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

Supporting Information: On the Effects of Solvation on the Back Reaction and Storage Capabilities of Solar Thermal Energy Storage Systems

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1 Structures

1.1 m062x_parent-DHA_an

Gibbs free energy: -802.220463
Electronic and ZPE: -802.176540

Atom	X	Y	Z
C	-4.574371	-0.305068	-0.248813
C	-4.122870	-1.318882	0.532906
C	-2.767704	-1.821704	0.563439
C	-3.786861	0.434538	-1.219126
C	-1.676939	-1.063813	0.332558
C	-2.482844	0.731652	-1.108438
C	-1.745782	0.436399	0.170637
H	-5.644011	-0.118087	-0.254349
H	-4.860367	-1.881553	1.097466
H	-2.630836	-2.877709	0.778694
H	-1.962732	1.202245	-1.936293
C	-0.294761	-1.485967	0.241544
H	-0.000314	-2.527867	0.269627
C	0.559938	-0.453773	0.136558
C	-0.231088	0.872401	0.224383
H	-2.289207	0.887333	1.006503
C	0.147953	1.802626	-0.851642
C	0.034768	1.525360	1.520847
N	0.439736	2.508359	-1.708385
N	0.218562	1.999677	2.550003
H	-4.308085	0.753094	-2.117473
C	2.019353	-0.493264	-0.011383
C	2.643324	-1.677077	-0.435277
C	2.821237	0.623518	0.257951
C	4.022499	-1.744923	-0.564487
H	2.043751	-2.545233	-0.683524
C	4.204216	0.553182	0.125290
H	2.383836	1.559585	0.586123
C	4.810261	-0.629553	-0.282987
H	4.484367	-2.667659	-0.896065
H	4.805962	1.427786	0.343060
H	5.887568	-0.682108	-0.388854

1.2 m062x_parent-DHA_ch

Gibbs free energy: -802.212533
Electronic and ZPE: -802.168711

Atom	X	Y	Z
C	-4.569556	-0.308113	-0.255971
C	-4.122066	-1.311563	0.540349
C	-2.767808	-1.814832	0.582240
C	-3.777913	0.418176	-1.232246
C	-1.675787	-1.061173	0.345306
C	-2.474609	0.715848	-1.119674
C	-1.743285	0.437049	0.166215
H	-5.638820	-0.118593	-0.265414
H	-4.862102	-1.864323	1.111574
H	-2.633547	-2.868651	0.810405
H	-1.949207	1.177366	-1.949332
C	-0.293031	-1.482812	0.259570
H	0.004367	-2.523682	0.298986
C	0.560896	-0.451360	0.144372
C	-0.229711	0.874915	0.221553
H	-2.291852	0.896097	0.994439
C	0.148977	1.798009	-0.860440
C	0.030365	1.536431	1.514704
N	0.433809	2.499832	-1.722765
N	0.206669	2.021963	2.539963
H	-4.294946	0.725853	-2.136827
C	2.019406	-0.493040	-0.006284
C	2.639802	-1.673639	-0.441663
C	2.822779	0.619776	0.270646
C	4.017944	-1.744127	-0.573082
H	2.035956	-2.535949	-0.700486
C	4.204591	0.546876	0.135973
H	2.385389	1.552783	0.606885
C	4.807430	-0.633248	-0.282370
H	4.477872	-2.664207	-0.914894
H	4.808443	1.418538	0.359409
H	5.884552	-0.686834	-0.390320

1.3 m062x_parent-DHA_dcm

Gibbs free energy: -802.218613
Electronic and ZPE: -802.174736

Atom	X	Y	Z
C	-4.573076	-0.305748	-0.250559
C	-4.122542	-1.317170	0.534588
C	-2.767637	-1.820263	0.567603
C	-3.784572	0.430538	-1.222408
C	-1.676545	-1.063428	0.335260
C	-2.480692	0.727641	-1.111297
C	-1.745133	0.436317	0.169504
H	-5.642603	-0.118055	-0.256924
H	-4.860624	-1.877455	1.100812
H	-2.631511	-2.875828	0.785691
H	-1.959232	1.195721	-1.939736
C	-0.294242	-1.485423	0.245090
H	0.000865	-2.527113	0.275558
C	0.560318	-0.453396	0.137872
C	-0.230688	0.872743	0.223847
H	-2.289963	0.889044	1.003522
C	0.147853	1.802291	-0.852891
C	0.033602	1.527104	1.519904
N	0.437229	2.508380	-1.710163
N	0.215057	2.003837	2.548365
H	-4.304747	0.746392	-2.122323
C	2.019519	-0.493228	-0.010621
C	2.642879	-1.676360	-0.436686
C	2.821533	0.622818	0.260194
C	4.021820	-1.744669	-0.566177
H	2.042504	-2.543360	-0.687197
C	4.204251	0.552066	0.127274
H	2.384029	1.558251	0.589890
C	4.809768	-0.630113	-0.282831
H	4.483444	-2.666836	-0.899760
H	4.806291	1.426185	0.346087
H	5.887053	-0.682772	-0.389037

1.4 m062x_parent-DHA_m

Gibbs free energy: -802.220400
Electronic and ZPE: -802.176479

Atom	X	Y	Z
C	-4.574326	-0.305091	-0.248868
C	-4.122856	-1.318827	0.532963
C	-2.767699	-1.821659	0.563573
C	-3.786785	0.434404	-1.219233
C	-1.676924	-1.063804	0.332642
C	-2.482772	0.731516	-1.108533
C	-1.745760	0.436392	0.170599
H	-5.643963	-0.118085	-0.254428
H	-4.860372	-1.881419	1.097579
H	-2.630857	-2.877651	0.778917
H	-1.962614	1.202023	-1.936409
C	-0.294741	-1.485951	0.241648
H	-0.000272	-2.527845	0.269807
C	0.559953	-0.453763	0.136593
C	-0.231074	0.872409	0.224366
H	-2.289232	0.887382	1.006405
C	0.147943	1.802625	-0.851674
C	0.034730	1.525406	1.520821
N	0.439633	2.508386	-1.708426
N	0.218440	1.999802	2.549956
H	-4.307974	0.752870	-2.117633
C	2.019361	-0.493263	-0.011365
C	2.643316	-1.677053	-0.435325
C	2.821246	0.623497	0.258016
C	4.022482	-1.744913	-0.564539
H	2.043719	-2.545173	-0.683646
C	4.204216	0.553150	0.125352
H	2.383839	1.559543	0.586235
C	4.810247	-0.629567	-0.282979
H	4.484346	-2.667630	-0.896179
H	4.805969	1.427740	0.343155
H	5.887554	-0.682123	-0.388854

1.5 m062x_parent-DHA_t

Gibbs free energy: -802.213500
Electronic and ZPE: -802.169676

Atom	X	Y	Z
C	-4.570027	-0.307717	-0.255235
C	-4.122104	-1.312405	0.539389
C	-2.767767	-1.815717	0.579883
C	-3.778832	0.420015	-1.230878
C	-1.675869	-1.061597	0.343662
C	-2.475429	0.717544	-1.118515
C	-1.743553	0.436860	0.166668
H	-5.639320	-0.118423	-0.264195
H	-4.861850	-1.866286	1.109875
H	-2.633274	-2.869830	0.806442
H	-1.950580	1.179918	-1.948040
C	-0.293188	-1.483286	0.257131
H	0.003835	-2.524299	0.295056
C	0.560861	-0.451749	0.143217
C	-0.229838	0.874489	0.221980
H	-2.291645	0.894917	0.995734
C	0.148724	1.798963	-0.858922
C	0.030772	1.534657	1.515738
N	0.434040	2.501918	-1.720154
N	0.207607	2.018719	2.541597
H	-4.296303	0.728888	-2.134794
C	2.019473	-0.493080	-0.007092
C	2.640409	-1.674119	-0.440798
C	2.822560	0.620322	0.268713
C	4.018674	-1.744210	-0.571865
H	2.037172	-2.537255	-0.698189
C	4.204515	0.547828	0.134353
H	2.385127	1.553756	0.603769
C	4.807846	-0.632652	-0.282482
H	4.478938	-2.664648	-0.912227
H	4.808011	1.419963	0.356912
H	5.884998	-0.686045	-0.390138

1.6 m062x_parent-TS-WH_an

Gibbs free energy: -802.174990
Electronic and ZPE: -802.129571

Atom	X	Y	Z
C	4.455999	-0.978063	0.566048
C	3.666977	-2.029058	0.159811
C	2.363822	-1.990841	-0.375887
C	1.594008	-0.902640	-0.729860
C	2.030473	0.461078	-0.827162
C	3.174877	1.027621	-0.234243
C	4.204949	0.403177	0.432664
C	0.162411	-1.089958	-0.899051
C	-0.662335	-0.143958	-0.392018
C	-0.060860	1.145302	0.081952
C	-0.022646	1.356621	1.479728
N	0.077661	1.481461	2.626916
C	-0.125075	2.296056	-0.730426
N	-0.133585	3.211924	-1.440250
H	5.398999	-1.239748	1.033905
H	4.063680	-3.022744	0.338807
H	1.878716	-2.957750	-0.479948
H	1.584135	1.037486	-1.626273
H	3.262294	2.104468	-0.348471
H	-0.212204	-2.052960	-1.228357
C	-2.106253	-0.387065	-0.167051
C	-2.997918	0.691090	-0.096292
C	-2.613697	-1.685635	-0.012836
C	-4.358746	0.477318	0.095348
H	-2.629439	1.704643	-0.206664
C	-3.972195	-1.897642	0.179952
H	-1.940855	-2.535345	-0.011344
C	-4.850863	-0.816946	0.230744
H	-5.033790	1.324254	0.138377
H	-4.344872	-2.907683	0.306070
H	-5.910660	-0.984004	0.385320
H	4.977890	1.056944	0.823380

1.7 m062x_parent-TS-WH_ch

Gibbs free energy: -802.159893
Electronic and ZPE: -802.115232

Atom	X	Y	Z
C	4.305093	-1.145222	0.771536
C	3.619408	-2.084129	0.025714
C	2.397452	-1.936392	-0.647749
C	1.628449	-0.798229	-0.825595
C	2.100289	0.560696	-0.661962
C	3.125285	0.984918	0.195375
C	4.041733	0.227780	0.899792
C	0.222263	-0.946538	-1.069569
C	-0.627377	-0.046003	-0.491112
C	-0.102165	1.249338	-0.019944
C	-0.333542	1.593559	1.342694
N	-0.446358	1.835085	2.466801
C	-0.003566	2.339293	-0.920406
N	0.121325	3.200419	-1.682261
H	5.172305	-1.509784	1.312857
H	4.022469	-3.091473	0.040019
H	1.952794	-2.859806	-1.011899
H	1.823788	1.252971	-1.444136
H	3.223794	2.063621	0.287171
H	-0.153114	-1.892302	-1.446199
C	-2.032438	-0.399513	-0.193146
C	-3.010263	0.602349	-0.159689
C	-2.415438	-1.723139	0.060352
C	-4.338287	0.285853	0.096451
H	-2.729140	1.631911	-0.352852
C	-3.742726	-2.037960	0.317388
H	-1.664247	-2.504272	0.093853
C	-4.708371	-1.034492	0.332656
H	-5.084272	1.071887	0.111785
H	-4.022503	-3.064809	0.523350
H	-5.743897	-1.280293	0.538754
H	4.722444	0.780814	1.538784

1.8 m062x_parent-TS-WH_dcm

Gibbs free energy: -802.171339
Electronic and ZPE: -802.126176

Atom	X	Y	Z
C	4.437382	-1.014445	0.610050
C	3.658991	-2.047542	0.137562
C	2.370428	-1.985934	-0.425864
C	1.605523	-0.881839	-0.745598
C	2.055413	0.481761	-0.791467
C	3.183294	1.021460	-0.148256
C	4.192954	0.370087	0.526588
C	0.178375	-1.058762	-0.930491
C	-0.652277	-0.122552	-0.408608
C	-0.073737	1.170581	0.067942
C	-0.121010	1.417015	1.461999
N	-0.091936	1.572091	2.608856
C	-0.094389	2.304695	-0.771605
N	-0.066049	3.205195	-1.499841
H	5.366233	-1.298211	1.093519
H	4.051118	-3.048129	0.285723
H	1.887471	-2.947328	-0.580819
H	1.636542	1.085260	-1.584810
H	3.277168	2.101314	-0.223181
H	-0.198030	-2.017576	-1.270439
C	-2.089548	-0.391234	-0.172664
C	-3.002549	0.670246	-0.131102
C	-2.568570	-1.695191	0.017760
C	-4.358097	0.433381	0.067226
H	-2.653122	1.687096	-0.270980
C	-3.922256	-1.930258	0.217624
H	-1.875887	-2.528594	0.043564
C	-4.822596	-0.866914	0.238815
H	-5.050989	1.266617	0.087451
H	-4.274281	-2.943703	0.372753
H	-5.878651	-1.051561	0.399134
H	4.954345	1.006493	0.965521

1.9 m062x_parent-TS-WH_m

Gibbs free energy: -802.174860
Electronic and ZPE: -802.129455

Atom	X	Y	Z
C	4.455523	-0.979286	0.567456
C	3.666770	-2.029713	0.159062
C	2.364077	-1.990701	-0.377547
C	1.594453	-0.901926	-0.730362
C	2.031378	0.461810	-0.825907
C	3.175315	1.027463	-0.231375
C	4.204756	0.402104	0.435726
C	0.162997	-1.088886	-0.900105
C	-0.661951	-0.143236	-0.392550
C	-0.061291	1.146155	0.081611
C	-0.026324	1.358663	1.479376
N	0.071234	1.484527	2.626666
C	-0.124004	2.296361	-0.731723
N	-0.131228	3.211718	-1.442205
H	5.398078	-1.241719	1.035806
H	4.063285	-3.023658	0.337039
H	1.879002	-2.957449	-0.483312
H	1.585895	1.039162	-1.624791
H	3.262971	2.104434	-0.344285
H	-0.211696	-2.051722	-1.229837
C	-2.105661	-0.387219	-0.167279
C	-2.998096	0.690377	-0.097850
C	-2.612099	-1.685980	-0.011568
C	-4.358763	0.475808	0.093924
H	-2.630285	1.704047	-0.209434
C	-3.970454	-1.898782	0.181376
H	-1.938528	-2.535118	-0.008973
C	-4.849907	-0.818676	0.230810
H	-5.034457	1.322277	0.135903
H	-4.342404	-2.908942	0.308695
H	-5.909591	-0.986338	0.385514
H	4.977384	1.055304	0.828001

1.10 m062x_parent-TS-WH_t

Gibbs free energy: -802.161736
Electronic and ZPE: -802.116977

Atom	X	Y	Z
C	4.323969	-1.129679	0.753393
C	3.623104	-2.082715	0.041491
C	2.392270	-1.945267	-0.619088
C	1.626424	-0.808921	-0.816285
C	2.097396	0.551355	-0.678897
C	3.137874	0.991161	0.152557
C	4.066196	0.247273	0.854523
C	0.217225	-0.960136	-1.053615
C	-0.629939	-0.055427	-0.481737
C	-0.098988	1.240185	-0.009252
C	-0.312387	1.573476	1.357982
N	-0.411773	1.805076	2.485757
C	-0.014938	2.335121	-0.903758
N	0.098502	3.200562	-1.662949
H	5.199052	-1.484297	1.288507
H	4.022316	-3.091102	0.073060
H	1.940165	-2.875084	-0.956507
H	1.802133	1.233319	-1.463322
H	3.237598	2.071271	0.223304
H	-0.158604	-1.907515	-1.425590
C	-2.039432	-0.398688	-0.191320
C	-3.009688	0.610607	-0.158904
C	-2.433972	-1.719986	0.057257
C	-4.341388	0.303825	0.090765
H	-2.720169	1.638654	-0.347558
C	-3.764805	-2.025063	0.307979
H	-1.689544	-2.507501	0.091678
C	-4.722875	-1.014205	0.321855
H	-5.081202	1.095702	0.105073
H	-4.053327	-3.050271	0.509980
H	-5.761118	-1.252508	0.522975
H	4.759329	0.812365	1.469059

1.11 m062x_parent-TS-ZI_an

Gibbs free energy: -802.177565
Electronic and ZPE: -802.132870

Atom	X	Y	Z
C	-4.571038	-0.637789	0.265688
C	-3.794606	-1.737531	0.512829
C	-2.406548	-1.912893	0.282432
C	-4.181732	0.572540	-0.361528
C	-1.520460	-1.096339	-0.376501
C	-2.995531	0.896167	-0.971011
C	-1.801872	0.140843	-1.047555
H	-5.607391	-0.692343	0.579526
H	-4.286455	-2.571804	1.002441
H	-1.982884	-2.823982	0.695045
H	-4.964572	1.320660	-0.442557
H	-2.969875	1.845600	-1.497003
C	-0.080079	-1.372785	-0.333154
C	0.715161	-0.303812	-0.123854
C	0.015061	1.008059	0.086798
C	0.430369	2.144114	-0.643421
C	-0.650035	1.230885	1.309831
N	0.746893	3.047984	-1.293627
N	-1.278414	1.359253	2.274850
H	-1.143798	0.379338	-1.874584
H	0.290149	-2.391531	-0.328253
C	2.185934	-0.385000	-0.025701
C	2.901127	0.540290	0.743414
C	2.890215	-1.390476	-0.701708
C	4.283682	0.444992	0.857695
H	2.372001	1.330411	1.265354
C	4.271348	-1.480619	-0.590993
H	2.355498	-2.089398	-1.335623
C	4.972328	-0.565275	0.192332
H	4.823188	1.163167	1.464291
H	4.803892	-2.258893	-1.125457
H	6.050951	-0.634107	0.274705

