97248	0.25818	0.28679

38
67-DHA cyclohexane Energy: -955.644051

C	-3.61700	0.91768	-0.02218
C	-2.83204	2.11482	-0.01280
C	-1.46701	2.32605	-0.02586
C	-0.44439	1.38737	-0.16779
C	-0.61028	-0.03054	-0.60566
C	-1.80758	-0.84096	-0.33944
C	0.93856	1.63934	-0.01152
C	1.70767	0.50783	-0.06434
C	0.75584	-0.69195	-0.15154
C	1.16728	-1.72862	-1.10836
N	1.44792	-2.52362	-1.88762
H	-3.42548	3.01905	0.08905
H	-1.14473	3.35395	0.11876
H	-0.51848	0.01439	-1.71276
H	-1.64632	-1.91207	-0.44788
H	1.33455	2.63064	0.17681
C	3.14842	0.38197	0.01789
C	3.76634	-0.83616	0.35061
C	3.96997	1.49982	-0.22311
C	5.14813	-0.92775	0.44583
H	3.17032	-1.71798	0.55977
C	5.34764	1.40328	-0.12138
H	3.52071	2.44243	-0.51534
C	5.94586	0.18851	0.21325
H	5.60246	-1.87617	0.70828
H	5.96170	2.27536	-0.31567
H	7.02452	0.11345	0.28691
C	0.59335	-1.29186	1.18551
N	0.45864	-1.73601	2.23583
C	-3.12078	-0.44451	-0.12274
C	-4.08532	-1.49997	-0.02467
C	-5.43035	-1.26912	0.13313
C	-5.90634	0.05042	0.19957
C	-5.00756	1.09989	0.12239
H	-3.72279	-2.52056	-0.08725
H	-6.11829	-2.10380	0.19967
H	-5.38155	2.11650	0.18604
H	-6.96503	0.24883	0.31537

38
67-DHA ethanol Energy: -955.656611
C -3.62246 0.91689 -0.03256
C -2.83374 2.11741 -0.03700
C -1.47232 2.32436 -0.04054
C -0.44779 1.37873 -0.16611
C -0.61864 -0.04363 -0.59880
C -1.81282 -0.85084 -0.28576
C 0.92830 1.63484 -0.01377
C 1.70505 0.50364 -0.07588
C 0.75621 -0.69951 -0.16946
C 1.16929 -1.72008 -1.14298
N 1.46354 -2.49842 -1.93377
H -3.42767 3.02321 0.04358
H -1.14672 3.35306 0.08886
H -0.56027 -0.00615 -1.70658
H -1.65139 -1.92548 -0.34799
H 1.31983 2.62765 0.17470
C 3.14259 0.38301 0.01603
C 3.76994 -0.84342 0.30789
C 3.96028 1.51647 -0.17328
C 5.15203 -0.92836 0.41129
H 3.18238 -1.73904 0.47906
C 5.33784 1.42500 -0.06438
H 3.50851 2.46849 -0.42774
C 5.94412 0.20201 0.22757
H 5.61122 -1.88269 0.64222
H 5.94597 2.30915 -0.21822
H 7.02260 0.13226 0.30747
C 0.62098 -1.31424 1.16478
N 0.51143 -1.75574 2.21922
C -3.12535 -0.44818 -0.09003
C -4.09228 -1.50324 0.03318
C -5.43821 -1.26647 0.16819
C -5.91301 0.05532 0.18792
C -5.01187 1.10397 0.09092
H -3.72976 -2.52530 0.00364
H -6.12843 -2.09761 0.25204
H -5.38706 2.12143 0.12266
H -6.97274 0.25810 0.28496

38
67-DHA toluene Energy: -955.645607

C	-3.61747	0.91775	-0.02321
C	-2.83205	2.11525	-0.01494
C	-1.46741	2.32593	-0.02702
C	-0.44458	1.38649	-0.16736
C	-0.61094	-0.03187	-0.60497
C	-1.80819	-0.84196	-0.33441
C	0.93760	1.63885	-0.01156
C	1.70753	0.50732	-0.06539
C	0.75586	-0.69274	-0.15270
C	1.16728	-1.72857	-1.11049
N	1.44900	-2.52261	-1.89031
H	-3.42549	3.01966	0.08499
H	-1.14475	3.35388	0.11623
H	-0.52198	0.01225	-1.71209
H	-1.64710	-1.91353	-0.43843
H	1.33322	2.63026	0.17682
C	3.14793	0.38202	0.01751
C	3.76695	-0.83695	0.34613
C	3.96903	1.50156	-0.21868
C	5.14880	-0.92782	0.44178
H	3.17190	-1.72024	0.55187
C	5.34673	1.40558	-0.11662
H	3.51945	2.44517	-0.50704
C	5.94590	0.18996	0.21371
H	5.60371	-1.87683	0.70108
H	5.96013	2.27895	-0.30715
H	7.02456	0.11549	0.28767
C	0.59575	-1.29351	1.18437
N	0.46313	-1.73707	2.23522
C	-3.12120	-0.44480	-0.11984
C	-4.08610	-1.50033	-0.01978
C	-5.43119	-1.26880	0.13566
C	-5.90697	0.05108	0.19789
C	-5.00789	1.10050	0.11920
H	-3.72359	-2.52110	-0.07930
H	-6.11943	-2.10311	0.20359
H	-5.38200	2.11722	0.17999
H	-6.96577	0.24998	0.31182

38
67-TS vacuum Energy: -955.634082

C	-3.48646	0.89650	0.02402
C	-2.73684	2.12756	-0.01493
C	-1.40159	2.37857	-0.19281
C	-0.37411	1.44031	-0.41592
C	-0.56566	0.08793	-1.00256
C	-1.78408	-0.63884	-1.06430
C	0.97803	1.63991	-0.08200
C	1.69861	0.46405	-0.01218
C	0.73614	-0.68028	-0.06224
C	1.16388	-1.88846	-0.75096
N	1.45215	-2.82307	-1.35463
H	-3.33121	3.00234	0.23594
H	-1.07655	3.40077	-0.01395
H	-0.03723	0.04239	-1.96436
H	-1.72716	-1.55512	-1.64727
H	1.39051	2.61531	0.14968
C	3.14060	0.31317	0.07494
C	3.72111	-0.83505	0.63707
C	3.98615	1.33978	-0.37929
C	5.09994	-0.95103	0.73787
H	3.09048	-1.63065	1.01942
C	5.36239	1.22330	-0.26736
H	3.55443	2.21809	-0.84703
C	5.92523	0.07605	0.28905
H	5.53153	-1.84333	1.17623
H	6.00113	2.02142	-0.62824
H	7.00213	-0.01709	0.36961
C	0.11792	-0.97877	1.22297
N	-0.39315	-1.20280	2.22781
C	-3.03258	-0.38269	-0.44729
C	-3.95411	-1.46075	-0.39941
C	-5.22428	-1.32855	0.11958
C	-5.65632	-0.08466	0.59384
C	-4.79764	0.99758	0.52452
H	-3.62735	-2.42445	-0.77543
H	-5.88574	-2.18660	0.15323
H	-5.14146	1.96829	0.86721
H	-6.65448	0.03602	0.99718