1.12 m062x_parent-TS-ZI_ch

Gibbs free energy: -802.163109
Electronic and ZPE: -802.118629

Atom	X	Y	Z
C	-4.581454	-0.623342	0.203245
C	-3.794531	-1.698987	0.527469
C	-2.404898	-1.872336	0.341347
C	-4.186540	0.553833	-0.470707
C	-1.505280	-1.083507	-0.344232
C	-2.985474	0.856760	-1.067634
C	-1.787373	0.112485	-1.075840
H	-5.622280	-0.671869	0.503153
H	-4.289141	-2.507618	1.057062
H	-1.981576	-2.751154	0.819097
H	-4.968672	1.296266	-0.599906
H	-2.950061	1.784491	-1.630564
C	-0.067923	-1.361636	-0.276740
C	0.730758	-0.289026	-0.074454
C	0.042780	1.014975	0.149724
C	0.474152	2.168839	-0.544188
C	-0.742904	1.191468	1.307380
N	0.797737	3.086588	-1.169942
N	-1.461511	1.278822	2.211531
H	-1.078363	0.360075	-1.856076
H	0.299476	-2.381196	-0.247030
C	2.202235	-0.377579	-0.012038
C	2.935327	0.529173	0.760707
C	2.887245	-1.371312	-0.722856
C	4.318639	0.426602	0.843172
H	2.416702	1.309648	1.306594
C	4.269221	-1.469470	-0.643038
H	2.334400	-2.050852	-1.362617
C	4.988484	-0.572624	0.144008
H	4.873983	1.131724	1.450659
H	4.788665	-2.237077	-1.205308
H	6.068511	-0.646205	0.201854

1.13 m062x_parent-TS-ZI_dcm

Gibbs free energy: -802.174194
Electronic and ZPE: -802.129630

Atom	X	Y	Z
C	-4.574304	-0.635269	0.249841
C	-3.794825	-1.729108	0.516420
C	-2.406015	-1.903621	0.297125
C	-4.184304	0.567480	-0.388795
C	-1.517157	-1.093375	-0.368288
C	-2.994305	0.886574	-0.994717
C	-1.799241	0.134091	-1.053929
H	-5.611902	-0.688844	0.559725
H	-4.287051	-2.557488	1.015857
H	-1.982100	-2.807193	0.725716
H	-4.967449	1.313936	-0.481829
H	-2.966486	1.830811	-1.529882
C	-0.077051	-1.369760	-0.319572
C	0.719012	-0.300138	-0.112128
C	0.022072	1.010350	0.102262
C	0.438734	2.150243	-0.621055
C	-0.669103	1.222017	1.312615
N	0.754241	3.057221	-1.267298
N	-1.315931	1.340997	2.266484
H	-1.128051	0.374992	-1.869402
H	0.292901	-2.388653	-0.309728
C	2.190038	-0.383298	-0.022639
C	2.909482	0.537047	0.747975
C	2.889739	-1.385249	-0.708184
C	4.292300	0.440035	0.854290
H	2.382771	1.324412	1.276327
C	4.271179	-1.477196	-0.605329
H	2.350642	-2.078883	-1.344291
C	4.976527	-0.566901	0.179682
H	4.835603	1.154738	1.461556
H	4.800709	-2.252218	-1.147526
H	6.055586	-0.636671	0.255729

1.14 m062x_parent-TS-ZI_m

Gibbs free energy: -802.177452
Electronic and ZPE: -802.132762

Atom	X	Y	Z
C	-4.571136	-0.637679	0.265126
C	-3.794609	-1.737224	0.512956
C	-2.406522	-1.912573	0.282944
C	-4.181797	0.572381	-0.362504
C	-1.520336	-1.096255	-0.376224
C	-2.995462	0.895837	-0.971863
C	-1.801754	0.140600	-1.047785
H	-5.607533	-0.692182	0.578827
H	-4.286476	-2.571286	1.002917
H	-1.982856	-2.823406	0.696123
H	-4.964645	1.320447	-0.443961
H	-2.969723	1.845086	-1.498183
C	-0.079961	-1.372698	-0.332687
C	0.715296	-0.303699	-0.123442
C	0.015284	1.008119	0.087343
C	0.430622	2.144320	-0.642623
C	-0.650719	1.230533	1.309952
N	0.747090	3.048311	-1.292685
N	-1.279751	1.358546	2.274589
H	-1.143217	0.379158	-1.874419
H	0.290266	-2.391446	-0.327628
C	2.186080	-0.384938	-0.025589
C	2.901409	0.540176	0.743593
C	2.890214	-1.390269	-0.701951
C	4.283976	0.444836	0.857589
H	2.372357	1.330186	1.265772
C	4.271360	-1.480457	-0.591517
H	2.355351	-2.089002	-1.335955
C	4.972481	-0.565293	0.191882
H	4.823607	1.162888	1.464218
H	4.803809	-2.258600	-1.126270
H	6.051122	-0.634143	0.274027

1.15 m062x_parent-TS-ZI_t

Gibbs free energy: -802.164994
Electronic and ZPE: -802.120427

Atom	X	Y	Z
C	-4.580357	-0.626147	0.210579
C	-3.794001	-1.704453	0.525699
C	-2.404373	-1.877357	0.334206
C	-4.186926	0.555446	-0.457645
C	-1.507053	-1.084768	-0.348566
C	-2.987765	0.861446	-1.056182
C	-1.789924	0.116219	-1.072687
H	-5.620637	-0.676022	0.512121
H	-4.287766	-2.516496	1.050669
H	-1.980430	-2.760023	0.804273
H	-4.969537	1.298342	-0.580772
H	-2.953966	1.791984	-1.614543
C	-0.069019	-1.362303	-0.284619
C	0.729199	-0.290333	-0.080950
C	0.039941	1.014726	0.142599
C	0.467959	2.166620	-0.556047
C	-0.731106	1.195711	1.309136
N	0.789241	3.082925	-1.185318
N	-1.438405	1.287355	2.221844
H	-1.086511	0.363616	-1.858076
H	0.298978	-2.381749	-0.258977
C	2.200627	-0.378250	-0.014051
C	2.931430	0.530188	0.759016
C	2.888071	-1.372938	-0.721335
C	4.314659	0.428310	0.845527
H	2.411407	1.311498	1.302420
C	4.269952	-1.470280	-0.637624
H	2.337516	-2.054250	-1.361153
C	4.986889	-0.571812	0.149824
H	4.867998	1.134618	1.453475
H	4.791107	-2.238746	-1.197117
H	6.066770	-0.644883	0.210715

1.16 m062x_parent-VHF-cis_an

Gibbs free energy: -802.211842
Electronic and ZPE: -802.166263

Atom	X	Y	Z
C	1.641096	-0.690756	-0.149755
C	0.294472	-0.768922	-0.485380
H	-0.022824	-1.681935	-0.979296
C	-0.761236	0.150344	-0.222451
C	-0.610859	1.530777	-0.166792
C	0.557724	2.188757	-0.638729
C	-1.634335	2.399618	0.315224
N	1.500136	2.724355	-1.033735
N	-2.430248	3.130667	0.718057
C	-2.118851	-0.432775	-0.076426
C	-2.297149	-1.568347	0.721019
C	-3.217795	0.111135	-0.749704
C	-3.558494	-2.134200	0.863784
H	-1.445636	-1.993539	1.241310
C	-4.474856	-0.466241	-0.618538
H	-3.082859	0.969215	-1.398867
C	-4.648465	-1.584440	0.193546
H	-3.690235	-3.004605	1.495890
H	-5.317838	-0.046819	-1.155132
H	-5.630799	-2.030543	0.298765
C	2.493931	-1.730673	-0.683591
H	1.959504	-2.516862	-1.209609
C	3.846979	-1.848865	-0.679947
H	4.235929	-2.714522	-1.207186
C	4.846547	-0.989284	-0.121508
H	5.872762	-1.252958	-0.354978
C	4.651570	0.078138	0.693094
H	5.535052	0.591787	1.057365
C	3.401718	0.580531	1.177620
H	3.486753	1.346791	1.942186
C	2.130569	0.265736	0.816536
H	1.355576	0.805638	1.351275

1.17 m062x_parent-VHF-cis_ch

Gibbs free energy: -802.201230
Electronic and ZPE: -802.155702

Atom	X	Y	Z
C	1.624446	-0.697995	-0.162695
C	0.298029	-0.748279	-0.538817
H	-0.017536	-1.628573	-1.090823
C	-0.766216	0.172649	-0.250583
C	-0.609024	1.542256	-0.184438
C	0.582574	2.194774	-0.618159
C	-1.636539	2.420333	0.284031
N	1.542305	2.725431	-0.972372
N	-2.433425	3.156522	0.671400
C	-2.115373	-0.424357	-0.086791
C	-2.262387	-1.580970	0.686341
C	-3.236868	0.122819	-0.717584
C	-3.512876	-2.163475	0.848506
H	-1.393031	-2.008553	1.174512
C	-4.483672	-0.470481	-0.566662
H	-3.129974	1.000344	-1.345014
C	-4.625097	-1.609334	0.220926
H	-3.619501	-3.049544	1.463553
H	-5.345040	-0.043674	-1.066931
H	-5.600318	-2.066964	0.342227
C	2.487120	-1.742908	-0.685634
H	1.956575	-2.535747	-1.206474
C	3.836994	-1.851127	-0.676557
H	4.235796	-2.718177	-1.194866
C	4.829836	-0.972356	-0.124367
H	5.858033	-1.214353	-0.373446
C	4.623897	0.084621	0.695092
H	5.500747	0.617678	1.048160
C	3.366786	0.557802	1.202804
H	3.445742	1.309378	1.982588
C	2.102970	0.234951	0.839342
H	1.318759	0.750980	1.384789

1.18 m062x_parent-VHF-cis_dcm

Gibbs free energy: -802.209346
Electronic and ZPE: -802.163807

Atom	X	Y	Z
C	1.636651	-0.691076	-0.155696
C	0.295774	-0.761666	-0.503470
H	-0.020929	-1.665381	-1.014770
C	-0.762873	0.157081	-0.231819
C	-0.611409	1.534455	-0.172360
C	0.562460	2.192250	-0.635241
C	-1.635450	2.405050	0.308708
N	1.507868	2.728678	-1.020782
N	-2.430323	3.137553	0.709840
C	-2.117523	-0.430883	-0.079848
C	-2.285245	-1.573416	0.709940
C	-3.223980	0.114063	-0.739505
C	-3.543094	-2.144785	0.859189
H	-1.427822	-1.999260	1.219982
C	-4.477692	-0.468761	-0.601921
H	-3.098261	0.978265	-1.382202
C	-4.640515	-1.593757	0.202524
H	-3.666536	-3.020254	1.486003
H	-5.326802	-0.047222	-1.127024
H	-5.620489	-2.043786	0.313035
C	2.492496	-1.732287	-0.686527
H	1.959531	-2.519114	-1.213319
C	3.844538	-1.848858	-0.679245
H	4.236239	-2.714408	-1.204828
C	4.842347	-0.986094	-0.119140
H	5.869312	-1.245055	-0.354932
C	4.644002	0.077885	0.697397
H	5.525582	0.595310	1.061129
C	3.391514	0.573715	1.185768
H	3.474192	1.335531	1.955072
C	2.122698	0.258564	0.821341
H	1.344968	0.792874	1.357886

1.19 m062x_parent-VHF-cis_m

Gibbs free energy: -802.211756
Electronic and ZPE: -802.166179

Atom	X	Y	Z
C	1.640945	-0.690738	-0.150001
C	0.294523	-0.768646	-0.486058
H	-0.022748	-1.681332	-0.980600
C	-0.761297	0.150588	-0.222801
C	-0.610891	1.530913	-0.166993
C	0.557857	2.188901	-0.638649
C	-1.634377	2.399806	0.315030
N	1.500353	2.724541	-1.033359
N	-2.430243	3.130892	0.717849
C	-2.118800	-0.432713	-0.076550
C	-2.296705	-1.568543	0.720616
C	-3.218025	0.111235	-0.749327
C	-3.557920	-2.134606	0.863617
H	-1.444972	-1.993761	1.240529
C	-4.474962	-0.466344	-0.617924
H	-3.083429	0.969539	-1.398259
C	-4.648169	-1.584799	0.193877
H	-3.689352	-3.005201	1.495526
H	-5.318173	-0.046845	-1.154097
H	-5.630416	-2.031050	0.299290
C	2.493891	-1.730690	-0.683742
H	1.959523	-2.516879	-1.209828
C	3.846902	-1.848850	-0.679927
H	4.235950	-2.714494	-1.207124
C	4.846408	-0.989193	-0.121373
H	5.872652	-1.252722	-0.354890
C	4.651306	0.078094	0.693314
H	5.534720	0.591847	1.057610
C	3.401354	0.580285	1.177927
H	3.486295	1.346382	1.942668
C	2.130292	0.265509	0.816679
H	1.355200	0.805231	1.351460

1.20 m062x_parent-VHF-cis_t

Gibbs free energy: -802.202511
Electronic and ZPE: -802.156984

Atom	X	Y	Z
C	1.626136	-0.696527	-0.162339
C	0.297762	-0.749676	-0.534833
H	-0.017874	-1.633163	-1.081545
C	-0.765896	0.170633	-0.248449
C	-0.609639	1.541313	-0.183062
C	0.579202	2.194882	-0.621392
C	-1.636376	2.418227	0.288079
N	1.536490	2.726820	-0.980635
N	-2.432403	3.153935	0.678501
C	-2.115606	-0.425354	-0.086015
C	-2.264979	-1.580324	0.689178
C	-3.235387	0.121542	-0.720246
C	-3.516324	-2.161569	0.849835
H	-1.397023	-2.007620	1.180043
C	-4.482989	-0.470591	-0.570898
H	-3.126300	0.997385	-1.349712
C	-4.626848	-1.607841	0.218744
H	-3.624906	-3.046382	1.466322
H	-5.342960	-0.044480	-1.074148
H	-5.602620	-2.064609	0.338788
C	2.487929	-1.740894	-0.686401
H	1.957149	-2.532502	-1.208786
C	3.838059	-1.850719	-0.676860
H	4.235823	-2.717447	-1.196413
C	4.831671	-0.974834	-0.122594
H	5.859770	-1.219653	-0.369167
C	4.626714	0.083041	0.696524
H	5.504225	0.613482	1.051784
C	3.370050	0.559895	1.200720
H	3.449340	1.312864	1.979120
C	2.105604	0.238662	0.836411
H	1.322272	0.757640	1.380242

1.21 m062x_3-amino-DHA_an

Gibbs free energy: -857.564167
Electronic and ZPE: -857.519343

Atom	X	Y	Z
C	4.536496	0.080730	-0.422174
C	4.161010	1.039973	0.461830
C	2.826410	1.585267	0.593943
C	3.674589	-0.555957	-1.402608
C	1.706469	0.875771	0.361787
C	2.370835	-0.825861	-1.232888
C	1.735368	-0.608052	0.113716
H	5.597761	-0.135299	-0.500682
H	4.943801	1.534073	1.029124
H	2.759527	2.632278	0.877236
H	4.133557	-0.812208	-2.353167
H	1.777929	-1.208644	-2.057454
C	0.319508	1.342001	0.308206
C	-0.545844	0.301106	0.160217
C	0.225746	-1.019902	0.248086
H	2.334894	-1.114202	0.876044
C	0.030268	-1.649947	1.573122
C	-0.207368	-1.982527	-0.780941
N	-0.102621	-2.099241	2.621710
N	-0.547904	-2.711247	-1.599927
C	-2.000364	0.348508	-0.012600
C	-2.829920	-0.684817	0.450421
C	-2.599903	1.424128	-0.688725
C	-4.206688	-0.630295	0.268225
H	-2.409730	-1.539337	0.969529
C	-3.977029	1.476082	-0.866763
H	-1.981010	2.205765	-1.114055
C	-4.788712	0.452855	-0.384255
H	-4.825893	-1.438608	0.640210
H	-4.415059	2.314336	-1.396656
H	-5.862636	0.493972	-0.524181
N	0.015351	2.674823	0.357462
H	-0.915471	2.919060	0.667545
H	0.723327	3.284092	0.740180

1.22 m062x_3-amino-DHA_ch

Gibbs free energy: -857.554273
Electronic and ZPE: -857.509400

Atom	X	Y	Z
C	4.536468	0.099288	-0.414264
C	4.153891	1.057343	0.466900
C	2.815509	1.592909	0.596587
C	3.680550	-0.544751	-1.394585
C	1.700023	0.876856	0.364019
C	2.378608	-0.822394	-1.227724
C	1.735656	-0.607118	0.115719
H	5.599000	-0.112940	-0.487659
H	4.932882	1.554794	1.036884
H	2.740716	2.641009	0.875366
H	4.143139	-0.801384	-2.343326
H	1.790217	-1.214390	-2.051120
C	0.311721	1.334034	0.310947
C	-0.547448	0.292392	0.159260
C	0.227336	-1.027087	0.242586
H	2.334306	-1.109383	0.881520
C	0.030578	-1.662386	1.564350
C	-0.197174	-1.984942	-0.793738
N	-0.099568	-2.118811	2.610152
N	-0.522444	-2.712206	-1.620095
C	-2.002165	0.342844	-0.013087
C	-2.835759	-0.675221	0.471970
C	-2.592719	1.408967	-0.710225
C	-4.211553	-0.613289	0.290700
H	-2.417865	-1.521165	1.006401
C	-3.969197	1.467444	-0.887624
H	-1.964446	2.172714	-1.154862
C	-4.786056	0.460449	-0.382319
H	-4.836187	-1.409977	0.678115
H	-4.402727	2.295518	-1.437094
H	-5.859820	0.505396	-0.522862
N	-0.004434	2.669139	0.367362
H	-0.938975	2.890374	0.684076
H	0.695274	3.270564	0.775805

1.23 m062x_3-amino-DHA_dcm

Gibbs free energy: -857.561851
Electronic and ZPE: -857.517044

Atom	X	Y	Z
C	4.535652	0.085478	-0.421950
C	4.159243	1.043011	0.463302
C	2.823932	1.586100	0.596355
C	3.674479	-0.551070	-1.402978
C	1.704897	0.875557	0.363269
C	2.371221	-0.822912	-1.233534
C	1.735289	-0.607959	0.113289
H	5.597130	-0.129685	-0.500319
H	4.941648	1.536777	1.031509
H	2.755439	2.633002	0.880033
H	4.133601	-0.805612	-2.353930
H	1.778538	-1.205889	-2.058150
C	0.317658	1.339767	0.309767
C	-0.546252	0.298867	0.160096
C	0.226091	-1.021781	0.246671
H	2.335461	-1.114198	0.875091
C	0.031237	-1.652721	1.571281
C	-0.205020	-1.984157	-0.783242
N	-0.099973	-2.103480	2.619447
N	-0.541370	-2.714070	-1.602857
C	-2.000804	0.347184	-0.012860
C	-2.831564	-0.682043	0.455934
C	-2.597721	1.420362	-0.694703
C	-4.208071	-0.625500	0.273865
H	-2.412145	-1.534423	0.979100
C	-3.974646	1.474094	-0.872804
H	-1.976142	2.197271	-1.125002
C	-4.787892	0.455223	-0.384222
H	-4.828806	-1.430763	0.649811
H	-4.411350	2.309620	-1.408137
H	-5.861742	0.497378	-0.524558
N	0.010707	2.673120	0.361407
H	-0.920750	2.911924	0.673948
H	0.717185	3.280618	0.749397

1.24 m062x_3-amino-DHA_m

Gibbs free energy: -857.564089
Electronic and ZPE: -857.519266

Atom	X	Y	Z
C	4.536458	0.080908	-0.422175
C	4.160943	1.040074	0.461895
C	2.826318	1.585289	0.594054
C	3.674574	-0.555752	-1.402641
C	1.706410	0.875760	0.361852
C	2.370838	-0.825727	-1.232931
C	1.735365	-0.608048	0.113690
H	5.597731	-0.135088	-0.500688
H	4.943723	1.534151	1.029226
H	2.759381	2.632292	0.877375
H	4.133543	-0.811918	-2.353223
H	1.777933	-1.208489	-2.057506
C	0.319439	1.341918	0.308271
C	-0.545861	0.301022	0.160211
C	0.225760	-1.019972	0.248030
H	2.334922	-1.114212	0.875985
C	0.030314	-1.650051	1.573052
C	-0.207276	-1.982599	-0.781022
N	-0.102506	-2.099397	2.621626
N	-0.547647	-2.711380	-1.600020
C	-2.000382	0.348457	-0.012612
C	-2.829986	-0.684710	0.450631
C	-2.599822	1.423985	-0.688957
C	-4.206746	-0.630111	0.268443
H	-2.409828	-1.539150	0.969896
C	-3.976941	1.476007	-0.866996
H	-1.980827	2.205444	-1.114475
C	-4.788686	0.452947	-0.384253
H	-4.826009	-1.438306	0.640581
H	-4.414919	2.314159	-1.397096
H	-5.862607	0.494105	-0.524194
N	0.015181	2.674756	0.357619
H	-0.915664	2.918803	0.667783
H	0.723104	3.283967	0.740518

1.25 m062x_3-amino-DHA_t

Gibbs free energy: -857.555494
Electronic and ZPE: -857.510634

Atom	X	Y	Z
C	4.535995	0.097107	-0.416227
C	4.154746	1.054594	0.466281
C	2.816949	1.591441	0.597110
C	3.678932	-0.545059	-1.396834
C	1.700808	0.876486	0.364176
C	2.376802	-0.821765	-1.229352
C	1.735516	-0.607290	0.115003
H	5.598320	-0.115652	-0.490828
H	4.934512	1.551024	1.036052
H	2.743300	2.639212	0.877255
H	4.140674	-0.800767	-2.346231
H	1.787371	-1.211639	-2.053021
C	0.312701	1.334863	0.311076
C	-0.547257	0.293422	0.159474
C	0.227108	-1.026255	0.243291
H	2.334771	-1.110513	0.879670
C	0.031045	-1.660672	1.565679
C	-0.198575	-1.985172	-0.791660
N	-0.098749	-2.116118	2.611960
N	-0.525519	-2.713391	-1.616517
C	-2.001923	0.343589	-0.013071
C	-2.835105	-0.676263	0.469286
C	-2.593384	1.410885	-0.707794
C	-4.210992	-0.615149	0.287826
H	-2.417035	-1.523321	1.001856
C	-3.969913	1.468634	-0.885405
H	-1.966078	2.176675	-1.150173
C	-4.786258	0.459754	-0.382807
H	-4.835026	-1.413258	0.673296
H	-4.403889	2.297877	-1.432738
H	-5.860021	0.504253	-0.523441
N	-0.001923	2.669699	0.366952
H	-0.935829	2.893774	0.683464
H	0.699096	3.272113	0.771760

1.26 m062x_3-amino-TS-WH_an

Gibbs free energy: -857.518461
Electronic and ZPE: -857.472618

Atom	X	Y	Z
C	4.623288	-0.460782	0.230716
C	3.840166	-1.522966	0.600298
C	2.448907	-1.707634	0.416016
C	1.552875	-0.943580	-0.296369
C	1.822909	0.225045	-1.066065
C	3.021971	0.970170	-1.092129
C	4.226912	0.688218	-0.494036
C	0.103404	-1.246866	-0.221402
C	-0.701819	-0.158968	-0.080015
C	-0.019249	1.153726	0.112739
C	-0.444736	2.271979	-0.637325
N	-0.779060	3.162004	-1.299415
H	5.667042	-0.499122	0.521373
H	4.336729	-2.313396	1.153958
H	2.025168	-2.575056	0.912284
H	1.111996	0.441765	-1.853262
H	2.986608	1.872343	-1.694458
C	-2.176140	-0.233579	0.010019
C	-2.914026	-1.044908	-0.863655
C	-2.869734	0.544323	0.945665
C	-4.301068	-1.096075	-0.784534
H	-2.398325	-1.614376	-1.630598
C	-4.256476	0.488912	1.027200
H	-2.314107	1.193449	1.614819
C	-4.977353	-0.334311	0.165468
H	-4.855146	-1.722593	-1.474378
H	-4.775684	1.092233	1.763308
H	-6.058906	-0.373219	0.225847
H	5.011915	1.418614	-0.664580
C	0.700148	1.408470	1.297026
N	1.366715	1.556351	2.234869
N	-0.265494	-2.568949	-0.056004
H	-1.258231	-2.739584	0.022368
H	0.185948	-3.233949	-0.670530

1.27 m062x_3-amino-TS-WH_ch

Gibbs free energy: -857.495565
Electronic and ZPE: -857.449580

Atom	X	Y	Z
C	4.245698	-0.981710	1.063169
C	3.537913	-1.982062	0.412716
C	2.360473	-1.880278	-0.335077
C	1.644114	-0.741282	-0.688657
C	2.166668	0.603108	-0.649146
C	3.182364	1.091403	0.168337
C	4.049851	0.398782	1.003402
C	0.240166	-0.877529	-1.012208
C	-0.602353	0.065735	-0.451328
C	-0.112774	1.389070	-0.064391
C	0.075000	2.397012	-1.039871
N	0.268403	3.187046	-1.863847
H	5.068604	-1.315810	1.687241
H	3.888746	-2.994658	0.583399
H	1.897960	-2.826575	-0.595369
H	1.881042	1.248139	-1.466814
H	3.329979	2.167060	0.115003
C	-2.003465	-0.278646	-0.099829
C	-3.014320	0.673355	-0.281035
C	-2.338400	-1.516954	0.463980
C	-4.328264	0.385810	0.066698
H	-2.763442	1.641556	-0.701226
C	-3.650672	-1.798509	0.821954
H	-1.559763	-2.250166	0.645148
C	-4.650316	-0.850815	0.617886
H	-5.099876	1.131600	-0.085948
H	-3.891830	-2.754943	1.271919
H	-5.674171	-1.071891	0.897372
H	4.731798	1.004205	1.591173
C	-0.389321	1.845243	1.254469
N	-0.558533	2.181210	2.347421
N	-0.198383	-2.100065	-1.534967
H	-1.189898	-2.117799	-1.737135
H	0.326282	-2.388455	-2.351424

1.28 m062x_3-amino-TS-WH_dcm

Gibbs free energy: -857.512440
Electronic and ZPE: -857.465307

Atom	X	Y	Z
C	4.582674	-0.636467	0.221380
C	3.732449	-1.715584	0.265643
C	2.356300	-1.773512	-0.037181
C	1.534244	-0.798822	-0.566583
C	1.901152	0.506966	-0.982530
C	3.127481	1.162403	-0.771994
C	4.285553	0.673012	-0.206887
C	0.073881	-1.051205	-0.639760
C	-0.714478	-0.053303	-0.171403
C	-0.037580	1.154421	0.394502
C	-0.331542	2.443025	-0.086764
N	-0.547289	3.488971	-0.540033
H	5.600330	-0.806156	0.554626
H	4.160017	-2.644105	0.630083
H	1.869224	-2.717264	0.187599
H	1.213854	0.993549	-1.662451
H	3.165038	2.188656	-1.123230
C	-2.191086	-0.194439	-0.061920
C	-3.044873	0.731746	-0.672308
C	-2.750977	-1.243065	0.675831
C	-4.424479	0.604273	-0.553921
H	-2.626314	1.551441	-1.246165
C	-4.132321	-1.368812	0.794800
H	-2.097768	-1.953544	1.173151
C	-4.972350	-0.446338	0.178693
H	-5.073535	1.326772	-1.035842
H	-4.550201	-2.184080	1.374725
H	-6.048157	-0.542593	0.271176
H	5.107919	1.378782	-0.144263
C	0.636519	1.045628	1.623011
N	1.262867	0.893916	2.588804
N	-0.335646	-2.333690	-0.981667
H	-1.335036	-2.434381	-1.107287
H	0.171699	-2.741021	-1.757513

1.29 m062x_3-amino-TS-WH_m

Gibbs free energy: -857.518327
Electronic and ZPE: -857.472482

Atom	X	Y	Z
C	4.623183	-0.460471	0.230710
C	3.840178	-1.522888	0.599988
C	2.449012	-1.707784	0.415572
C	1.552800	-0.943535	-0.296466
C	1.822820	0.224938	-1.066345
C	3.022012	0.969757	-1.093063
C	4.226840	0.688209	-0.494481
C	0.103363	-1.246707	-0.221113
C	-0.701835	-0.158807	-0.079732
C	-0.019386	1.153864	0.113116
C	-0.445279	2.272360	-0.636372
N	-0.779835	3.162604	-1.298039
H	5.666818	-0.498503	0.521840
H	4.336808	-2.313232	1.153722
H	2.025283	-2.575257	0.911756
H	1.111532	0.441848	-1.853144
H	2.986779	1.871561	-1.695948
C	-2.176178	-0.233534	0.010041
C	-2.913858	-1.044568	-0.864063
C	-2.869904	0.543901	0.945949
C	-4.300904	-1.095810	-0.785194
H	-2.397954	-1.613777	-1.631065
C	-4.256651	0.488401	1.027240
H	-2.314368	1.192733	1.615460
C	-4.977349	-0.334446	0.165014
H	-4.854870	-1.722044	-1.475386
H	-4.776001	1.091390	1.763516
H	-6.058914	-0.373375	0.225172
H	5.011806	1.418622	-0.665146
C	0.700906	1.408149	1.296976
N	1.368115	1.555700	2.234405
N	-0.265617	-2.568818	-0.055102
H	-1.258367	-2.738815	0.024692
H	0.184188	-3.233716	-0.670964

1.30 m062x_3-amino-TS-WH_t

Gibbs free energy: -857.497461
Electronic and ZPE: -857.451502

Atom	X	Y	Z
C	4.291179	-0.962512	1.019400
C	3.551638	-1.974908	0.426928
C	2.355400	-1.883677	-0.292849
C	1.644263	-0.750351	-0.671788
C	2.168736	0.590150	-0.672187
C	3.213636	1.093261	0.099196
C	4.106343	0.417823	0.920665
C	0.234097	-0.891082	-0.981775
C	-0.606213	0.056688	-0.431345
C	-0.114570	1.380908	-0.035894
C	0.061297	2.397582	-1.002324
N	0.245492	3.195134	-1.821949
H	5.130775	-1.284891	1.627151
H	3.895171	-2.985554	0.621849
H	1.876605	-2.832435	-0.511472
H	1.846712	1.226008	-1.483336
H	3.362075	2.166807	0.016436
C	-2.015591	-0.276281	-0.099658
C	-3.018235	0.678785	-0.308146
C	-2.366515	-1.506082	0.472612
C	-4.339583	0.401457	0.019627
H	-2.755204	1.641354	-0.733843
C	-3.686328	-1.777261	0.811418
H	-1.594845	-2.240962	0.675821
C	-4.677558	-0.827358	0.579158
H	-5.104710	1.149173	-0.154895
H	-3.939873	-2.727226	1.268246
H	-5.707214	-1.040180	0.843320
H	4.813072	1.034574	1.465724
C	-0.379198	1.820476	1.289433
N	-0.542108	2.141495	2.388356
N	-0.201731	-2.118878	-1.493391
H	-1.193584	-2.142816	-1.693243
H	0.322668	-2.413806	-2.307700

1.31 m062x_3-amino-TS-ZI_an

Gibbs free energy: -857.518464
Electronic and ZPE: -857.472618

Atom	X	Y	Z
C	-4.623085	-0.460652	0.230780
C	-3.840007	-1.522883	0.600349
C	-2.448807	-1.707732	0.415867
C	-4.226785	0.688098	-0.494390
C	-1.552742	-0.943656	-0.296458
C	-3.021872	0.969907	-1.092634
C	-1.822735	0.224944	-1.066214
H	-5.666775	-0.498820	0.521690
H	-4.336571	-2.313205	1.154162
H	-2.025108	-2.575247	0.912006
H	-2.986583	1.871874	-1.695271
C	-0.103258	-1.246857	-0.221420
C	0.701827	-0.158888	-0.079916
C	0.018988	1.153631	0.113056
H	-1.111636	0.441756	-1.853228
C	0.443961	2.272004	-0.637104
C	-0.700055	1.408094	1.297618
N	0.777814	3.162105	-1.299334
N	-1.366307	1.555722	2.235726
H	-5.011819	1.418416	-0.665128
C	2.176171	-0.233377	0.009942
C	2.914009	-1.044056	-0.864358
C	2.869757	0.543787	0.946204
C	4.301068	-1.095175	-0.785398
H	2.398228	-1.613116	-1.631551
C	4.256510	0.488442	1.027556
H	2.314102	1.192225	1.616003
C	4.977370	-0.334035	0.165088
H	4.855138	-1.721172	-1.475721
H	4.775746	1.091200	1.764104
H	6.058933	-0.372885	0.225326
N	0.265789	-2.568895	-0.055798
H	-0.185185	-3.233920	-0.670657
H	1.258582	-2.739212	0.022692