38
67-TS acetonitrile Energy: -955.652684

C	-3.48466	0.90044	0.03276
C	-2.72860	2.13105	-0.02351
C	-1.39691	2.37274	-0.22094
C	-0.37488	1.42108	-0.43584
C	-0.57738	0.06914	-1.02296
C	-1.80275	-0.64893	-1.07225
C	0.97206	1.62597	-0.10064
C	1.70030	0.45233	-0.02342
C	0.74900	-0.70230	-0.07196
C	1.18691	-1.90597	-0.75653
N	1.48872	-2.83912	-1.35637
H	-3.31592	3.01111	0.22401
H	-1.06327	3.39544	-0.06511
H	-0.04726	0.01366	-1.98145
H	-1.75998	-1.56742	-1.65255
H	1.37903	2.60469	0.12489
C	3.14036	0.31401	0.07882
C	3.72905	-0.83224	0.64149
C	3.97948	1.35295	-0.36517
C	5.10883	-0.93544	0.75117
H	3.10639	-1.63467	1.02287
C	5.35644	1.24713	-0.24637
H	3.54426	2.23242	-0.82675
C	5.92734	0.10170	0.30887
H	5.54658	-1.82313	1.19263
H	5.98940	2.05332	-0.59869
H	7.00442	0.01887	0.39616
C	0.12361	-1.00040	1.20631
N	-0.40758	-1.21357	2.20368
C	-3.04371	-0.38238	-0.44443
C	-3.97724	-1.45394	-0.39258
C	-5.24124	-1.31058	0.13866
C	-5.65701	-0.06361	0.62301
C	-4.78918	1.01275	0.54746
H	-3.66529	-2.41852	-0.77892
H	-5.91198	-2.16137	0.17286
H	-5.12264	1.98616	0.89198
H	-6.65051	0.06530	1.03504

38
67-TS cyclohexane Energy: -955.641048

C	-3.48746	0.89789	0.02684
C	-2.73406	2.12743	-0.01378
C	-1.39947	2.37442	-0.19726
C	-0.37439	1.43170	-0.41930
C	-0.57046	0.07950	-1.00631
C	-1.79119	-0.64367	-1.06393
C	0.97623	1.63361	-0.08652
C	1.70050	0.45888	-0.01367
C	0.74287	-0.68948	-0.05890
C	1.17208	-1.89756	-0.74437
N	1.46219	-2.83302	-1.34612
H	-3.32489	3.00414	0.23830
H	-1.07080	3.39612	-0.02318
H	-0.03928	0.02836	-1.96551
H	-1.73927	-1.56144	-1.64488
H	1.38652	2.61050	0.14206
C	3.14217	0.31373	0.07527
C	3.72811	-0.83234	0.63787
C	3.98355	1.34443	-0.37976
C	5.10768	-0.94303	0.73736
H	3.10207	-1.62997	1.02363
C	5.36046	1.23257	-0.26981
H	3.54875	2.22224	-0.84539
C	5.92862	0.08712	0.28616
H	5.54321	-1.83283	1.17682
H	5.99559	2.03320	-0.63131
H	7.00591	-0.00187	0.36545
C	0.12249	-0.98487	1.22453
N	-0.39374	-1.20330	2.22818
C	-3.03828	-0.38257	-0.44664
C	-3.96588	-1.45709	-0.40269
C	-5.23518	-1.32002	0.11671
C	-5.66131	-0.07509	0.59532
C	-4.79792	1.00394	0.52841
H	-3.64418	-2.42084	-0.78284
H	-5.90113	-2.17469	0.14734
H	-5.13774	1.97539	0.87266
H	-6.65882	0.04900	0.99922

38
67-TS ethanol Energy: -955.652236

C	-3.48507	0.90031	0.03248
C	-2.72892	2.13072	-0.02262
C	-1.39703	2.37255	-0.21925
C	-0.37492	1.42129	-0.43465
C	-0.57721	0.06932	-1.02172
C	-1.80235	-0.64896	-1.07133
C	0.97223	1.62616	-0.09981
C	1.70043	0.45253	-0.02277
C	0.74899	-0.70194	-0.07069
C	1.18642	-1.90586	-0.75519
N	1.48767	-2.83916	-1.35507
H	-3.31628	3.01066	0.22529
H	-1.06354	3.39514	-0.06234
H	-0.04688	0.01382	-1.98014
H	-1.75913	-1.56751	-1.65152
H	1.37932	2.60485	0.12566
C	3.14060	0.31408	0.07853
C	3.72947	-0.83207	0.64108
C	3.97959	1.35272	-0.36629
C	5.10929	-0.93548	0.74983
H	3.10688	-1.63431	1.02294
C	5.35660	1.24674	-0.24836
H	3.54417	2.23207	-0.82793
C	5.92767	0.10138	0.30677
H	5.54716	-1.82320	1.19111
H	5.98947	2.05273	-0.60136
H	7.00480	0.01836	0.39332
C	0.12410	-0.99972	1.20796
N	-0.40599	-1.21300	2.20588
C	-3.04376	-0.38245	-0.44446
C	-3.97726	-1.45399	-0.39351
C	-5.24169	-1.31073	0.13663
C	-5.65792	-0.06381	0.62069
C	-4.79007	1.01251	0.54604
H	-3.66486	-2.41854	-0.77953
H	-5.91239	-2.16158	0.17029
H	-5.12378	1.98585	0.89054
H	-6.65176	0.06500	1.03195

38
67-TS toluene Energy: -955.642416

C	-3.48758	0.89819	0.02739
C	-2.73357	2.12757	-0.01409
C	-1.39915	2.37381	-0.19870
C	-0.37450	1.43015	-0.42027
C	-0.57138	0.07797	-1.00728
C	-1.79258	-0.64462	-1.06395
C	0.97580	1.63250	-0.08761
C	1.70072	0.45797	-0.01428
C	0.74398	-0.69120	-0.05907
C	1.17379	-1.89898	-0.74423
N	1.46474	-2.83436	-1.34573
H	-3.32381	3.00468	0.23783
H	-1.06982	3.39549	-0.02600
H	-0.04002	0.02600	-1.96621
H	-1.74160	-1.56267	-1.64452
H	1.38570	2.60965	0.14042
C	3.14229	0.31385	0.07543
C	3.72906	-0.83202	0.63792
C	3.98302	1.34549	-0.37910
C	5.10873	-0.94170	0.73767
H	3.10376	-1.63020	1.02378
C	5.36003	1.23450	-0.26903
H	3.54779	2.22337	-0.84417
C	5.92899	0.08921	0.28670
H	5.54488	-1.83115	1.17721
H	5.99459	2.03575	-0.63010
H	7.00633	0.00103	0.36615
C	0.12336	-0.98648	1.22401
N	-0.39389	-1.20412	2.22735
C	-3.03929	-0.38260	-0.44634
C	-3.96790	-1.45655	-0.40250
C	-5.23693	-1.31854	0.11729
C	-5.66194	-0.07333	0.59648
C	-4.79775	1.00518	0.52948
H	-3.64720	-2.42039	-0.78325
H	-5.90365	-2.17262	0.14773
H	-5.13684	1.97684	0.87379
H	-6.65924	0.05144	1.00065

38
67-VHF vacuum Energy: -955.667949

C	-3.86462	-1.02808	-0.12847
C	-2.74318	-1.94101	-0.25567
C	-1.40194	-1.74246	-0.24069
C	-0.61177	-0.55007	-0.09874
C	-1.20940	0.74472	0.01906
C	-2.51238	1.12346	0.06238
C	0.79965	-0.76752	-0.10053
C	1.88946	0.05695	-0.01470
C	1.80133	1.52917	0.09684
C	1.72205	2.14863	1.35772
N	1.63890	2.63198	2.40467
H	-3.04613	-2.97713	-0.37822
H	-0.81810	-2.65206	-0.35296
H	-0.52814	1.57882	0.08466
H	-2.66415	2.19503	0.15378
H	1.07175	-1.81239	-0.21964
C	3.26283	-0.50743	-0.00927
C	4.32774	0.16246	-0.62464
C	3.52395	-1.73106	0.62187
C	5.60245	-0.39075	-0.63677
H	4.16488	1.11227	-1.12070
C	4.79804	-2.28200	0.60639
H	2.72961	-2.23769	1.15846
C	5.84355	-1.61637	-0.02648
H	6.40913	0.14034	-1.12910
H	4.97828	-3.22659	1.10723
H	6.83936	-2.04416	-0.03329
C	1.85769	2.35697	-1.03923
N	1.89544	3.01009	-1.99289
C	-3.75748	0.37732	0.01921
C	-4.93702	1.13050	0.12822
C	-6.19084	0.54276	0.09793
C	-6.29578	-0.83814	-0.04735
C	-5.14525	-1.60145	-0.15882
H	-4.85506	2.20635	0.23973
H	-7.08005	1.15572	0.18566
H	-5.22775	-2.67708	-0.27341
H	-7.26827	-1.31553	-0.07426

38

67-VHF acetonitrile Energy: -955.669382

C	-3.74067	1.04576	0.03719
C	-2.70708	2.05546	-0.14514
C	-1.38013	1.94598	-0.37552
C	-0.55705	0.77000	-0.54810
C	-1.13469	-0.49986	-0.92884
C	-2.40348	-0.94985	-0.80574
C	0.82237	0.95735	-0.39976
C	1.83824	0.02596	-0.18276
C	1.53239	-1.39611	0.01802
C	1.61488	-2.32735	-1.04124
N	1.69599	-3.04776	-1.93961
H	-3.06780	3.07150	-0.01378
H	-0.83299	2.88513	-0.38842
H	-0.46830	-1.18707	-1.43281
H	-2.56765	-1.96007	-1.17106
H	1.13550	1.99389	-0.32477
C	3.24105	0.42813	0.00630
C	4.17143	-0.43983	0.60609
C	3.70344	1.68468	-0.43005
C	5.49301	-0.05350	0.79661
H	3.87174	-1.42687	0.93939
C	5.02343	2.06278	-0.24068
H	3.03737	2.36403	-0.94739
C	5.92696	1.20004	0.38000
H	6.18470	-0.74068	1.27016
H	5.35334	3.03424	-0.59091
H	6.95850	1.49923	0.52391
C	1.25737	-1.87618	1.31779
N	1.00989	-2.20564	2.39665
C	-3.59918	-0.33274	-0.25248
C	-4.69954	-1.18317	-0.04975
C	-5.90371	-0.71497	0.44825
C	-6.04399	0.64274	0.73399
C	-4.97913	1.50225	0.51890
H	-4.59274	-2.23551	-0.29040
H	-6.73008	-1.39811	0.60418
H	-5.09606	2.55996	0.72907
H	-6.98225	1.02865	1.11498

38
67-VHF cyclohexane Energy: -955.664263

C	-3.86604	1.02223	0.12583
C	-2.75041	1.94365	0.26762
C	-1.40999	1.75654	0.26694
C	-0.60699	0.56542	0.13091
C	-1.20068	-0.73769	0.02418
C	-2.49868	-1.12316	-0.02842
C	0.79163	0.79016	0.12993
C	1.88930	-0.04085	0.03417
C	1.78260	-1.50389	-0.08720
C	1.68748	-2.10819	-1.35820
N	1.59389	-2.56873	-2.41342
H	-3.06255	2.97749	0.38627
H	-0.83269	2.66964	0.38402
H	-0.51477	-1.57050	-0.01875
H	-2.64431	-2.19677	-0.10614
H	1.06184	1.83492	0.25060
C	3.26442	0.50748	0.01438
C	4.34604	-0.22610	0.52383
C	3.52338	1.77474	-0.53116
C	5.63127	0.30247	0.51860
H	4.18987	-1.20943	0.95207
C	4.80788	2.29940	-0.53321
H	2.71983	2.33975	-0.98916
C	5.86915	1.56844	-0.00469
H	6.44836	-0.28018	0.92844
H	4.98399	3.27749	-0.96655
H	6.87245	1.97817	-0.01175
C	1.84225	-2.34466	1.04365
N	1.88369	-3.00045	1.99396
C	-3.74971	-0.38198	-0.01210
C	-4.92228	-1.14333	-0.13719
C	-6.17987	-0.56193	-0.13241
C	-6.29429	0.81925	0.00402
C	-5.14963	1.58967	0.13196
H	-4.83252	-2.21935	-0.24087
H	-7.06416	-1.18004	-0.23254
H	-5.24001	2.66528	0.24019
H	-7.26950	1.29171	0.01168