1.32 m062x_3-amino-TS-ZI_ch

Gibbs free energy: -857.501626
Electronic and ZPE: -857.455586

Atom	X	Y	Z
C	-4.636271	-0.464345	0.160092
C	-3.837935	-1.498611	0.588140
C	-2.448406	-1.674374	0.437817
C	-4.239941	0.659171	-0.593019
C	-1.539786	-0.916041	-0.280338
C	-3.020698	0.942179	-1.168114
C	-1.813582	0.220166	-1.086068
H	-5.683128	-0.506949	0.438782
H	-4.334031	-2.269242	1.170814
H	-2.018773	-2.515830	0.971950
H	-2.979867	1.831446	-1.789001
C	-0.096865	-1.220707	-0.184364
C	0.716286	-0.136790	-0.042193
C	0.048163	1.166499	0.183889
H	-1.059622	0.466612	-1.822679
C	0.486509	2.311106	-0.520986
C	-0.774541	1.359815	1.312485
N	0.821222	3.221194	-1.152982
N	-1.517005	1.452878	2.197826
H	-5.027879	1.376736	-0.802803
C	2.191184	-0.226730	0.010462
C	2.897848	-1.041484	-0.884658
C	2.912131	0.538179	0.933896
C	4.284695	-1.106885	-0.840230
H	2.354633	-1.598356	-1.642033
C	4.299090	0.467446	0.981501
H	2.375967	1.189363	1.616205
C	4.989594	-0.357226	0.098248
H	4.817365	-1.731406	-1.548636
H	4.842303	1.062922	1.706359
H	6.072040	-0.405437	0.130992
N	0.266990	-2.548691	0.015645
H	-0.119868	-3.209504	-0.646240
H	1.257547	-2.696232	0.153498

1.33 m062x_3-amino-TS-ZI_dcm

Gibbs free energy: -857.514548
Electronic and ZPE: -857.468625

Atom	X	Y	Z
C	-4.627369	-0.465588	0.214028
C	-3.839312	-1.521603	0.594817
C	-2.448113	-1.701712	0.418757
C	-4.232535	0.679557	-0.514602
C	-1.549998	-0.936164	-0.293081
C	-3.024796	0.963061	-1.108417
C	-1.823425	0.224417	-1.070757
H	-5.671656	-0.506619	0.502427
H	-4.334784	-2.309347	1.153572
H	-2.021609	-2.563332	0.922604
H	-2.989403	1.863196	-1.713771
C	-0.101513	-1.238328	-0.212916
C	0.705739	-0.151876	-0.071345
C	0.028390	1.159657	0.130812
H	-1.101068	0.451568	-1.844363
C	0.453969	2.283474	-0.610867
C	-0.715448	1.399223	1.302942
N	0.785182	3.177991	-1.268198
N	-1.399495	1.534631	2.229873
H	-5.018723	1.407211	-0.691751
C	2.180393	-0.231917	0.009906
C	2.910337	-1.041773	-0.871496
C	2.880848	0.539345	0.945302
C	4.297413	-1.097227	-0.800930
H	2.387677	-1.605649	-1.637951
C	4.267664	0.479172	1.018635
H	2.330090	1.187167	1.619541
C	4.980912	-0.341802	0.148880
H	4.846168	-1.721039	-1.497494
H	4.792943	1.078034	1.754013
H	6.062755	-0.383387	0.202299
N	0.266659	-2.561969	-0.038430
H	-0.166966	-3.226135	-0.666693
H	1.259224	-2.725747	0.056857

1.34 m062x_3-amino-TS-ZI_m

Gibbs free energy: -857.518330
Electronic and ZPE: -857.472482

Atom	X	Y	Z
C	-4.623252	-0.460880	0.230238
C	-3.839990	-1.522919	0.600114
C	-2.448786	-1.707572	0.415912
C	-4.227019	0.687798	-0.494971
C	-1.552663	-0.943395	-0.296357
C	-3.022024	0.969688	-1.093089
C	-1.822812	0.224942	-1.066350
H	-5.666959	-0.499174	0.521073
H	-4.336505	-2.313195	1.154048
H	-2.024976	-2.574901	0.912277
H	-2.986746	1.871623	-1.695775
C	-0.103205	-1.246540	-0.221149
C	0.701961	-0.158630	-0.079651
C	0.019344	1.153877	0.113642
H	-1.111333	0.442155	-1.852904
C	0.444294	2.272411	-0.636283
C	-0.700496	1.407860	1.297811
N	0.778010	3.162644	-1.298398
N	-1.367305	1.555111	2.235579
H	-5.012092	1.418042	-0.665858
C	2.176317	-0.233335	0.009931
C	2.913891	-1.043971	-0.864622
C	2.870131	0.543597	0.946194
C	4.300951	-1.095250	-0.785932
H	2.397884	-1.612831	-1.631815
C	4.256886	0.488074	1.027290
H	2.314639	1.192004	1.616151
C	4.977492	-0.334334	0.164560
H	4.854846	-1.721156	-1.476479
H	4.776322	1.090679	1.763820
H	6.059065	-0.373284	0.224576
N	0.265821	-2.568631	-0.055210
H	-0.184557	-3.233643	-0.670523
H	1.258611	-2.738716	0.023878

1.35 m062x_3-amino-TS-ZI_t

Gibbs free energy: -857.503638
Electronic and ZPE: -857.457641

Atom	X	Y	Z
C	-4.635210	-0.465262	0.167920
C	-3.837731	-1.502080	0.589676
C	-2.447790	-1.677761	0.435471
C	-4.239928	0.661283	-0.582310
C	-1.541313	-0.918407	-0.282377
C	-3.022458	0.944700	-1.160311
C	-1.815760	0.221022	-1.084226
H	-5.681643	-0.508072	0.448191
H	-4.333166	-2.275211	1.169419
H	-2.018029	-2.521814	0.965417
H	-2.983030	1.835267	-1.779409
C	-0.097339	-1.222560	-0.189158
C	0.714996	-0.138497	-0.046982
C	0.045669	1.166127	0.176751
H	-1.065943	0.465420	-1.825717
C	0.480757	2.308149	-0.533500
C	-0.764863	1.364577	1.312862
N	0.813615	3.216479	-1.169329
N	-1.498062	1.462026	2.205609
H	-5.028063	1.379810	-0.787651
C	2.189904	-0.227336	0.009961
C	2.899929	-1.040671	-0.883871
C	2.907879	0.537582	0.935900
C	4.286843	-1.104768	-0.835654
H	2.359677	-1.597836	-1.643127
C	4.294839	0.468171	0.987286
H	2.369616	1.187773	1.617550
C	4.988653	-0.355197	0.105235
H	4.821865	-1.728505	-1.542970
H	4.835459	1.063470	1.714246
H	6.071040	-0.402480	0.140937
N	0.267077	-2.550091	0.006563
H	-0.126712	-3.211114	-0.650958
H	1.258063	-2.700038	0.138140

1.36 m062x_3-amino-VHF-cis_an

Gibbs free energy: -857.543549
Electronic and ZPE: -857.496476

Atom	X	Y	Z
C	1.544103	-0.713464	0.021449
C	2.459110	-1.833756	0.285163
C	3.805176	-1.811997	0.284270
C	4.674521	-0.689259	-0.007558
C	4.361967	0.381514	-0.767268
C	3.095970	0.644883	-1.421798
C	1.874535	0.182048	-1.089250
C	-0.501379	1.602844	0.297334
C	-0.729370	0.257289	0.325809
C	0.337120	-0.696740	0.659886
C	0.717820	2.195228	0.758271
C	-1.463094	2.543249	-0.199422
N	1.671683	2.717053	1.135482
N	-2.199010	3.328785	-0.606859
C	-2.068790	-0.302304	0.046416
C	-2.170070	-1.440454	-0.763955
C	-3.227039	0.269769	0.582021
C	-3.415583	-1.971922	-1.065104
C	-4.471573	-0.278685	0.294037
H	-3.154457	1.122831	1.247190
C	-4.567787	-1.391628	-0.536104
H	-5.364264	0.160903	0.722837
N	-0.042703	-1.697868	1.566775
H	1.982394	-2.787430	0.504755
H	4.308119	-2.738849	0.545814
H	5.695792	-0.772552	0.351185
H	5.153310	1.096003	-0.973967
H	3.139196	1.337390	-2.257373
H	1.040854	0.526012	-1.697080
H	-1.268398	-1.894808	-1.161036
H	-3.489349	-2.842555	-1.705885
H	-5.539545	-1.814648	-0.763308
H	-0.775396	-1.414350	2.204636
H	0.728117	-2.093433	2.089251

1.37 m062x_3-amino-VHF-cis_ch

Gibbs free energy: -857.532374
Electronic and ZPE: -857.485464

Atom	X	Y	Z
C	1.543045	-0.712364	0.003058
C	2.447214	-1.842011	0.260218
C	3.792848	-1.829710	0.273248
C	4.670951	-0.706971	0.012974
C	4.372626	0.379696	-0.727858
C	3.118277	0.660898	-1.395481
C	1.891315	0.198834	-1.087992
C	-0.500011	1.609279	0.288882
C	-0.731159	0.264893	0.313547
C	0.334783	-0.694449	0.635849
C	0.726028	2.196086	0.742332
C	-1.464917	2.556349	-0.192066
N	1.686026	2.709931	1.114029
N	-2.206588	3.344786	-0.582419
C	-2.073097	-0.297565	0.043168
C	-2.174492	-1.458362	-0.734204
C	-3.233968	0.288743	0.557072
C	-3.418858	-1.997168	-1.025004
C	-4.477619	-0.264831	0.278086
H	-3.165549	1.164440	1.192222
C	-4.572224	-1.400549	-0.519619
H	-5.371698	0.191604	0.686003
N	-0.039169	-1.708905	1.536136
H	1.957255	-2.794007	0.458864
H	4.287304	-2.765078	0.521401
H	5.686133	-0.799388	0.386719
H	5.167119	1.098885	-0.903253
H	3.175949	1.370719	-2.215412
H	1.065739	0.559642	-1.697416
H	-1.271300	-1.927254	-1.109990
H	-3.490653	-2.886438	-1.640112
H	-5.543927	-1.827120	-0.740940
H	-0.812813	-1.455161	2.136333
H	0.730095	-2.056310	2.094105

1.38 m062x_3-amino-VHF-cis_dcm

Gibbs free energy: -857.540810
Electronic and ZPE: -857.493859

Atom	X	Y	Z
C	1.544061	-0.713369	0.015663
C	2.455820	-1.836760	0.275968
C	3.801845	-1.817769	0.279639
C	4.674079	-0.694757	-0.000991
C	4.366089	0.381903	-0.753776
C	3.103609	0.651656	-1.411814
C	1.880313	0.188608	-1.087593
C	-0.500305	1.603589	0.294717
C	-0.729817	0.258215	0.321634
C	0.335927	-0.697846	0.651493
C	0.720555	2.193997	0.754528
C	-1.462110	2.546483	-0.197846
N	1.675711	2.713709	1.131199
N	-2.198575	3.333799	-0.600705
C	-2.070493	-0.300907	0.045445
C	-2.173345	-1.445406	-0.755710
C	-3.228574	0.276426	0.575670
C	-3.419229	-1.977650	-1.053322
C	-4.473608	-0.272182	0.290886
H	-3.156025	1.135688	1.232728
C	-4.570907	-1.391498	-0.530217
H	-5.366008	0.173064	0.714439
N	-0.043236	-1.704828	1.553745
H	1.975391	-2.790337	0.488242
H	4.302076	-2.747484	0.536428
H	5.693524	-0.781558	0.362123
H	5.158608	1.097868	-0.950443
H	3.151240	1.350689	-2.241663
H	1.049353	0.538989	-1.695587
H	-1.271963	-1.904826	-1.147468
H	-3.493658	-2.853456	-1.686982
H	-5.543204	-1.814523	-0.755226
H	-0.787268	-1.430331	2.182183
H	0.727185	-2.088933	2.085312

1.39 m062x_3-amino-VHF-cis_m

Gibbs free energy: -857.543453
Electronic and ZPE: -857.496386

Atom	X	Y	Z
C	1.544124	-0.713457	0.021200
C	2.458991	-1.833888	0.284746
C	3.805057	-1.812250	0.284067
C	4.674538	-0.689498	-0.007247
C	4.362193	0.381551	-0.766637
C	3.096349	0.645221	-1.421312
C	1.874825	0.182373	-1.089142
C	-0.501334	1.602847	0.297212
C	-0.729385	0.257293	0.325610
C	0.337066	-0.696829	0.659491
C	0.717920	2.195160	0.758116
C	-1.463056	2.543350	-0.199368
N	1.671824	2.716916	1.135313
N	-2.198990	3.328964	-0.606619
C	-2.068871	-0.302251	0.046368
C	-2.170266	-1.440605	-0.763700
C	-3.227079	0.270019	0.581850
C	-3.415816	-1.972067	-1.064682
C	-4.471655	-0.278406	0.294021
H	-3.154449	1.123284	1.246751
C	-4.567967	-1.391553	-0.535824
H	-5.364308	0.161391	0.722685
N	-0.042762	-1.698257	1.566107
H	1.982122	-2.787566	0.504001
H	4.307876	-2.739231	0.545400
H	5.695731	-0.772964	0.351680
H	5.153599	1.096095	-0.972898
H	3.139770	1.338036	-2.256621
H	1.041271	0.526648	-1.696974
H	-1.268632	-1.895150	-1.160643
H	-3.489654	-2.842868	-1.705229
H	-5.539763	-1.814547	-0.762919
H	-0.775909	-1.415132	2.203615
H	0.728030	-2.093423	2.088928

1.40 m062x_3-amino-VHF-cis_t

Gibbs free energy: -857.533689
Electronic and ZPE: -857.486792

Atom	X	Y	Z
C	1.543156	-0.712206	0.005376
C	2.448376	-1.841027	0.262601
C	3.794117	-1.828181	0.273581
C	4.671814	-0.705861	0.009899
C	4.372128	0.379698	-0.732224
C	3.116206	0.660153	-1.397286
C	1.889727	0.198276	-1.086874
C	-0.500049	1.608394	0.289963
C	-0.731117	0.263809	0.314885
C	0.334635	-0.695008	0.638315
C	0.725128	2.195496	0.744876
C	-1.464051	2.555020	-0.193208
N	1.684174	2.710254	1.117883
N	-2.204435	3.343504	-0.586003
C	-2.072799	-0.298061	0.043569
C	-2.174266	-1.457008	-0.736598
C	-3.233375	0.287454	0.559062
C	-3.418807	-1.994829	-1.028606
C	-4.477207	-0.265339	0.279019
H	-3.164580	1.161103	1.197039
C	-4.572057	-1.399171	-0.521494
H	-5.371128	0.189905	0.688586
N	-0.040522	-1.708832	1.538263
H	1.959794	-2.793191	0.463499
H	4.289104	-2.762936	0.522834
H	5.687873	-0.798172	0.381227
H	5.166607	1.098007	-0.911291
H	3.172104	1.368976	-2.218206
H	1.063289	0.558528	-1.695427
H	-1.271256	-1.924897	-1.114111
H	-3.490824	-2.882494	-1.645964
H	-5.543832	-1.825176	-0.743492
H	-0.809932	-1.451994	2.142661
H	0.728890	-2.061784	2.092499

1.41 m062x_A-NBD_an

Gibbs free energy: -769.370811
Electronic and ZPE: -769.326524

Atom	X	Y	Z
C	1.265046	-2.615254	1.156499
H	0.904212	-3.149463	2.025615
C	2.392811	-1.920709	1.019059
H	3.171457	-1.755451	1.751952
C	0.478070	-2.462561	-0.155611
H	-0.327134	-3.173849	-0.324784
C	2.366428	-1.294180	-0.384699
H	3.310917	-0.915056	-0.764475
C	1.666246	-2.443594	-1.150284
H	1.375813	-2.169689	-2.165763
H	2.233923	-3.374424	-1.146060
C	0.062856	-0.977695	-0.260753
C	1.209814	-0.280847	-0.389472
C	-1.348627	-0.584122	-0.158457
C	-2.162698	-1.227734	0.782122
C	-1.922018	0.368217	-1.008885
C	-3.508234	-0.896495	0.900030
H	-1.734782	-1.982183	1.434984
C	-3.271510	0.682617	-0.904588
H	-1.306507	0.852481	-1.756596
C	-4.066576	0.059078	0.055323
H	-4.121479	-1.391153	1.644647
H	-3.705524	1.414996	-1.575991
H	-5.118075	0.310020	0.137297
C	1.489593	1.161228	-0.336029
O	2.613717	1.615872	-0.371729
O	0.396704	1.921659	-0.225378
C	0.589078	3.345451	-0.131211
H	1.354202	3.646972	-0.846568
H	-0.368388	3.765264	-0.436158
C	0.949117	3.756428	1.282339
H	1.905479	3.327303	1.582468
H	1.027027	4.843846	1.340107
H	0.179110	3.431188	1.983887

1.42 m062x_A-NBD_ch

Gibbs free energy: -769.364565
Electronic and ZPE: -769.320625

Atom	X	Y	Z
C	1.444716	-2.517450	1.137343
H	1.115124	-3.080952	2.000315
C	2.518269	-1.739538	1.019109
H	3.270499	-1.517245	1.763948
C	0.665456	-2.414288	-0.184762
H	-0.084009	-3.181045	-0.369559
C	2.465342	-1.109840	-0.382099
H	3.383747	-0.656601	-0.744227
C	1.862706	-2.303554	-1.161781
H	1.567030	-2.046922	-2.180340
H	2.497606	-3.189970	-1.151626
C	0.143418	-0.962276	-0.287604
C	1.238130	-0.185003	-0.400478
C	-1.292219	-0.673407	-0.171063
C	-2.044448	-1.377741	0.777066
C	-1.946511	0.233525	-1.011149
C	-3.408976	-1.151315	0.911596
H	-1.550814	-2.095726	1.424741
C	-3.314536	0.443208	-0.890160
H	-1.377016	0.764486	-1.762932
C	-4.048493	-0.240536	0.075988
H	-3.973880	-1.691803	1.662712
H	-3.811091	1.141419	-1.554771
H	-5.115165	-0.071005	0.170592
C	1.421851	1.270666	-0.301799
O	2.508010	1.786483	-0.167426
O	0.279335	1.966959	-0.358421
C	0.376358	3.390204	-0.183372
H	1.221699	3.761801	-0.763348
H	-0.548625	3.775885	-0.610616
C	0.503274	3.754439	1.282645
H	1.435287	3.370740	1.698004
H	0.498873	4.840563	1.395924
H	-0.334047	3.346282	1.851079