38

67-VHF ethanol Energy: -955.669294

C	-3.74470	1.04565	0.04061
C	-2.70768	2.05320	-0.13328
C	-1.38028	1.94172	-0.36052
C	-0.55853	0.76559	-0.53700
C	-1.13730	-0.50345	-0.91775
C	-2.40732	-0.95128	-0.79929
C	0.82165	0.95285	-0.39170
C	1.83990	0.02341	-0.17950
C	1.53934	-1.39999	0.02017
C	1.61681	-2.32843	-1.04187
N	1.69280	-3.04697	-1.94221
H	-3.06625	3.06957	0.00146
H	-0.83158	2.88002	-0.36778
H	-0.47030	-1.19299	-1.41758
H	-2.57132	-1.96160	-1.16440
H	1.13410	1.98954	-0.31566
C	3.24249	0.42952	0.00474
C	4.17629	-0.43306	0.60675
C	3.70070	1.68487	-0.43899
C	5.49726	-0.04246	0.79230
H	3.87972	-1.41896	0.94603
C	5.02017	2.06736	-0.25445
H	3.03167	2.35953	-0.95870
C	5.92718	1.21006	0.36846
H	6.19173	-0.72552	1.26778
H	5.34684	3.03781	-0.61048
H	6.95831	1.51247	0.50854
C	1.27439	-1.88461	1.32026
N	1.03567	-2.21920	2.39953
C	-3.60481	-0.33241	-0.25181
C	-4.70817	-1.18065	-0.05709
C	-5.91409	-0.71083	0.43523
C	-6.05278	0.64640	0.72365
C	-4.98461	1.50382	0.51681
H	-4.60250	-2.23271	-0.29944
H	-6.74287	-1.39245	0.58489
H	-5.10006	2.56123	0.72932
H	-6.99220	1.03357	1.10047

38

67-VHF toluene Energy: -955.666369

C	-3.86652	1.02076	0.12229
C	-2.75258	1.94399	0.26720
C	-1.41212	1.75961	0.27054
C	-0.60609	0.56904	0.13728
C	-1.19864	-0.73581	0.03582
C	-2.49575	-1.12304	-0.01893
C	0.79035	0.79682	0.13348
C	1.88977	-0.03492	0.03538
C	1.77638	-1.49725	-0.07886
C	1.67591	-2.10689	-1.34717
N	1.57847	-2.57022	-2.40073
H	-3.06684	2.97744	0.38375
H	-0.83667	2.67380	0.38783
H	-0.51175	-1.56828	0.00017
H	-2.63967	-2.19729	-0.09138
H	1.05774	1.84231	0.25178
C	3.26547	0.50816	0.01037
C	4.35317	-0.25104	0.46880
C	3.52381	1.79472	-0.49057
C	5.64151	0.26999	0.46026
H	4.20131	-1.25104	0.85815
C	4.81130	2.31106	-0.49664
H	2.71775	2.38397	-0.91160
C	5.87798	1.55428	-0.01666
H	6.46214	-0.33358	0.83082
H	4.98539	3.30428	-0.89495
H	6.88347	1.95853	-0.02626
C	1.83718	-2.33091	1.05769
N	1.88004	-2.97881	2.01319
C	-3.74786	-0.38345	-0.01136
C	-4.91876	-1.14699	-0.14006
C	-6.17699	-0.56704	-0.14319
C	-6.29377	0.81451	-0.01088
C	-5.15085	1.58683	0.12087
H	-4.82711	-2.22319	-0.24017
H	-7.06006	-1.18642	-0.24611
H	-5.24312	2.66256	0.22603
H	-7.26964	1.28564	-0.00924

38

78-DHA vacuum Energy: -955.674682

C	-4.28063	1.21006	-0.36276
C	-3.35651	0.15034	-0.13455
C	-1.97373	0.49096	0.01168
C	-1.54909	1.77239	-0.31618
C	-2.46918	2.76223	-0.64815
C	-3.84460	2.48682	-0.62226
H	-5.34023	0.97675	-0.39000
H	-0.49633	2.02546	-0.31027
H	-2.11687	3.75625	-0.89746
H	-4.56007	3.27460	-0.82808
C	-3.84400	-1.17880	-0.18176
H	-4.92514	-1.27019	-0.11456
C	-1.09913	-0.61535	0.54831
H	-1.64180	-1.07471	1.38044
C	-0.82704	-1.65110	-0.51914
C	-3.18124	-2.36452	-0.57163
C	-1.84187	-2.55316	-0.88722
H	-3.84187	-3.20299	-0.77142
H	-1.56608	-3.44239	-1.44552
C	0.47812	-1.50583	-0.98033
C	0.36163	-0.26231	1.01230
C	1.20385	-0.57300	-0.22476
H	0.89403	-2.06606	-1.80805
C	0.51806	1.07348	1.61013
C	0.73269	-1.24046	2.06407
N	1.04825	-2.01248	2.85427
N	0.65877	2.09605	2.11229
C	5.19355	0.70127	-0.92150
C	4.43369	0.14758	-1.95320
C	3.13520	-0.26440	-1.72056
C	2.54810	-0.13097	-0.43870
C	3.33628	0.42479	0.59449
C	4.63631	0.83235	0.34985
H	6.21165	1.02395	-1.10672
H	4.85935	0.04488	-2.94524
H	2.54573	-0.66663	-2.53706
H	2.94153	0.51262	1.59971
H	5.22433	1.24925	1.15949

38
78-DHA acetonitrile Energy: -955.689528

C	3.66108	1.85940	-0.00150
C	2.75198	2.93263	-0.03351
C	3.48034	0.45902	0.00853
C	1.37217	2.90362	-0.01439
H	0.85690	3.85484	0.08270
C	0.54550	1.76634	-0.08272
C	2.25869	-0.27642	-0.17614
C	0.93709	0.37453	-0.52131
H	0.92482	0.42667	-1.62447
C	-0.84467	1.82517	0.06298
C	-0.36438	-0.46070	-0.15628
C	-1.46751	0.59726	-0.04350
H	-1.36708	2.75283	0.26372
C	-0.66197	-1.45827	-1.19605
C	-0.22890	-1.11104	1.16266
N	-0.16279	-1.57184	2.21258
N	-0.88057	-2.20492	-2.04052
C	-5.63133	-0.23952	0.17725
C	-5.17776	1.06423	-0.03143
C	-3.82322	1.32956	-0.11247
C	-2.86937	0.29336	0.01827
C	-3.34754	-1.01864	0.22766
C	-4.70713	-1.27452	0.30494
H	-6.69368	-0.44527	0.23723
H	-5.88928	1.87494	-0.14085
H	-3.49061	2.34343	-0.30342
H	-2.65656	-1.84402	0.35610
H	-5.04855	-2.28955	0.47257
H	4.70023	2.16732	0.06695
H	3.20790	3.91701	-0.00477
C	4.68190	-0.29923	0.19866
H	5.60510	0.25198	0.34152
C	2.32551	-1.67140	-0.18725
H	1.43452	-2.26096	-0.36340
C	3.50553	-2.37046	0.01734
H	3.49268	-3.45380	0.01972
C	4.70287	-1.66798	0.21492
H	5.63390	-2.19966	0.37207

38
78-DHA cyclohexane Energy: -955.689551

C	3.66108	1.85940	-0.00150
C	2.75198	2.93263	-0.03351
C	3.48034	0.45902	0.00853
C	1.37217	2.90362	-0.01439
H	0.85690	3.85484	0.08270
C	0.54550	1.76634	-0.08272
C	2.25869	-0.27642	-0.17614
C	0.93709	0.37453	-0.52131
H	0.92482	0.42667	-1.62447
C	-0.84467	1.82517	0.06298
C	-0.36438	-0.46070	-0.15628
C	-1.46751	0.59726	-0.04350
H	-1.36708	2.75283	0.26372
C	-0.66197	-1.45827	-1.19605
C	-0.22890	-1.11104	1.16266
N	-0.16279	-1.57184	2.21258
N	-0.88057	-2.20492	-2.04052
C	-5.63133	-0.23952	0.17725
C	-5.17776	1.06423	-0.03143
C	-3.82322	1.32956	-0.11247
C	-2.86937	0.29336	0.01827
C	-3.34754	-1.01864	0.22766
C	-4.70713	-1.27452	0.30494
H	-6.69368	-0.44527	0.23723
H	-5.88928	1.87494	-0.14085
H	-3.49061	2.34343	-0.30342
H	-2.65656	-1.84402	0.35610
H	-5.04855	-2.28955	0.47257
H	4.70023	2.16732	0.06695
H	3.20790	3.91701	-0.00477
C	4.68190	-0.29923	0.19866
H	5.60510	0.25198	0.34152
C	2.32551	-1.67140	-0.18725
H	1.43452	-2.26096	-0.36340
C	3.50553	-2.37046	0.01734
H	3.49268	-3.45380	0.01972
C	4.70287	-1.66798	0.21492
H	5.63390	-2.19966	0.37207

38

78-DHA ethanol Energy: -955.703066

C	3.66148	1.85814	-0.01679
C	2.75032	2.93204	-0.04565
C	3.48003	0.45680	0.00464
C	1.37413	2.90321	-0.02053
H	0.85782	3.85387	0.07407
C	0.54377	1.76243	-0.08743
C	2.25871	-0.27944	-0.16976
C	0.93812	0.37096	-0.53212
H	0.93202	0.42358	-1.63385
C	-0.83919	1.82622	0.05622
C	-0.36368	-0.46305	-0.16978
C	-1.46870	0.59437	-0.05860
H	-1.35895	2.75495	0.25745
C	-0.65558	-1.46359	-1.20771
C	-0.23743	-1.10606	1.15446
N	-0.18381	-1.54776	2.21340
N	-0.87518	-2.20963	-2.05233
C	-5.63105	-0.23848	0.18635
C	-5.17459	1.07003	0.00673
C	-3.82064	1.33547	-0.08017
C	-2.86475	0.29235	0.01253
C	-3.34790	-1.02556	0.19531
C	-4.70729	-1.27931	0.28026
H	-6.69323	-0.44301	0.25155
H	-5.88465	1.88530	-0.07356
H	-3.48926	2.35430	-0.24370
H	-2.66050	-1.85768	0.29681
H	-5.05007	-2.29711	0.42756
H	4.70078	2.16713	0.04398
H	3.20671	3.91613	-0.02075
C	4.68195	-0.29785	0.20135
H	5.60581	0.25452	0.33422
C	2.32505	-1.67294	-0.15962
H	1.43563	-2.26708	-0.32925
C	3.50728	-2.37215	0.05183
H	3.49387	-3.45537	0.06513
C	4.70357	-1.66864	0.23619
H	5.63557	-2.19744	0.39668

38

78-DHA toluene Energy: -955.691280

C	3.66112	1.85950	-0.00537
C	2.75154	2.93263	-0.03558
C	3.48052	0.45897	0.00694
C	1.37219	2.90338	-0.01405
H	0.85676	3.85441	0.08367
C	0.54518	1.76565	-0.08214
C	2.25880	-0.27681	-0.17459
C	0.93718	0.37394	-0.52186
H	0.92565	0.42637	-1.62480
C	-0.84409	1.82496	0.06316
C	-0.36428	-0.46122	-0.15740
C	-1.46775	0.59661	-0.04508
H	-1.36627	2.75263	0.26427
C	-0.66056	-1.45926	-1.19703
C	-0.23061	-1.11075	1.16226
N	-0.16687	-1.56947	2.21324
N	-0.87869	-2.20598	-2.04155
C	-5.63155	-0.23896	0.17706
C	-5.17729	1.06554	-0.02650
C	-3.82276	1.33061	-0.10778
C	-2.86890	0.29311	0.01725
C	-3.34804	-1.01976	0.22182
C	-4.70766	-1.27511	0.29951
H	-6.69395	-0.44435	0.23732
H	-5.88843	1.87716	-0.13147
H	-3.49002	2.34527	-0.29412
H	-2.65776	-1.84634	0.34619
H	-5.04953	-2.29060	0.46344
H	4.70033	2.16773	0.06055
H	3.20736	3.91706	-0.00766
C	4.68243	-0.29853	0.19708
H	5.60581	0.25306	0.33720
C	2.32564	-1.67155	-0.18167
H	1.43474	-2.26196	-0.35543
C	3.50625	-2.37039	0.02318
H	3.49337	-3.45372	0.02807
C	4.70362	-1.66755	0.21696
H	5.63497	-2.19866	0.37402