1.43 m062x_A-NBD_dcm

Gibbs free energy: -769.369153
Electronic and ZPE: -769.325049

Atom	X	Y	Z
C	1.394961	-2.546969	1.147123
H	1.056409	-3.101042	2.012763
C	2.486198	-1.794932	1.019461
H	3.249645	-1.590604	1.758342
C	0.610274	-2.431114	-0.170489
H	-0.156733	-3.181933	-0.346952
C	2.437842	-1.167445	-0.383241
H	3.364241	-0.738781	-0.754732
C	1.803118	-2.349154	-1.156107
H	1.506538	-2.088303	-2.173262
H	2.417813	-3.249614	-1.149014
C	0.120338	-0.968804	-0.274875
C	1.231345	-0.214878	-0.395207
C	-1.309250	-0.648521	-0.165432
C	-2.081069	-1.331114	0.783268
C	-1.939015	0.267937	-1.014917
C	-3.441304	-1.072620	0.909923
H	-1.607876	-2.058001	1.436205
C	-3.302846	0.509213	-0.901933
H	-1.355296	0.781700	-1.768117
C	-4.056343	-0.152198	0.065689
H	-4.021649	-1.596208	1.661142
H	-3.780509	1.214388	-1.572887
H	-5.119237	0.042078	0.154475
C	1.440578	1.237946	-0.316294
O	2.542145	1.741037	-0.257052
O	0.308849	1.948791	-0.298345
C	0.429670	3.376572	-0.163628
H	1.241218	3.725016	-0.802577
H	-0.514917	3.761922	-0.544979
C	0.645551	3.772927	1.283172
H	1.591397	3.381281	1.658354
H	0.667015	4.861264	1.367337
H	-0.166313	3.397136	1.908005

1.44 m062x_A-NBD_m

Gibbs free energy: -769.370774
Electronic and ZPE: -769.326477

Atom	X	Y	Z
C	1.266896	-2.614243	1.156347
H	0.906375	-3.148683	2.025452
C	2.394181	-1.918909	1.019006
H	3.172627	-1.753067	1.751975
C	0.479941	-2.462116	-0.155843
H	-0.324754	-3.173966	-0.325103
C	2.367482	-1.292397	-0.384750
H	3.311725	-0.912562	-0.764419
C	1.668191	-2.442294	-1.150405
H	1.377657	-2.168589	-2.165911
H	2.236538	-3.372714	-1.146128
C	0.063673	-0.977536	-0.261005
C	1.210146	-0.279895	-0.389650
C	-1.348089	-0.585011	-0.158545
C	-2.161513	-1.229153	0.782227
C	-1.922368	0.366760	-1.008995
C	-3.507292	-0.899002	0.900285
H	-1.732874	-1.983146	1.435144
C	-3.272105	0.680065	-0.904553
H	-1.307341	0.851442	-1.756828
C	-4.066533	0.056001	0.055529
H	-4.120026	-1.394055	1.645061
H	-3.706808	1.412008	-1.575988
H	-5.118225	0.306095	0.137616
C	1.489022	1.162341	-0.335706
O	2.612928	1.617603	-0.369464
O	0.395494	1.922171	-0.226977
C	0.587020	3.345995	-0.131862
H	1.353212	3.648208	-0.845792
H	-0.370139	3.765473	-0.438237
C	0.944488	3.756557	1.282467
H	1.900586	3.327813	1.583972
H	1.021730	4.843993	1.340845
H	0.173496	3.430579	1.982586

1.45 m062x_A-NBD_t

Gibbs free energy: -769.365249
Electronic and ZPE: -769.321299

Atom	X	Y	Z
C	1.442206	-2.519128	1.138235
H	1.112114	-3.081979	2.001449
C	2.517030	-1.743034	1.018969
H	3.270375	-1.522052	1.763118
C	0.662222	-2.415345	-0.183388
H	-0.088393	-3.181142	-0.367272
C	2.463869	-1.113481	-0.382336
H	3.382728	-0.662057	-0.745554
C	1.858885	-2.306442	-1.161378
H	1.562836	-2.049565	-2.179756
H	2.492489	-3.193772	-1.151695
C	0.142196	-0.962705	-0.286285
C	1.237951	-0.186820	-0.399833
C	-1.293148	-0.671981	-0.170407
C	-2.046653	-1.374892	0.777847
C	-1.945929	0.235209	-1.011520
C	-3.411051	-1.146661	0.911525
H	-1.554382	-2.093278	1.426105
C	-3.313831	0.446613	-0.891434
H	-1.375576	0.765025	-1.763505
C	-4.049086	-0.235634	0.074914
H	-3.976968	-1.686004	1.662689
H	-3.809200	1.144972	-1.556759
H	-5.115592	-0.064749	0.168885
C	1.422750	1.268728	-0.302899
O	2.510243	1.784371	-0.175101
O	0.280636	1.965305	-0.352988
C	0.378267	3.389304	-0.181879
H	1.220299	3.759637	-0.767368
H	-0.548959	3.773597	-0.605347
C	0.512411	3.757140	1.282543
H	1.446017	3.373975	1.694841
H	0.509173	4.843549	1.392774
H	-0.322518	3.351217	1.856061

1.46 m062x_A-QC_an

Gibbs free energy: -769.346847
Electronic and ZPE: -769.302511

Atom	X	Y	Z
C	0.455001	-2.095742	1.208051
H	0.013110	-2.412237	2.142122
C	1.858556	-1.499671	1.009213
H	2.562109	-1.203879	1.773832
C	0.109838	-2.658290	-0.148459
H	-0.772609	-3.277429	-0.246376
C	2.204161	-1.753317	-0.419528
H	3.202390	-1.531126	-0.772292
C	1.355568	-2.873618	-0.978527
H	1.167740	-2.753814	-2.047851
H	1.808591	-3.852075	-0.801335
C	-0.102894	-1.181409	0.141805
C	1.305831	-0.574029	-0.077805
C	-1.418741	-0.512960	0.036344
C	-2.331788	-0.549591	1.089755
C	-1.779051	0.139611	-1.148108
C	-3.585898	0.046921	0.963319
H	-2.058137	-1.042968	2.016584
C	-3.024225	0.741872	-1.272800
H	-1.070939	0.178162	-1.969705
C	-3.934458	0.696040	-0.215950
H	-4.285359	0.009311	1.791187
H	-3.289373	1.246707	-2.195310
H	-4.906773	1.165627	-0.313885
C	1.754872	0.811494	-0.232320
O	2.920498	1.142795	-0.282603
O	0.736193	1.674298	-0.291679
C	1.062379	3.073918	-0.391593
H	1.889288	3.195392	-1.091019
H	0.168121	3.528368	-0.815140
C	1.388951	3.654073	0.969550
H	2.280169	3.186405	1.389303
H	1.574328	4.726024	0.877922
H	0.555189	3.508964	1.658531

1.47 m062x_A-QC_ch

Gibbs free energy: -769.340675
Electronic and ZPE: -769.296524

Atom	X	Y	Z
C	0.496003	-2.107320	1.187123
H	0.052733	-2.453640	2.109988
C	1.887568	-1.474896	1.013942
H	2.580436	-1.179272	1.788228
C	0.174851	-2.651473	-0.183269
H	-0.692999	-3.287423	-0.302022
C	2.251249	-1.695370	-0.416140
H	3.246363	-1.438731	-0.754268
C	1.433892	-2.824442	-1.003400
H	1.253997	-2.690124	-2.072592
H	1.906494	-3.795990	-0.838510
C	-0.073387	-1.186032	0.133705
C	1.324036	-0.543872	-0.058278
C	-1.402992	-0.543503	0.035496
C	-2.310958	-0.604144	1.091016
C	-1.780740	0.107847	-1.143257
C	-3.577758	-0.035482	0.971885
H	-2.021847	-1.093648	2.015184
C	-3.038725	0.682095	-1.261060
H	-1.075022	0.167427	-1.965405
C	-3.944285	0.610247	-0.202688
H	-4.273421	-0.091782	1.801924
H	-3.318027	1.185465	-2.180246
H	-4.927467	1.057778	-0.295622
C	1.744851	0.853948	-0.201021
O	2.898810	1.215733	-0.191550
O	0.703337	1.684454	-0.330374
C	0.997067	3.088850	-0.421296
H	1.854554	3.229718	-1.079961
H	0.111127	3.518018	-0.887483
C	1.246248	3.682877	0.950735
H	2.136434	3.246888	1.404811
H	1.397706	4.761011	0.866082
H	0.390255	3.506828	1.604326

1.48 m062x_A-QC_dcm

Gibbs free energy: -769.345504
Electronic and ZPE: -769.301109

Atom	X	Y	Z
C	0.450274	-2.099983	1.203137
H	0.006166	-2.419618	2.135114
C	1.855187	-1.505236	1.009297
H	2.558545	-1.213737	1.775719
C	0.106369	-2.656639	-0.156156
H	-0.777232	-3.273422	-0.258536
C	2.202821	-1.754302	-0.419817
H	3.201921	-1.531293	-0.769661
C	1.353449	-2.871202	-0.984436
H	1.167842	-2.747359	-2.053743
H	1.804341	-3.851162	-0.809810
C	-0.104308	-1.180537	0.139695
C	1.306053	-0.574905	-0.074577
C	-1.419319	-0.510082	0.036014
C	-2.334418	-0.553665	1.087113
C	-1.777332	0.150247	-1.144555
C	-3.588456	0.042712	0.961995
H	-2.061936	-1.052075	2.011598
C	-3.022478	0.752326	-1.267975
H	-1.067269	0.194812	-1.964076
C	-3.934954	0.698892	-0.213726
H	-4.289539	-0.000306	1.788243
H	-3.285943	1.263051	-2.187744
H	-4.907405	1.168423	-0.310733
C	1.758860	0.810280	-0.226359
O	2.924688	1.139630	-0.264763
O	0.741053	1.673594	-0.299304
C	1.070293	3.072052	-0.395176
H	1.904267	3.192721	-1.086525
H	0.180330	3.528069	-0.826207
C	1.385868	3.650978	0.969232
H	2.274794	3.183854	1.394299
H	1.570691	4.723380	0.880907
H	0.547043	3.503253	1.651456

1.49 m062x_A-QC_m

Gibbs free energy: -769.346805
Electronic and ZPE: -769.302464

Atom	X	Y	Z
C	0.454494	-2.095927	1.207876
H	0.012487	-2.412442	2.141886
C	1.858192	-1.500139	1.009185
H	2.561796	-1.204600	1.773854
C	0.109265	-2.658227	-0.148717
H	-0.773330	-3.277134	-0.246775
C	2.203808	-1.753698	-0.419571
H	3.202101	-1.531652	-0.772248
C	1.354993	-2.873746	-0.978740
H	1.167244	-2.753784	-2.048062
H	1.807781	-3.852329	-0.801633
C	-0.103147	-1.181330	0.141725
C	1.305734	-0.574250	-0.077729
C	-1.418865	-0.512617	0.036328
C	-2.332074	-0.549549	1.089580
C	-1.778926	0.140445	-1.147919
C	-3.586104	0.047118	0.963179
H	-2.058594	-1.043269	2.016277
C	-3.024022	0.742861	-1.272574
H	-1.070679	0.179249	-1.969384
C	-3.934424	0.696704	-0.215895
H	-4.285691	0.009273	1.790931
H	-3.288979	1.248073	-2.194933
H	-4.906683	1.166416	-0.313804
C	1.755160	0.811180	-0.232142
O	2.920859	1.142188	-0.282054
O	0.736675	1.674198	-0.291908
C	1.063231	3.073720	-0.391627
H	1.890389	3.195041	-1.090793
H	0.169195	3.528413	-0.815388
C	1.389570	3.653707	0.969649
H	2.280631	3.185871	1.389542
H	1.575129	4.725643	0.878179
H	0.555623	3.508633	1.658412

1.50 m062x_A-QC_t

Gibbs free energy: -769.341459
Electronic and ZPE: -769.297239

Atom	X	Y	Z
C	0.488176	-2.106775	1.188998
H	0.044340	-2.449173	2.113042
C	1.882129	-1.480496	1.013297
H	2.576535	-1.186125	1.786696
C	0.163699	-2.652180	-0.180034
H	-0.706819	-3.284832	-0.296827
C	2.243707	-1.704945	-0.416643
H	3.239698	-1.453692	-0.756201
C	1.421136	-2.831639	-1.001182
H	1.240736	-2.698399	-2.070398
H	1.890005	-3.804770	-0.835116
C	-0.078332	-1.185063	0.134320
C	1.321444	-0.548868	-0.060426
C	-1.405604	-0.537916	0.035484
C	-2.315031	-0.597020	1.089973
C	-1.780008	0.116003	-1.143005
C	-3.579928	-0.024107	0.970067
H	-2.028706	-1.088747	2.013832
C	-3.036084	0.694515	-1.261533
H	-1.073368	0.174122	-1.964484
C	-3.943093	0.624346	-0.204183
H	-4.276695	-0.079219	1.799261
H	-3.312705	1.199918	-2.180413
H	-4.924674	1.075270	-0.297631
C	1.747730	0.846941	-0.204228
O	2.903808	1.203484	-0.200872
O	0.709987	1.682743	-0.326334
C	1.009446	3.086254	-0.417609
H	1.864245	3.223892	-1.080335
H	0.123316	3.519563	-0.879467
C	1.267264	3.678127	0.953695
H	2.156985	3.237545	1.404284
H	1.423765	4.755483	0.868714
H	0.413072	3.506286	1.610749

1.51 m062x_A-TS_an

Gibbs free energy: -769.279704
Electronic and ZPE: -769.236493

Atom	X	Y	Z
C	-0.123970	2.036708	1.307287
H	0.425297	1.835720	2.211012
C	-1.472770	1.776878	1.064495
H	-2.155186	1.295349	1.756762
C	0.411823	2.520707	-0.038695
H	1.400786	2.958211	-0.075475
C	-1.791314	2.032170	-0.366127
H	-2.832607	2.116561	-0.649154
C	-0.787690	3.117071	-0.765650
H	-0.638911	3.152814	-1.844873
H	-1.045239	4.106427	-0.384364
C	0.270101	1.047332	-0.123372
C	-1.077973	0.705074	-0.715919
C	1.467199	0.191650	-0.048540
C	2.533128	0.476409	0.815331
C	1.603703	-0.846777	-0.976964
C	3.697846	-0.277023	0.768257
H	2.457392	1.282957	1.535920
C	2.784257	-1.579544	-1.039974
H	0.787365	-1.068587	-1.650182
C	3.828164	-1.307106	-0.161743
H	4.507425	-0.055992	1.454031
H	2.881949	-2.373269	-1.771739
H	4.740033	-1.891957	-0.200592
C	-1.815148	-0.486219	-0.532336
O	-3.043102	-0.590884	-0.647610
O	-1.052655	-1.586780	-0.236123
C	-1.736876	-2.830385	-0.070925
H	-2.530232	-2.912860	-0.813984
H	-0.984001	-3.592866	-0.275204
C	-2.286280	-2.974725	1.336354
H	-3.027737	-2.200916	1.539456
H	-2.762534	-3.950326	1.457902
H	-1.482929	-2.893265	2.071470

1.52 m062x_A-TS_ch

Gibbs free energy: -769.268351
Electronic and ZPE: -769.225451

Atom	X	Y	Z
C	-0.134059	2.052355	1.325482
H	0.409444	1.799337	2.219356
C	-1.467047	1.740348	1.031436
H	-2.151174	1.209493	1.684505
C	0.423258	2.515307	-0.017162
H	1.413919	2.950337	-0.052667
C	-1.774372	2.035903	-0.389173
H	-2.811138	2.109358	-0.690858
C	-0.761988	3.119448	-0.763346
H	-0.594603	3.158493	-1.839727
H	-1.023348	4.107835	-0.380665
C	0.283190	1.042613	-0.141916
C	-1.059059	0.706628	-0.723657
C	1.472394	0.183075	-0.054335
C	2.541202	0.477395	0.803339
C	1.602000	-0.869890	-0.966496
C	3.701914	-0.280276	0.767132
H	2.465778	1.294740	1.512255
C	2.780410	-1.606239	-1.019742
H	0.782605	-1.096252	-1.634017
C	3.825905	-1.324356	-0.148063
H	4.513789	-0.053421	1.448465
H	2.874402	-2.411329	-1.739441
H	4.735616	-1.913232	-0.179520
C	-1.816577	-0.478293	-0.527370
O	-3.042467	-0.548503	-0.589138
O	-1.062932	-1.594641	-0.271633
C	-1.776436	-2.817135	-0.081873
H	-2.585131	-2.883187	-0.810373
H	-1.045599	-3.599939	-0.290179
C	-2.309137	-2.934186	1.334663
H	-3.047430	-2.155263	1.528189
H	-2.787967	-3.905518	1.479936
H	-1.495557	-2.842474	2.057389