38
78-TS vacuum Energy: -955.673140

C	3.49365	1.74690	0.31726
C	2.65920	2.83922	0.03840
C	1.31065	2.84991	-0.27637
C	0.46485	1.73185	-0.38147
C	0.91217	0.36640	-0.77351
H	4.45912	2.01324	0.73844
H	3.11048	3.81415	0.19420
H	0.82007	3.82053	-0.29408
C	-0.91616	1.77927	-0.14159
C	-1.49622	0.53303	0.08326
C	-0.44679	-0.46180	0.35591
C	-0.65716	-1.82316	-0.07863
C	0.22883	-0.37289	1.63529
N	-0.77868	-2.89276	-0.48538
N	0.78773	-0.29789	2.63815
H	0.40407	0.04688	-1.68581
H	-1.46500	2.71284	-0.08764
C	-2.91257	0.22170	0.00610
C	-3.46594	-0.86058	0.71134
C	-3.77104	1.03198	-0.75838
C	-4.82573	-1.12417	0.64643
H	-2.83070	-1.48176	1.33342
C	-5.13096	0.77024	-0.81115
H	-3.35579	1.85229	-1.33401
C	-5.66414	-0.31085	-0.11200
H	-5.23538	-1.96198	1.19878
H	-5.77734	1.40128	-1.41062
H	-6.72703	-0.51825	-0.15862
C	2.36730	-1.52470	-1.16309
C	3.47463	-2.28422	-0.89938
H	3.54528	-3.29277	-1.28908
C	4.52011	-1.75522	-0.09946
H	5.38580	-2.36463	0.13202
C	4.44702	-0.46880	0.34745
H	5.26814	-0.04526	0.91619
H	1.55678	-1.94600	-1.74861
C	3.32764	0.37705	0.05958
C	2.21036	-0.21380	-0.63499

38
78-TS acetonitrile Energy: -955.692038

C	3.48466	1.76803	0.33462
C	2.64343	2.85587	0.04066
C	1.30036	2.85303	-0.28102
C	0.46148	1.72006	-0.36863
C	0.92389	0.36675	-0.78244
H	4.44371	2.04311	0.76423
H	3.08922	3.83462	0.18544
H	0.80237	3.81840	-0.32629
C	-0.91053	1.76515	-0.11451
C	-1.50155	0.51515	0.08913
C	-0.46262	-0.49669	0.34183
C	-0.67656	-1.84638	-0.11697
C	0.22313	-0.43755	1.61334
N	-0.80093	-2.91127	-0.53648
N	0.79837	-0.38512	2.60936
H	0.42061	0.04954	-1.69758
H	-1.45385	2.70056	-0.04319
C	-2.91758	0.22120	0.01520
C	-3.47826	-0.88301	0.68531
C	-3.77524	1.06812	-0.71459
C	-4.84090	-1.13312	0.61817
H	-2.84836	-1.52808	1.28823
C	-5.13732	0.81731	-0.77019
H	-3.35995	1.90914	-1.25884
C	-5.67658	-0.28605	-0.10848
H	-5.25606	-1.98418	1.14557
H	-5.78149	1.47592	-1.34134
H	-6.74132	-0.48267	-0.15679
C	2.40017	-1.50926	-1.16493
C	3.51414	-2.26043	-0.89534
H	3.60357	-3.26336	-1.29553
C	4.54636	-1.72491	-0.08206
H	5.41768	-2.32543	0.15118
C	4.45735	-0.43984	0.36961
H	5.27213	-0.00937	0.94215
H	1.60326	-1.92991	-1.76953
C	3.33078	0.39720	0.07386
C	2.22576	-0.20289	-0.63223

38
78-TS cyclohexane Energy: -955.680241

C	3.49151	1.75433	0.32270
C	2.65391	2.84463	0.03945
C	1.30716	2.85002	-0.27731
C	0.46416	1.72655	-0.37685
C	0.91756	0.36536	-0.77605
H	4.45453	2.02436	0.74690
H	3.10244	3.82112	0.19236
H	0.81360	3.81872	-0.30358
C	-0.91375	1.77349	-0.13281
C	-1.49853	0.52603	0.08460
C	-0.45352	-0.47470	0.35262
C	-0.66478	-1.83235	-0.08935
C	0.22367	-0.39411	1.63024
N	-0.78764	-2.90037	-0.50033
N	0.78408	-0.32458	2.63297
H	0.41085	0.04543	-1.68869
H	-1.46016	2.70803	-0.07240
C	-2.91478	0.22145	0.00797
C	-3.47146	-0.86776	0.70180
C	-3.77249	1.04427	-0.74573
C	-4.83227	-1.12634	0.63567
H	-2.83875	-1.49680	1.31856
C	-5.13321	0.78671	-0.79990
H	-3.35691	1.87150	-1.31093
C	-5.66915	-0.30160	-0.11300
H	-5.24411	-1.96832	1.17994
H	-5.77845	1.42712	-1.39051
H	-6.73274	-0.50496	-0.16062
C	2.38061	-1.52001	-1.16291
C	3.49121	-2.27574	-0.89840
H	3.56830	-3.28256	-1.29131
C	4.53268	-1.74360	-0.09535
H	5.40080	-2.34947	0.13612
C	4.45349	-0.45767	0.35326
H	5.27240	-0.03123	0.92293
H	1.57458	-1.94191	-1.75421
C	3.33051	0.38401	0.06398
C	2.21724	-0.21071	-0.63345

38
78-TS ethanol Energy: -955.691589

C	3.48481	1.76709	0.33408
C	2.64382	2.85509	0.04056
C	1.30066	2.85274	-0.28120
C	0.46153	1.72026	-0.36948
C	0.92353	0.36648	-0.78232
H	4.44396	2.04192	0.76366
H	3.08972	3.83371	0.18593
H	0.80297	3.81832	-0.32566
C	-0.91076	1.76554	-0.11593
C	-1.50149	0.51568	0.08880
C	-0.46220	-0.49540	0.34285
C	-0.67570	-1.84577	-0.11433
C	0.22329	-0.43410	1.61453
N	-0.79979	-2.91107	-0.53286
N	0.79795	-0.37964	2.61075
H	0.41989	0.04879	-1.69710
H	-1.45419	2.70095	-0.04536
C	-2.91748	0.22113	0.01476
C	-3.47793	-0.88241	0.68602
C	-3.77521	1.06681	-0.71628
C	-4.84045	-1.13308	0.61882
H	-2.84789	-1.52666	1.28967
C	-5.13720	0.81552	-0.77192
H	-3.36000	1.90724	-1.26153
C	-5.67623	-0.28720	-0.10901
H	-5.25540	-1.98375	1.14704
H	-5.78146	1.47320	-1.34405
H	-6.74089	-0.48427	-0.15738
C	2.39918	-1.50996	-1.16509
C	3.51302	-2.26133	-0.89579
H	3.60189	-3.26444	-1.29567
C	4.54568	-1.72600	-0.08299
H	5.41687	-2.32677	0.15011
C	4.45709	-0.44092	0.36866
H	5.27205	-0.01067	0.94111
H	1.60184	-1.93065	-1.76909
C	3.33066	0.39630	0.07327
C	2.22529	-0.20347	-0.63250

38
78-TS toluene Energy: -955.681625

C	3.49086	1.75562	0.32394
C	2.65281	2.84562	0.03959
C	1.30648	2.85011	-0.27780
C	0.46393	1.72563	-0.37620
C	0.91842	0.36521	-0.77670
H	4.45337	2.02627	0.74886
H	3.10093	3.82237	0.19186
H	0.81245	3.81847	-0.30603
C	-0.91337	1.77249	-0.13131
C	-1.49896	0.52481	0.08487
C	-0.45468	-0.47700	0.35195
C	-0.66603	-1.83399	-0.09128
C	0.22311	-0.39783	1.62905
N	-0.78901	-2.90179	-0.50290
N	0.78444	-0.32915	2.63138
H	0.41195	0.04521	-1.68941
H	-1.45935	2.70720	-0.06984
C	-2.91517	0.22139	0.00847
C	-3.47235	-0.86922	0.70008
C	-3.77283	1.04657	-0.74306
C	-4.83335	-1.12696	0.63375
H	-2.84004	-1.49975	1.31572
C	-5.13368	0.78968	-0.79748
H	-3.35730	1.87519	-1.30623
C	-5.67004	-0.30009	-0.11298
H	-5.24555	-1.96978	1.17646
H	-5.77876	1.43185	-1.38631
H	-6.73374	-0.50277	-0.16075
C	2.38295	-1.51908	-1.16312
C	3.49409	-2.27417	-0.89831
H	3.57251	-3.28059	-1.29199
C	4.53467	-1.74156	-0.09438
H	5.40322	-2.34679	0.13714
C	4.45431	-0.45576	0.35466
H	5.27277	-0.02883	0.92460
H	1.57787	-1.94095	-1.75573
C	3.33076	0.38524	0.06494
C	2.21834	-0.21011	-0.63329

38
78-VHF vacuum Energy: -955.723043

C	-5.21033	0.01455	0.10495
C	-3.86460	0.05646	0.49256
C	-2.94397	-0.79701	-0.17671
C	-3.43446	-1.63459	-1.18944
C	-4.77359	-1.65982	-1.55222
C	-5.67152	-0.82572	-0.89902
H	-5.91144	0.66860	0.61221
H	-2.73502	-2.28345	-1.70529
H	-5.10907	-2.32382	-2.34002
H	-6.72120	-0.82523	-1.16773
C	-3.53824	0.98598	1.56432
H	-4.39229	1.54974	1.92649
C	-1.51460	-0.88278	0.07414
H	-1.00625	-1.57884	-0.58542
C	-0.71316	-0.22363	0.97185
C	-2.35538	1.25263	2.18185
C	-1.06856	0.71262	1.95460
H	-2.40193	1.99937	2.96923
H	-0.27274	1.08933	2.58511
C	0.74575	-0.53089	0.88959
C	1.41052	1.19649	-0.75237
C	1.68456	0.10012	0.12117
H	1.10771	-1.34035	1.51712
C	2.41043	1.69647	-1.62771
C	0.16569	1.86289	-0.85887
N	-0.81897	2.45068	-0.98472
N	3.20542	2.11929	-2.34938
C	5.70578	-1.35870	0.37543
C	4.66815	-2.22405	0.04653
C	3.36575	-1.74593	-0.04367
C	3.09097	-0.39814	0.19052
C	4.13776	0.46579	0.51650
C	5.43793	-0.01388	0.61142
H	6.72173	-1.73014	0.44428
H	4.87207	-3.27081	-0.14716
H	2.55721	-2.41694	-0.31472
H	3.93416	1.51492	0.70341
H	6.24270	0.66480	0.86875

38
78-VHF acetonitrile Energy: -955.723074

C	5.07924	-0.00587	0.07425
C	3.77419	-0.50754	-0.01971
C	2.75367	0.11352	0.75248
C	3.10880	1.19950	1.57011
C	4.41061	1.67583	1.64828
C	5.40642	1.06887	0.89236
H	5.85703	-0.47736	-0.51680
H	2.33324	1.67822	2.15821
H	4.64175	2.51457	2.29417
H	6.42847	1.42563	0.93630
C	3.59412	-1.64372	-0.91883
H	4.51118	-1.95647	-1.40905
C	1.34650	-0.23967	0.75713
H	0.73686	0.40014	1.38708
C	0.66314	-1.23431	0.08193
C	2.49230	-2.37398	-1.22488
C	1.15151	-2.22958	-0.76686
H	2.64880	-3.18745	-1.92678
H	0.43177	-2.94170	-1.15405
C	-0.80588	-1.22475	0.22246
C	-1.20225	0.93225	-0.90704
C	-1.63643	-0.18408	-0.15515
H	-1.27765	-2.10357	0.65124
C	-2.03089	2.07981	-1.06696
C	0.02737	1.01385	-1.60898
N	0.99519	1.12339	-2.22892
N	-2.66753	3.03225	-1.19604
C	-5.75398	-0.46286	0.97950
C	-4.75287	-0.62524	1.93315
C	-3.41584	-0.52908	1.56242
C	-3.07140	-0.26000	0.23554
C	-4.08071	-0.09840	-0.71771
C	-5.41591	-0.20324	-0.34648
H	-6.79589	-0.54066	1.26806
H	-5.01150	-0.82435	2.96657
H	-2.63455	-0.64622	2.30617
H	-3.82128	0.08892	-1.75448
H	-6.19200	-0.08711	-1.09392