1.53 m062x_A-TS_dcm

Gibbs free energy: -769.276971
Electronic and ZPE: -769.233762

Atom	X	Y	Z
C	-0.118898	2.040855	1.311431
H	0.428399	1.825629	2.213028
C	-1.465021	1.772779	1.056748
H	-2.149136	1.280907	1.739935
C	0.423379	2.517734	-0.033891
H	1.414270	2.951076	-0.071050
C	-1.780073	2.038600	-0.371671
H	-2.820019	2.123647	-0.659230
C	-0.770837	3.119813	-0.765394
H	-0.617641	3.155627	-1.843947
H	-1.025943	4.109906	-0.383919
C	0.277067	1.044888	-0.127961
C	-1.070888	0.708568	-0.717933
C	1.469636	0.184795	-0.049621
C	2.538390	0.471207	0.810465
C	1.600453	-0.859714	-0.971806
C	3.700115	-0.286293	0.766094
H	2.465963	1.282361	1.526408
C	2.778549	-1.596471	-1.032489
H	0.782036	-1.081952	-1.642193
C	3.824850	-1.322320	-0.158108
H	4.511903	-0.064273	1.448988
H	2.872211	-2.394845	-1.759696
H	4.734670	-1.910529	-0.195211
C	-1.816957	-0.478550	-0.530943
O	-3.044650	-0.571750	-0.636515
O	-1.060351	-1.584506	-0.239666
C	-1.755145	-2.821702	-0.072889
H	-2.547653	-2.898980	-0.817552
H	-1.007596	-3.590494	-0.273284
C	-2.310033	-2.958665	1.333083
H	-3.051599	-2.183121	1.528618
H	-2.788440	-3.932935	1.457403
H	-1.508931	-2.875115	2.070463

1.54 m062x_A-TS_m

Gibbs free energy: -769.279610
Electronic and ZPE: -769.236399

Atom	X	Y	Z
C	-0.123796	2.036806	1.307442
H	0.425394	1.835303	2.211098
C	-1.472504	1.776710	1.064223
H	-2.154987	1.294805	1.756161
C	0.412237	2.520587	-0.038501
H	1.401272	2.957938	-0.075279
C	-1.790910	2.032399	-0.366322
H	-2.832152	2.116824	-0.649516
C	-0.787081	3.117174	-0.765611
H	-0.638139	3.152944	-1.844809
H	-1.044542	4.106550	-0.384299
C	0.270346	1.047231	-0.123535
C	-1.077723	0.705201	-0.716018
C	1.467287	0.191396	-0.048582
C	2.533326	0.476240	0.815135
C	1.603589	-0.847265	-0.976767
C	3.697945	-0.277326	0.768156
H	2.457711	1.282967	1.535545
C	2.784062	-1.580163	-1.039697
H	0.787173	-1.069110	-1.649873
C	3.828063	-1.307637	-0.161622
H	4.507610	-0.056237	1.453812
H	2.881609	-2.374066	-1.771288
H	4.739866	-1.892599	-0.200411
C	-1.815225	-0.485936	-0.532320
O	-3.043174	-0.590191	-0.647274
O	-1.052952	-1.586691	-0.236254
C	-1.737556	-2.830063	-0.070974
H	-2.530912	-2.912345	-0.814058
H	-0.984887	-3.592779	-0.275142
C	-2.287099	-2.974126	1.336283
H	-3.028507	-2.200215	1.539161
H	-2.763478	-3.949655	1.457943
H	-1.483790	-2.892642	2.071443

1.55 m062x_A-TS_t

Gibbs free energy: -769.269641
Electronic and ZPE: -769.226706

Atom	X	Y	Z
C	-0.130501	2.050498	1.323424
H	0.413280	1.802747	2.218629
C	-1.465724	1.745964	1.035218
H	-2.150144	1.220888	1.692668
C	0.424957	2.515378	-0.019496
H	1.415957	2.949446	-0.055240
C	-1.773828	2.037403	-0.386641
H	-2.810993	2.113325	-0.686351
C	-0.761196	3.120006	-0.763538
H	-0.595801	3.158524	-1.840222
H	-1.021044	4.108802	-0.381003
C	0.282990	1.042730	-0.139843
C	-1.060284	0.707586	-0.723095
C	1.472156	0.182428	-0.053514
C	2.541251	0.475226	0.804299
C	1.601279	-0.869530	-0.966978
C	3.701740	-0.282977	0.766836
H	2.466789	1.291825	1.514141
C	2.779298	-1.606490	-1.021405
H	0.781867	-1.094959	-1.634829
C	3.825191	-1.326084	-0.149555
H	4.513832	-0.057114	1.448223
H	2.872740	-2.410737	-1.742119
H	4.734641	-1.915290	-0.181915
C	-1.816772	-0.477137	-0.527871
O	-3.043030	-0.550340	-0.597003
O	-1.063250	-1.592094	-0.265363
C	-1.774496	-2.816723	-0.080442
H	-2.579463	-2.884416	-0.812872
H	-1.040809	-3.597491	-0.286272
C	-2.313238	-2.936957	1.333516
H	-3.052721	-2.158863	1.525935
H	-2.791924	-3.908945	1.474679
H	-1.502910	-2.846199	2.059987

1.56 m062x_B-NBD_an

Gibbs free energy: -709.002764
Electronic and ZPE: -708.961444

Atom	X	Y	Z
C	3.669599	-0.575969	-0.992006
H	4.328177	-0.366462	-1.824141
C	2.850190	-1.612554	-0.828816
C	2.080294	-1.382741	0.481974
H	1.588002	-2.248800	0.916626
C	3.456294	0.360961	0.207662
H	4.216190	1.118007	0.381169
C	3.202969	-0.700151	1.306341
C	2.010994	0.888773	0.092815
C	1.173120	-0.158425	0.253973
C	-0.280478	-0.229843	0.162104
C	-1.094869	0.875370	0.430114
C	-0.902290	-1.433624	-0.210794
C	-2.478251	0.801257	0.320597
H	-0.650099	1.809315	0.753975
C	-2.275747	-1.517838	-0.334829
H	-0.299856	-2.309686	-0.424871
C	-3.075607	-0.400224	-0.069693
H	-3.072986	1.675967	0.547897
H	-2.755243	-2.442709	-0.633499
C	1.688437	2.214125	-0.281314
N	1.458740	3.303177	-0.588827
O	-4.408769	-0.578146	-0.208878
C	-5.259859	0.528887	0.049061
H	-6.271999	0.175348	-0.127143
H	-5.163950	0.861964	1.085112
H	-5.038367	1.357356	-0.627645
H	2.680967	-2.447516	-1.495573
H	2.851937	-0.271771	2.245949
H	4.057412	-1.356109	1.471831

1.57 m062x_B-NBD_ch

Gibbs free energy: -708.995369
Electronic and ZPE: -708.954127

Atom	X	Y	Z
C	3.662375	-0.577275	-1.007375
H	4.312482	-0.363975	-1.845003
C	2.843964	-1.613996	-0.843960
C	2.080198	-1.387059	0.470547
H	1.590215	-2.253814	0.907206
C	3.455091	0.355029	0.196733
H	4.216386	1.111241	0.369421
C	3.208117	-0.710753	1.292033
C	2.010477	0.886001	0.092091
C	1.172284	-0.159763	0.251880
C	-0.281692	-0.231119	0.165154
C	-1.092663	0.883325	0.400493
C	-0.908544	-1.441866	-0.174010
C	-2.475863	0.809011	0.293773
H	-0.644570	1.827265	0.687900
C	-2.281896	-1.527190	-0.292997
H	-0.308653	-2.324384	-0.367586
C	-3.077649	-0.400851	-0.059499
H	-3.067221	1.693421	0.490507
H	-2.767041	-2.456741	-0.566301
C	1.695283	2.220934	-0.258817
N	1.472845	3.318040	-0.539132
O	-4.411695	-0.579752	-0.193553
C	-5.256177	0.536500	0.019086
H	-6.269550	0.181779	-0.149307
H	-5.165540	0.908104	1.043251
H	-5.028665	1.340400	-0.685836
H	2.671034	-2.442856	-1.517274
H	2.861788	-0.285906	2.235107
H	4.063162	-1.368376	1.449465

1.58 m062x_B-NBD_dcm

Gibbs free energy: -709.001081
Electronic and ZPE: -708.959779

Atom	X	Y	Z
C	3.667998	-0.576288	-0.995847
H	4.324561	-0.365506	-1.829201
C	2.848641	-1.612839	-0.833210
C	2.079948	-1.384188	0.478403
H	1.588083	-2.250540	0.913161
C	3.456030	0.359001	0.205235
H	4.216343	1.115664	0.379039
C	3.203786	-0.703602	1.302626
C	2.010982	0.887825	0.092692
C	1.172738	-0.158935	0.252918
C	-0.280962	-0.230197	0.162431
C	-1.094397	0.877822	0.421013
C	-0.904281	-1.436129	-0.200607
C	-2.477733	0.803734	0.312508
H	-0.648699	1.814808	0.734393
C	-2.277726	-1.520648	-0.322999
H	-0.302678	-2.314137	-0.408850
C	-3.076421	-0.400372	-0.066920
H	-3.071501	1.681389	0.530912
H	-2.758775	-2.447006	-0.614317
C	1.690960	2.215975	-0.274862
N	1.464220	3.307637	-0.574566
O	-4.409810	-0.578529	-0.204253
C	-5.259064	0.531549	0.041026
H	-6.271622	0.177701	-0.132516
H	-5.164183	0.875612	1.073767
H	-5.036000	1.352919	-0.644019
H	2.678473	-2.445859	-1.502130
H	2.853719	-0.276373	2.243152
H	4.058233	-1.360153	1.466154

1.59 m062x_B-NBD_m

Gibbs free energy: -709.002708
Electronic and ZPE: -708.961388

Atom	X	Y	Z
C	3.669548	-0.575982	-0.992136
H	4.328060	-0.366427	-1.824310
C	2.850138	-1.612565	-0.828975
C	2.080277	-1.382796	0.481841
H	1.587995	-2.248867	0.916490
C	3.456285	0.360885	0.207584
H	4.216196	1.117915	0.381110
C	3.202988	-0.700282	1.306212
C	2.010996	0.888736	0.092810
C	1.173104	-0.158445	0.253927
C	-0.280498	-0.229855	0.162105
C	-1.094853	0.875464	0.429770
C	-0.902365	-1.433716	-0.210430
C	-2.478234	0.801353	0.320294
H	-0.650049	1.809522	0.753248
C	-2.275822	-1.517942	-0.334401
H	-0.299963	-2.309851	-0.424296
C	-3.075639	-0.400228	-0.069595
H	-3.072933	1.676172	0.547268
H	-2.755375	-2.442869	-0.632800
C	1.688538	2.214191	-0.281079
N	1.458960	3.303343	-0.588307
O	-4.408810	-0.578159	-0.208705
C	-5.259834	0.528988	0.048780
H	-6.271990	0.175436	-0.127319
H	-5.163954	0.862466	1.084710
H	-5.038290	1.357198	-0.628235
H	2.680883	-2.447454	-1.495814
H	2.851985	-0.271945	2.245852
H	4.057428	-1.356263	1.471637

1.60 m062x_B-NBD_t

Gibbs free energy: -708.996293
Electronic and ZPE: -708.955043

Atom	X	Y	Z
C	3.663153	-0.576867	-1.005865
H	4.314150	-0.363638	-1.842839
C	2.844617	-1.613620	-0.842864
C	2.080133	-1.386842	0.471287
H	1.589929	-2.253680	0.907428
C	3.455191	0.355489	0.198091
H	4.216313	1.111730	0.371183
C	3.207406	-0.710118	1.293404
C	2.010473	0.886175	0.092433
C	1.172251	-0.159794	0.251944
C	-0.281652	-0.231129	0.164785
C	-1.092911	0.882548	0.403118
C	-0.908110	-1.441284	-0.177404
C	-2.476133	0.808391	0.296188
H	-0.645104	1.825602	0.693959
C	-2.281495	-1.526425	-0.296793
H	-0.308101	-2.323291	-0.372873
C	-3.077585	-0.400783	-0.060420
H	-3.067775	1.691986	0.495647
H	-2.766051	-2.455619	-0.572425
C	1.694843	2.220213	-0.260689
N	1.472428	3.316725	-0.543748
O	-4.411517	-0.579504	-0.194815
C	-5.256592	0.536260	0.021756
H	-6.269841	0.181680	-0.147377
H	-5.165435	0.904385	1.047021
H	-5.029399	1.342196	-0.680778
H	2.672033	-2.442833	-1.515840
H	2.860521	-0.285198	2.236228
H	4.062351	-1.367637	1.451574

1.61 m062x_B-QC_an

Gibbs free energy: -708.973119
Electronic and ZPE: -708.931731

Atom	X	Y	Z
C	3.193045	-0.163143	-0.924254
H	3.752305	0.117202	-1.804138
C	2.225555	-1.349441	-0.770090
C	2.073067	-1.503407	0.722410
H	1.554035	-2.371798	1.107281
C	3.521897	0.264509	0.473132
H	4.298164	1.000717	0.633296
C	3.222861	-0.846978	1.454203
C	2.217457	0.727128	-0.160892
C	1.244546	-0.473911	-0.024424
C	-0.229003	-0.404326	-0.069001
C	-0.910294	0.621151	0.583184
C	-0.980057	-1.374886	-0.742674
C	-2.302991	0.690917	0.574068
H	-0.353812	1.385647	1.116401
C	-2.363754	-1.326402	-0.749716
H	-0.473458	-2.176398	-1.270537
C	-3.035376	-0.290502	-0.092895
H	-2.793891	1.506242	1.089017
H	-2.946351	-2.078088	-1.270181
C	1.876723	2.076296	-0.438296
N	1.588235	3.168983	-0.668592
O	-4.392461	-0.320018	-0.163256
C	-5.108233	0.716049	0.487908
H	-6.161144	0.510849	0.313441
H	-4.909615	0.714880	1.562667
H	-4.852650	1.692676	0.069143
H	2.030081	-2.120647	-1.500995
H	2.928447	-0.464725	2.433574
H	4.077260	-1.517624	1.571245

1.62 m062x_B-QC_ch

Gibbs free energy: -708.965183
Electronic and ZPE: -708.923839

Atom	X	Y	Z
C	3.184012	-0.161077	-0.937064
H	3.743165	0.124823	-1.815322
C	2.209813	-1.343017	-0.793214
C	2.062982	-1.516553	0.697583
H	1.536184	-2.383558	1.075336
C	3.522136	0.243426	0.466611
H	4.303557	0.972716	0.634404
C	3.223005	-0.881549	1.432111
C	2.221151	0.724944	-0.157492
C	1.239218	-0.469817	-0.030416
C	-0.234371	-0.398879	-0.067918
C	-0.912258	0.661603	0.526067
C	-0.988154	-1.408821	-0.677441
C	-2.305003	0.726285	0.522460
H	-0.354776	1.462164	1.001207
C	-2.370598	-1.365045	-0.677519
H	-0.483074	-2.237429	-1.163949
C	-3.039745	-0.293728	-0.078188
H	-2.793468	1.572789	0.986958
H	-2.958160	-2.144225	-1.149108
C	1.900407	2.087832	-0.404074
N	1.639815	3.192502	-0.603503
O	-4.396666	-0.331791	-0.138037
C	-5.109480	0.741915	0.442212
H	-6.163004	0.525175	0.284292
H	-4.909956	0.813950	1.515234
H	-4.856565	1.689933	-0.040865
H	2.002561	-2.101091	-1.534725
H	2.936746	-0.512508	2.419195
H	4.072719	-1.561040	1.533848

1.63 m062x_B-QC_dcm

Gibbs free energy: -708.971218
Electronic and ZPE: -708.929911

Atom	X	Y	Z
C	3.190813	-0.163041	-0.927179
H	3.750245	0.119248	-1.806351
C	2.220669	-1.347615	-0.777092
C	2.069051	-1.507808	0.714754
H	1.547074	-2.375699	1.096855
C	3.521915	0.257238	0.472252
H	4.300045	0.990909	0.635357
C	3.221668	-0.858329	1.448303
C	2.218776	0.726248	-0.159217
C	1.242653	-0.472584	-0.026637
C	-0.230870	-0.402272	-0.069465
C	-0.911117	0.634593	0.564653
C	-0.982861	-1.385689	-0.723127
C	-2.303865	0.702752	0.557482
H	-0.354266	1.410632	1.080242
C	-2.366246	-1.338727	-0.727782
H	-0.476888	-2.196001	-1.238192
C	-3.037069	-0.291366	-0.088713
H	-2.793964	1.528246	1.056757
H	-2.950243	-2.099468	-1.233163
C	1.885398	2.079685	-0.428085
N	1.607172	3.176529	-0.649879
O	-4.394180	-0.323607	-0.155386
C	-5.108765	0.724761	0.474835
H	-6.161974	0.516001	0.306061
H	-4.909063	0.745901	1.549396
H	-4.854124	1.692920	0.035912
H	2.021827	-2.114558	-1.511597
H	2.929296	-0.480102	2.429906
H	4.074369	-1.531957	1.561157