38
78-VHF cyclohexane Energy: -955.719306

C	-5.16999	0.04021	0.07499
C	-3.83010	0.07084	0.48468
C	-2.91310	-0.81318	-0.14662
C	-3.39886	-1.67020	-1.14626
C	-4.73179	-1.68411	-1.53116
C	-5.62736	-0.81867	-0.91502
H	-5.86933	0.71780	0.55296
H	-2.70070	-2.34289	-1.63264
H	-5.06473	-2.36319	-2.30708
H	-6.67218	-0.80863	-1.20182
C	-3.50914	1.02389	1.54045
H	-4.36253	1.60674	1.87270
C	-1.48785	-0.90944	0.12605
H	-0.97443	-1.62298	-0.51092
C	-0.69503	-0.23570	1.02412
C	-2.33686	1.28951	2.17407
C	-1.04959	0.72808	1.97833
H	-2.38648	2.05498	2.94296
H	-0.25694	1.11039	2.61017
C	0.75878	-0.53716	0.95056
C	1.35128	1.13982	-0.76093
C	1.67395	0.08847	0.13770
H	1.14160	-1.31641	1.60324
C	2.31749	1.63133	-1.68336
C	0.09044	1.78001	-0.86586
N	-0.90251	2.35206	-0.99989
N	3.07692	2.04475	-2.44605
C	5.72992	-1.26992	0.35993
C	4.70523	-2.17111	0.08918
C	3.39018	-1.72647	0.01027
C	3.09129	-0.37575	0.19532
C	4.12397	0.52424	0.46489
C	5.43691	0.07732	0.54963
H	6.75522	-1.61608	0.42129
H	4.92881	-3.22015	-0.06636
H	2.59138	-2.42627	-0.21275
H	3.89967	1.57452	0.61961
H	6.23119	0.78259	0.76436

38
78-VHF Ethanol Energy: -955.722967

C	5.08164	-0.00383	0.05735
C	3.77459	-0.50182	-0.02969
C	2.76443	0.10888	0.76369
C	3.13073	1.18103	1.59427
C	4.43417	1.65376	1.66535
C	5.42010	1.05707	0.88852
H	5.85170	-0.46707	-0.55010
H	2.36268	1.65188	2.19835
H	4.67422	2.48185	2.32164
H	6.44324	1.41145	0.92627
C	3.58227	-1.62354	-0.94438
H	4.49305	-1.92993	-1.45006
C	1.35605	-0.24176	0.77829
H	0.75433	0.39162	1.42229
C	0.66436	-1.22521	0.09721
C	2.47588	-2.34791	-1.24807
C	1.14081	-2.20832	-0.77281
H	2.62296	-3.15106	-1.96379
H	0.41536	-2.91339	-1.16218
C	-0.80429	-1.21286	0.25329
C	-1.20774	0.91935	-0.91964
C	-1.63814	-0.18404	-0.14630
H	-1.27152	-2.07891	0.71212
C	-2.04501	2.05629	-1.10871
C	0.02747	1.00064	-1.61140
N	1.00002	1.11170	-2.22361
N	-2.68885	3.00016	-1.26228
C	-5.75561	-0.45061	0.99224
C	-4.75484	-0.58182	1.95101
C	-3.41784	-0.48993	1.57909
C	-3.07324	-0.25630	0.24569
C	-4.08207	-0.12590	-0.71266
C	-5.41723	-0.22636	-0.34002
H	-6.79749	-0.52480	1.28186
H	-5.01380	-0.75312	2.98933
H	-2.63686	-0.58283	2.32660
H	-3.82214	0.03445	-1.75383
H	-6.19299	-0.13401	-1.09111

38

78-VHF toluene Energy: -955.720879

C	-5.15947	-0.04315	-0.06645
C	-3.82181	-0.07037	-0.48458
C	-2.90299	0.81540	0.14156
C	-3.38438	1.67104	1.14496
C	-4.71474	1.68141	1.53812
C	-5.61230	0.81397	0.92696
H	-5.86032	-0.72192	-0.54049
H	-2.68466	2.34504	1.62725
H	-5.04455	2.35919	2.31651
H	-6.65523	0.80137	1.22045
C	-3.50568	-1.02193	-1.54301
H	-4.36054	-1.60466	-1.87172
C	-1.47961	0.91349	-0.13821
H	-0.96308	1.62703	0.49632
C	-0.69037	0.23930	-1.03986
C	-2.33666	-1.28659	-2.18293
C	-1.04837	-0.72517	-1.99172
H	-2.38961	-2.05123	-2.95236
H	-0.25772	-1.10784	-2.62599
C	0.76359	0.53625	-0.96841
C	1.33506	-1.12560	0.76403
C	1.67059	-0.08633	-0.14297
H	1.15272	1.30551	-1.62908
C	2.28966	-1.60770	1.70396
C	0.07241	-1.76345	0.86243
N	-0.92224	-2.33394	0.99192
N	3.03832	-2.01245	2.48169
C	5.73637	1.24284	-0.35655
C	4.71583	2.15446	-0.10519
C	3.39729	1.71965	-0.02888
C	3.09093	0.36826	-0.19668
C	4.11940	-0.54231	-0.44679
C	5.43582	-0.10513	-0.52926
H	6.76425	1.58154	-0.41628
H	4.94530	3.20415	0.03677
H	2.60164	2.42779	0.17848
H	3.88904	-1.59308	-0.58895
H	6.22684	-0.81834	-0.72934