1.64 m062x_B-QC_m

Gibbs free energy: -708.973058
Electronic and ZPE: -708.931670

Atom	X	Y	Z
C	3.192962	-0.163144	-0.924367
H	3.752230	0.117274	-1.804222
C	2.225357	-1.349365	-0.770367
C	2.072903	-1.503581	0.722106
H	1.553747	-2.371950	1.106861
C	3.521910	0.264210	0.473099
H	4.298257	1.000311	0.633376
C	3.222812	-0.847435	1.453971
C	2.217520	0.727098	-0.160821
C	1.244472	-0.473846	-0.024510
C	-0.229075	-0.404233	-0.069018
C	-0.910332	0.621701	0.582449
C	-0.980164	-1.375323	-0.741891
C	-2.303033	0.691398	0.573408
H	-0.353843	1.386661	1.114982
C	-2.363851	-1.326907	-0.748838
H	-0.473590	-2.177194	-1.269239
C	-3.035447	-0.290541	-0.092729
H	-2.793904	1.507130	1.087739
H	-2.946493	-2.078970	-1.268702
C	1.877084	2.076433	-0.437896
N	1.588984	3.169282	-0.667863
O	-4.392534	-0.320173	-0.162946
C	-5.108264	0.716403	0.487382
H	-6.161186	0.511060	0.313130
H	-4.909611	0.716121	1.562142
H	-4.852707	1.692695	0.067809
H	2.029739	-2.120395	-1.501421
H	2.928481	-0.465338	2.433431
H	4.077138	-1.518205	1.570850

1.65 m062x_B-QC_t

Gibbs free energy: -708.966112
Electronic and ZPE: -708.924807

Atom	X	Y	Z
C	3.185190	-0.161782	-0.935193
H	3.744435	0.123439	-1.813602
C	2.211548	-1.344086	-0.790325
C	2.063639	-1.515168	0.700663
H	1.537476	-2.382177	1.079236
C	3.521918	0.245515	0.467800
H	4.302812	0.975501	0.634929
C	3.222364	-0.877760	1.435163
C	2.220709	0.724943	-0.157826
C	1.239650	-0.470404	-0.029900
C	-0.233918	-0.399449	-0.068448
C	-0.912055	0.657339	0.532165
C	-0.987511	-1.405035	-0.685326
C	-2.304777	0.722667	0.528070
H	-0.354537	1.454071	1.013771
C	-2.370101	-1.360686	-0.686041
H	-0.482376	-2.230613	-1.176828
C	-3.039404	-0.293218	-0.079977
H	-2.793388	1.565991	0.998165
H	-2.957218	-2.136778	-1.163313
C	1.898405	2.086425	-0.408313
N	1.635797	3.190047	-0.611482
O	-4.396354	-0.330333	-0.140729
C	-5.109289	0.739394	0.447910
H	-6.162804	0.523947	0.288444
H	-4.909481	0.803088	1.521309
H	-4.856191	1.690827	-0.028093
H	2.005855	-2.103772	-1.530590
H	2.934947	-0.507031	2.421250
H	4.072506	-1.556344	1.538997

1.66 m062x_B-TS_an

Gibbs free energy: -708.910690
Electronic and ZPE: -708.869409

Atom	X	Y	Z
C	-2.870349	-0.662458	1.469220
H	-3.023436	-0.521211	2.531914
C	-1.978183	-1.542206	0.869554
C	-2.132885	-1.347974	-0.662518
H	-1.767216	-2.137479	-1.305140
C	-3.443728	0.205959	0.399489
H	-4.301386	0.816140	0.658921
C	-3.511522	-0.720873	-0.829413
C	-2.084970	0.908799	0.313361
C	-1.255544	-0.321778	-0.076041
C	0.207195	-0.334132	-0.091517
C	0.912158	0.749435	0.438592
C	0.939228	-1.406250	-0.634071
C	2.302999	0.781529	0.433981
H	0.364171	1.582283	0.862608
C	2.317068	-1.389956	-0.638502
H	0.426515	-2.263549	-1.055488
C	3.011882	-0.293411	-0.104149
H	2.813349	1.640745	0.847945
H	2.886282	-2.212767	-1.054688
C	-1.935887	2.119558	-0.361201
N	-1.789215	3.171014	-0.849227
O	4.357809	-0.367945	-0.158984
C	5.109673	0.713881	0.373192
H	6.153918	0.449150	0.233098
H	4.891184	1.640271	-0.162526
H	4.903838	0.844051	1.437939
H	-1.307015	-2.233628	1.351956
H	-3.594082	-0.151808	-1.756688
H	-4.306912	-1.466475	-0.773245

1.67 m062x_B-TS_ch

Gibbs free energy: -708.896289
Electronic and ZPE: -708.854951

Atom	X	Y	Z
C	-2.862946	-0.664633	1.463168
H	-2.993922	-0.505030	2.525903
C	-2.003072	-1.570669	0.863418
C	-2.131105	-1.346397	-0.666059
H	-1.766938	-2.127044	-1.321275
C	-3.434123	0.210580	0.396465
H	-4.288062	0.826455	0.655544
C	-3.507330	-0.712422	-0.836610
C	-2.076303	0.909035	0.319598
C	-1.253780	-0.311077	-0.095309
C	0.203304	-0.335017	-0.096720
C	0.905514	0.757351	0.420145
C	0.936831	-1.417378	-0.618401
C	2.295272	0.786140	0.420351
H	0.352972	1.598308	0.821070
C	2.313189	-1.405161	-0.614172
H	0.423171	-2.278750	-1.031200
C	3.005134	-0.298927	-0.094988
H	2.805052	1.653997	0.816566
H	2.887899	-2.232218	-1.013519
C	-1.919892	2.131238	-0.344498
N	-1.767368	3.180944	-0.826271
O	4.349982	-0.376904	-0.142833
C	5.100663	0.716784	0.356995
H	6.144920	0.448897	0.221384
H	4.880809	1.629276	-0.202511
H	4.898542	0.876461	1.419091
H	-1.313027	-2.245318	1.343292
H	-3.582371	-0.136493	-1.760244
H	-4.305460	-1.456593	-0.787836

1.68 m062x_B-TS_dcm

Gibbs free energy: -708.907394
Electronic and ZPE: -708.866090

Atom	X	Y	Z
C	-2.865842	-0.668181	1.467646
H	-3.012399	-0.525179	2.530950
C	-1.980872	-1.551358	0.864776
C	-2.130921	-1.346440	-0.666118
H	-1.765061	-2.131531	-1.314254
C	-3.440749	0.203912	0.401303
H	-4.298131	0.813645	0.662897
C	-3.509950	-0.719060	-0.830820
C	-2.083349	0.908028	0.317400
C	-1.254371	-0.318594	-0.081408
C	0.206970	-0.333192	-0.093638
C	0.911081	0.753871	0.430601
C	0.939566	-1.409151	-0.628325
C	2.301661	0.785133	0.427481
H	0.362008	1.590026	0.846394
C	2.316997	-1.394018	-0.630082
H	0.426775	-2.268442	-1.045841
C	3.010980	-0.293793	-0.101809
H	2.811733	1.647752	0.834622
H	2.887688	-2.218882	-1.039995
C	-1.937068	2.122198	-0.354678
N	-1.794491	3.174164	-0.840795
O	4.356598	-0.369596	-0.153765
C	5.108010	0.716570	0.368220
H	6.152304	0.450448	0.230845
H	4.889809	1.638105	-0.176105
H	4.902143	0.856796	1.431838
H	-1.303679	-2.238962	1.344322
H	-3.592373	-0.146223	-1.755748
H	-4.305030	-1.465480	-0.777535

1.69 m062x_B-TS_m

Gibbs free energy: -708.910581
Electronic and ZPE: -708.869297

Atom	X	Y	Z
C	-2.870169	-0.662720	1.469159
H	-3.023024	-0.521450	2.531880
C	-1.978242	-1.542550	0.869345
C	-2.132798	-1.347903	-0.662680
H	-1.767113	-2.137227	-1.305524
C	-3.443620	0.205852	0.399577
H	-4.301277	0.815995	0.659109
C	-3.511458	-0.720806	-0.829467
C	-2.084920	0.908762	0.313535
C	-1.255495	-0.321662	-0.076230
C	0.207196	-0.334087	-0.091593
C	0.912129	0.749619	0.438279
C	0.939251	-1.406357	-0.633837
C	2.302961	0.781683	0.433720
H	0.364107	1.582601	0.861977
C	2.317076	-1.390105	-0.638172
H	0.426537	-2.263738	-1.055094
C	3.011861	-0.293415	-0.104064
H	2.813301	1.641035	0.847415
H	2.886341	-2.213002	-1.054113
C	-1.935987	2.119647	-0.360941
N	-1.789521	3.171131	-0.848898
O	4.357778	-0.367998	-0.158790
C	5.109625	0.714001	0.372995
H	6.153872	0.449216	0.233008
H	4.891146	1.640203	-0.163058
H	4.903785	0.844558	1.437699
H	-1.306853	-2.233848	1.351621
H	-3.594028	-0.151582	-1.756642
H	-4.306828	-1.466450	-0.773419

1.70 m062x_B-TS_t

Gibbs free energy: -708.898073
Electronic and ZPE: -708.856746

Atom	X	Y	Z
C	-2.862325	-0.667008	1.463949
H	-2.995175	-0.510894	2.527010
C	-1.998362	-1.568445	0.862508
C	-2.130590	-1.346004	-0.666984
H	-1.766035	-2.126561	-1.321963
C	-3.434862	0.208466	0.398273
H	-4.289545	0.822748	0.658584
C	-3.507617	-0.713533	-0.835406
C	-2.077526	0.908623	0.320148
C	-1.253612	-0.312023	-0.093442
C	0.204102	-0.334334	-0.096639
C	0.906530	0.757588	0.420652
C	0.937564	-1.416052	-0.619576
C	2.296406	0.786767	0.420478
H	0.354488	1.598145	0.823122
C	2.314066	-1.403426	-0.616050
H	0.424098	-2.277368	-1.032649
C	3.006269	-0.297765	-0.096058
H	2.806178	1.654175	0.817677
H	2.888226	-2.230396	-1.016424
C	-1.924309	2.129731	-0.345358
N	-1.775194	3.180067	-0.827779
O	4.351199	-0.375531	-0.144101
C	5.101938	0.717369	0.358607
H	6.146216	0.449538	0.223317
H	4.882622	1.630835	-0.199373
H	4.898834	0.874832	1.420764
H	-1.309751	-2.245166	1.341499
H	-3.584506	-0.137360	-1.758726
H	-4.304924	-1.458467	-0.786206

1.71 m062x_C-NBD_an

Gibbs free energy: -783.081820
Electronic and ZPE: -783.039439

Atom	X	Y	Z
C	3.457927	-0.742919	1.306372
H	4.281219	-1.434450	1.482557
H	3.158483	-0.248101	2.231030
C	2.276240	-1.403930	0.549689
H	1.746923	-2.215931	1.041501
C	3.737048	0.244537	0.145500
H	4.540991	0.966647	0.256918
C	1.435636	-0.143263	0.280305
C	2.320688	0.844819	0.041298
C	2.994534	-1.744308	-0.767643
H	2.763544	-2.604486	-1.381523
C	3.862853	-0.764801	-1.007764
H	4.510129	-0.635641	-1.864479
C	2.055568	2.168687	-0.388023
N	1.873652	3.252545	-0.738981
C	-0.024773	-0.129765	0.208799
C	-0.706305	-1.297396	-0.161355
C	-0.761642	1.026822	0.498533
C	-2.088452	-1.301048	-0.264804
H	-0.149706	-2.200478	-0.385347
C	-2.144751	1.021046	0.404784
H	-0.252745	1.927593	0.820289
C	-2.811957	-0.142887	0.017786
H	-2.616658	-2.199121	-0.561613
H	-2.707713	1.916064	0.637125
C	-4.294085	-0.192232	-0.098643
O	-4.919827	-1.168450	-0.432441
O	-4.880395	0.971484	0.207054
H	-5.839421	0.875647	0.110494

1.72 m062x_C-NBD_ch

Gibbs free energy: -783.072739
Electronic and ZPE: -783.030492

Atom	X	Y	Z
C	3.456854	-0.760974	1.296451
H	4.278443	-1.456669	1.465662
H	3.159837	-0.272107	2.225226
C	2.271762	-1.410784	0.536249
H	1.741550	-2.223951	1.025910
C	3.735933	0.234507	0.142867
H	4.542383	0.953635	0.258554
C	1.433801	-0.144581	0.276477
C	2.322170	0.841525	0.045170
C	2.988347	-1.745971	-0.782967
H	2.755842	-2.598734	-1.406495
C	3.858167	-0.766994	-1.017494
H	4.500855	-0.633026	-1.876773
C	2.070062	2.176003	-0.361950
N	1.901661	3.269212	-0.687791
C	-0.026504	-0.128804	0.205764
C	-0.712550	-1.302375	-0.136250
C	-0.760576	1.036466	0.465518
C	-2.094437	-1.306602	-0.237303
H	-0.157780	-2.210895	-0.342464
C	-2.143535	1.031274	0.373016
H	-0.248590	1.945957	0.756015
C	-2.813876	-0.140316	0.017924
H	-2.629668	-2.207651	-0.512326
H	-2.706206	1.933033	0.578631
C	-4.295710	-0.192391	-0.096870
O	-4.924191	-1.172844	-0.402010
O	-4.881948	0.984078	0.177495
H	-5.838622	0.876155	0.079110

1.73 m062x_C-NBD_dcm

Gibbs free energy: -783.079745
Electronic and ZPE: -783.037436

Atom	X	Y	Z
C	3.457974	-0.747592	1.303608
H	4.280676	-1.440435	1.477716
H	3.159875	-0.253985	2.229394
C	2.274773	-1.405516	0.546847
H	1.745179	-2.217457	1.038653
C	3.736829	0.241536	0.144210
H	4.541767	0.962585	0.256115
C	1.435142	-0.143281	0.279898
C	2.321248	0.843965	0.042198
C	2.991700	-1.745100	-0.771353
H	2.759677	-2.603391	-1.387459
C	3.860683	-0.766126	-1.010711
H	4.506327	-0.636114	-1.868488
C	2.059673	2.170538	-0.381740
N	1.881788	3.256990	-0.726200
C	-0.025230	-0.129147	0.208617
C	-0.707635	-1.298394	-0.154777
C	-0.761549	1.029574	0.490782
C	-2.089689	-1.302396	-0.257830
H	-0.151167	-2.202610	-0.374625
C	-2.144600	1.023782	0.397136
H	-0.252041	1.932756	0.804642
C	-2.812376	-0.142238	0.017978
H	-2.619379	-2.201303	-0.549564
H	-2.707584	1.920556	0.622558
C	-4.294400	-0.192230	-0.098369
O	-4.920777	-1.169734	-0.424973
O	-4.880711	0.974709	0.199206
H	-5.839203	0.876420	0.101636

1.74 m062x_C-NBD_m

Gibbs free energy: -783.081750
Electronic and ZPE: -783.039372

Atom	X	Y	Z
C	3.457935	-0.743093	1.306265
H	4.281204	-1.434676	1.482368
H	3.158553	-0.248317	2.230967
C	2.276182	-1.403986	0.549593
H	1.746855	-2.215981	1.041410
C	3.737041	0.244421	0.145444
H	4.541027	0.966488	0.256871
C	1.435619	-0.143259	0.280301
C	2.320712	0.844789	0.041335
C	2.994410	-1.744339	-0.767779
H	2.763368	-2.604447	-1.381738
C	3.862757	-0.764857	-1.007882
H	4.509966	-0.635670	-1.864642
C	2.055723	2.168753	-0.387796
N	1.873959	3.252707	-0.738522
C	-0.024789	-0.129737	0.208803
C	-0.706349	-1.297428	-0.161110
C	-0.761641	1.026926	0.498262
C	-2.088492	-1.301095	-0.264550
H	-0.149750	-2.200550	-0.384953
C	-2.144748	1.021148	0.404513
H	-0.252726	1.927787	0.819735
C	-2.811971	-0.142863	0.017795
H	-2.616746	-2.199201	-0.561180
H	-2.707711	1.916230	0.636602
C	-4.294095	-0.192231	-0.098636
O	-4.919858	-1.168501	-0.432173
O	-4.880405	0.971602	0.206760
H	-5.839413	0.875685	0.110157

1.75 m062x_C-NBD_t

Gibbs free energy: -783.073883
Electronic and ZPE: -783.031632

Atom	X	Y	Z
C	3.457182	-0.758742	1.297503
H	4.278948	-1.453996	1.467434
H	3.160213	-0.268957	2.225794
C	2.272213	-1.409904	0.538177
H	1.742138	-2.222730	1.028475
C	3.736047	0.235518	0.142771
H	4.542348	0.954897	0.257566
C	1.434000	-0.144334	0.277151
C	2.322011	0.841915	0.044703
C	2.988574	-1.746088	-0.780953
H	2.756044	-2.599812	-1.403155
C	3.858148	-0.767118	-1.016655
H	4.501031	-0.633894	-1.875917
C	2.068491	2.175171	-0.365140
N	1.898990	3.267360	-0.694059
C	-0.026308	-0.128819	0.206402
C	-0.711748	-1.301712	-0.139109
C	-0.760752	1.035391	0.469792
C	-2.093658	-1.305930	-0.240514
H	-0.156642	-2.209491	-0.347643
C	-2.143722	1.030104	0.377047
H	-0.249173	1.943930	0.764006
C	-2.813637	-0.140620	0.018032
H	-2.627948	-2.206658	-0.518323
H	-2.706433	1.931115	0.585743
C	-4.295486	-0.192309	-0.097179
O	-4.923625	-1.172315	-0.405866
O	-4.881736	0.982636	0.180858
H	-5.838694	0.876388	0.082317

1.76 m062x_C-QC_an

Gibbs free energy: -783.055325
Electronic and ZPE: -783.012868

Atom	X	Y	Z
C	3.445374	-0.990435	1.409175
H	4.253297	-1.719300	1.504998
H	3.187507	-0.605573	2.397412
C	2.247923	-1.561180	0.682118
H	1.672416	-2.393791	1.065754
C	3.805945	0.112690	0.440406
H	4.632801	0.791513	0.600031
C	1.478612	-0.457696	-0.031076
C	2.527103	0.674677	-0.166814
C	2.387308	-1.391942	-0.804258
H	2.118596	-2.128247	-1.547747
C	3.428340	-0.270011	-0.957036
H	3.989185	-0.015312	-1.843468
C	2.291281	2.049365	-0.430713
N	2.094698	3.163726	-0.652536
C	0.014407	-0.320432	-0.033279
C	-0.791912	-1.344033	-0.546656
C	-0.594456	0.819637	0.501804
C	-2.172159	-1.233663	-0.515971
H	-0.332637	-2.227797	-0.976632
C	-1.977693	0.936276	0.525396
H	0.013930	1.618761	0.910304
C	-2.773090	-0.091383	0.017387
H	-2.796414	-2.025617	-0.912551
H	-2.439405	1.822833	0.941728
C	-4.254549	-0.010276	0.022318
O	-4.990364	-0.868400	-0.403106
O	-4.716198	1.129631	0.555769
H	-5.684266	1.117040	0.529818

1.77 m062x_C-QC_ch

Gibbs free energy: -783.045316
Electronic and ZPE: -783.003069

Atom	X	Y	Z
C	3.441854	-1.028677	1.388857
H	4.243161	-1.767033	1.469248
H	3.191457	-0.658103	2.384729
C	2.234922	-1.574091	0.658108
H	1.651120	-2.405119	1.032995
C	3.806165	0.088187	0.437264
H	4.638557	0.758355	0.605715
C	1.474435	-0.453196	-0.035361
C	2.533761	0.670869	-0.160469
C	2.371859	-1.383846	-0.826407
H	2.091144	-2.104550	-1.580886
C	3.421695	-0.268570	-0.966943
H	3.984890	-0.008632	-1.850487
C	2.318044	2.057637	-0.390191
N	2.146678	3.181192	-0.579252
C	0.009678	-0.311587	-0.036047
C	-0.796911	-1.356558	-0.503446
C	-0.597612	0.848572	0.452099
C	-2.176581	-1.248667	-0.472052
H	-0.336869	-2.255884	-0.900090
C	-1.981352	0.962829	0.476236
H	0.010718	1.668624	0.816213
C	-2.775863	-0.086449	0.016696
H	-2.805682	-2.054058	-0.832546
H	-2.445591	1.865787	0.852585
C	-4.257884	-0.011284	0.023271
O	-4.992698	-0.885573	-0.360646
O	-4.722055	1.152433	0.511328
H	-5.688870	1.126382	0.482146

1.78 m062x_C-QC_dcm

Gibbs free energy: -783.053089
Electronic and ZPE: -783.010687

Atom	X	Y	Z
C	3.443256	-1.004669	1.402403
H	4.248742	-1.736982	1.492921
H	3.187608	-0.625162	2.393343
C	2.242878	-1.566248	0.673065
H	1.664192	-2.398493	1.052833
C	3.806110	0.103497	0.440220
H	4.635165	0.778814	0.603611
C	1.476952	-0.455886	-0.032756
C	2.529445	0.673438	-0.163520
C	2.381872	-1.388760	-0.812383
H	2.109119	-2.118929	-1.560491
C	3.426414	-0.269421	-0.959663
H	3.987932	-0.012118	-1.844943
C	2.301613	2.052154	-0.416649
N	2.114980	3.169918	-0.628530
C	0.012716	-0.317116	-0.034329
C	-0.793718	-1.348558	-0.531651
C	-0.595855	0.830075	0.484638
C	-2.173777	-1.239021	-0.500825
H	-0.334194	-2.238028	-0.949688
C	-1.979255	0.945852	0.508441
H	0.012289	1.636549	0.878566
C	-2.774420	-0.089582	0.017001
H	-2.799060	-2.036294	-0.884992
H	-2.441551	1.838343	0.911215
C	-4.255965	-0.010116	0.022514
O	-4.991607	-0.873889	-0.389789
O	-4.718226	1.137295	0.541487
H	-5.686034	1.121781	0.514704

1.79 m062x_C-QC_m

Gibbs free energy: -783.055251
Electronic and ZPE: -783.012796

Atom	X	Y	Z
C	3.445277	-0.990995	1.408923
H	4.253102	-1.719997	1.504546
H	3.187492	-0.606339	2.397263
C	2.247716	-1.561381	0.681766
H	1.672082	-2.393977	1.065246
C	3.805953	0.112323	0.440411
H	4.632900	0.791001	0.600186
C	1.478545	-0.457622	-0.031146
C	2.527197	0.674627	-0.166678
C	2.387096	-1.391821	-0.804572
H	2.118233	-2.127886	-1.548244
C	3.428270	-0.269995	-0.957126
H	3.989144	-0.015194	-1.843512
C	2.291701	2.049470	-0.430175
N	2.095520	3.163970	-0.651623
C	0.014340	-0.320298	-0.033325
C	-0.791984	-1.344209	-0.546081
C	-0.594513	0.820051	0.501136
C	-2.172224	-1.233873	-0.515389
H	-0.332700	-2.228198	-0.975596
C	-1.977757	0.936656	0.524738
H	0.013861	1.619462	0.909083
C	-2.773147	-0.091310	0.017369
H	-2.796511	-2.026042	-0.911489
H	-2.439488	1.823447	0.940549
C	-4.254608	-0.010267	0.022327
O	-4.990420	-0.868609	-0.402602
O	-4.716278	1.129928	0.555228
H	-5.684338	1.117244	0.529251

1.80 m062x_C-QC_t

Gibbs free energy: -783.046572
Electronic and ZPE: -783.004319

Atom	X	Y	Z
C	3.441879	-1.026034	1.390455
H	4.243695	-1.763659	1.472013
H	3.190776	-0.654537	2.385770
C	2.235824	-1.573329	0.659656
H	1.652616	-2.404570	1.034953
C	3.806174	0.089901	0.437771
H	4.638210	0.760591	0.605795
C	1.474688	-0.453515	-0.035083
C	2.533174	0.671200	-0.160512
C	2.373062	-1.384314	-0.824898
H	2.093332	-2.105913	-1.578862
C	3.422292	-0.268536	-0.965936
H	3.985133	-0.008601	-1.849691
C	2.316256	2.056979	-0.393260
N	2.143413	3.179892	-0.585399
C	0.010030	-0.312277	-0.035822
C	-0.796562	-1.355693	-0.506775
C	-0.597452	0.846362	0.456063
C	-2.176280	-1.247580	-0.475473
H	-0.336602	-2.253904	-0.905911
C	-1.981142	0.960828	0.480153
H	0.010832	1.664804	0.823900
C	-2.775770	-0.086835	0.016742
H	-2.804789	-2.052122	-0.838839
H	-2.445053	1.862613	0.859705
C	-4.257715	-0.010992	0.023173
O	-4.992692	-0.884105	-0.364284
O	-4.721586	1.150686	0.514955
H	-5.688571	1.126420	0.486063

1.81 m062x_C-TS_an

Gibbs free energy: -782.988941
Electronic and ZPE: -782.947115

Atom	X	Y	Z
C	-3.589350	-1.158560	-1.098488
H	-4.352102	-1.916047	-0.914186
H	-3.547030	-0.910183	-2.158272
C	-2.230022	-1.577197	-0.546433
H	-1.684870	-2.439155	-0.906559
C	-3.761770	0.094540	-0.230104
H	-4.680275	0.666641	-0.281963
C	-1.511402	-0.329882	-0.207897
C	-2.431243	0.857041	-0.464037
C	-2.311114	-1.337087	0.960483
H	-1.705785	-1.774361	1.736332
C	-3.286953	-0.349520	1.108010
H	-3.531102	0.153110	2.037914
C	-2.237617	2.074463	0.197283
N	-2.080914	3.131782	0.665375
C	-0.047224	-0.256919	-0.090635
C	0.718338	-1.373402	0.278895
C	0.600040	0.935263	-0.430176
C	2.097800	-1.293252	0.314278
H	0.237634	-2.308400	0.543814
C	1.988195	1.010723	-0.407979
H	0.024018	1.801579	-0.727739
C	2.737919	-0.099339	-0.029631
H	2.692227	-2.151117	0.603890
H	2.483779	1.934206	-0.678768
C	4.225429	-0.059293	0.021915
O	4.919238	-0.991467	0.345115
O	4.727041	1.129341	-0.331139
H	5.693509	1.092770	-0.276805

1.82 m062x_C-TS_ch

Gibbs free energy: -782.973034
Electronic and ZPE: -782.931341

Atom	X	Y	Z
C	-3.593806	-1.180429	-1.071015
H	-4.356784	-1.934088	-0.869197
H	-3.552876	-0.950563	-2.135046
C	-2.232547	-1.589540	-0.513527
H	-1.689659	-2.451576	-0.878008
C	-3.759177	0.090464	-0.230021
H	-4.674251	0.667736	-0.286408
C	-1.511113	-0.328676	-0.224767
C	-2.430334	0.846903	-0.476004
C	-2.320983	-1.347869	0.990094
H	-1.682807	-1.738163	1.764317
C	-3.249970	-0.307390	1.107248
H	-3.442235	0.257577	2.013127
C	-2.235581	2.076717	0.171944
N	-2.082546	3.129957	0.642365
C	-0.049943	-0.255324	-0.101549
C	0.716034	-1.377843	0.251737
C	0.595704	0.943109	-0.420234
C	2.094404	-1.298951	0.291394
H	0.232718	-2.315702	0.503345
C	1.984226	1.017377	-0.393383
H	0.018493	1.814459	-0.699597
C	2.732605	-0.098236	-0.032660
H	2.694368	-2.157396	0.568160
H	2.482176	1.945079	-0.644724
C	4.220396	-0.062160	0.023970
O	4.912112	-0.996305	0.335933
O	4.725282	1.133573	-0.313384
H	5.690023	1.085877	-0.252286

1.83 m062x_C-TS_dcm

Gibbs free energy: -782.985274
Electronic and ZPE: -782.943476

Atom	X	Y	Z
C	-3.589571	-1.164487	-1.092363
H	-4.352290	-1.921304	-0.904190
H	-3.547192	-0.920579	-2.153156
C	-2.229865	-1.580425	-0.538568
H	-1.684634	-2.442024	-0.899675
C	-3.760859	0.092977	-0.230668
H	-4.678739	0.665974	-0.284047
C	-1.511053	-0.329493	-0.211804
C	-2.431010	0.854590	-0.467804
C	-2.313107	-1.339536	0.967408
H	-1.700248	-1.765272	1.743683
C	-3.278387	-0.339809	1.107837
H	-3.510204	0.178265	2.032387
C	-2.238149	2.074750	0.191016
N	-2.083728	3.131106	0.660134
C	-0.047693	-0.256405	-0.092613
C	0.718034	-1.374433	0.272770
C	0.598981	0.937446	-0.426837
C	2.097211	-1.294476	0.309031
H	0.236827	-2.310281	0.534418
C	1.987227	1.012673	-0.403825
H	0.022566	1.805001	-0.719747
C	2.736726	-0.098801	-0.030113
H	2.693074	-2.152485	0.595342
H	2.483206	1.937333	-0.669787
C	4.224328	-0.059589	0.022264
O	4.917713	-0.992090	0.343376
O	4.726559	1.130352	-0.328154
H	5.692677	1.091631	-0.272337

1.84 m062x_C-TS_m

Gibbs free energy: -782.988818
Electronic and ZPE: -782.946992

Atom	X	Y	Z
C	-3.589340	-1.158762	-1.098304
H	-4.352089	-1.916232	-0.913886
H	-3.547006	-0.910527	-2.158119
C	-2.230001	-1.577305	-0.546180
H	-1.684834	-2.439241	-0.906344
C	-3.761735	0.094478	-0.230137
H	-4.680223	0.666604	-0.282052
C	-1.511386	-0.329865	-0.208026
C	-2.431235	0.856960	-0.464166
C	-2.311182	-1.337180	0.960704
H	-1.705602	-1.774064	1.736574
C	-3.286671	-0.349208	1.107995
H	-3.530409	0.153943	2.037725
C	-2.237650	2.074469	0.197083
N	-2.081041	3.131753	0.665221
C	-0.047238	-0.256895	-0.090686
C	0.718329	-1.373428	0.278712
C	0.600004	0.935343	-0.430052
C	2.097782	-1.293285	0.314122
H	0.237608	-2.308453	0.543531
C	1.988162	1.010794	-0.407835
H	0.023968	1.801699	-0.727460
C	2.737879	-0.099315	-0.029640
H	2.692258	-2.151152	0.603627
H	2.483759	1.934315	-0.678467
C	4.225393	-0.059300	0.021923
O	4.919187	-0.991479	0.345071
O	4.727026	1.129367	-0.331079
H	5.693483	1.092725	-0.276700

1.85 m062x_C-TS_t

Gibbs free energy: -782.974969
Electronic and ZPE: -782.933274

Atom	X	Y	Z
C	-3.593048	-1.178204	-1.074225
H	-4.355993	-1.932362	-0.874444
H	-3.551876	-0.946305	-2.137786
C	-2.232023	-1.588263	-0.517281
H	-1.688687	-2.450206	-0.881166
C	-3.759319	0.090769	-0.230214
H	-4.674863	0.667317	-0.286257
C	-1.511021	-0.328818	-0.222809
C	-2.430394	0.848103	-0.475272
C	-2.319546	-1.346311	0.986619
H	-1.685437	-1.742023	1.761483
C	-3.254382	-0.312308	1.107479
H	-3.452623	0.245757	2.016357
C	-2.236191	2.076270	0.174778
N	-2.083431	3.129934	0.645286
C	-0.049538	-0.255554	-0.100152
C	0.716434	-1.377389	0.254977
C	0.596199	0.942202	-0.421222
C	2.094917	-1.298268	0.294102
H	0.233513	-2.314998	0.508148
C	1.984676	1.016679	-0.394993
H	0.019072	1.812934	-0.702691
C	2.733264	-0.098279	-0.032284
H	2.694284	-2.156626	0.572333
H	2.482243	1.943975	-0.648554
C	4.221031	-0.061604	0.023724
O	4.913040	-0.995457	0.337275
O	4.725415	1.133172	-0.315816
H	5.690393	1.087132	-0.255456

2 Imaginary frequencies and reduced masses

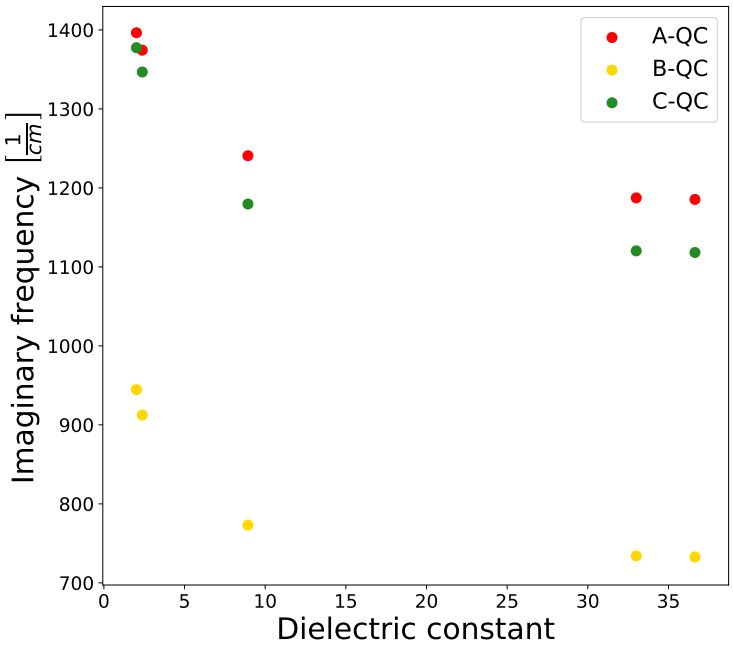

Figure 1: Imaginary frequency as a function of the dielectric constant for the NBD/QC systems.

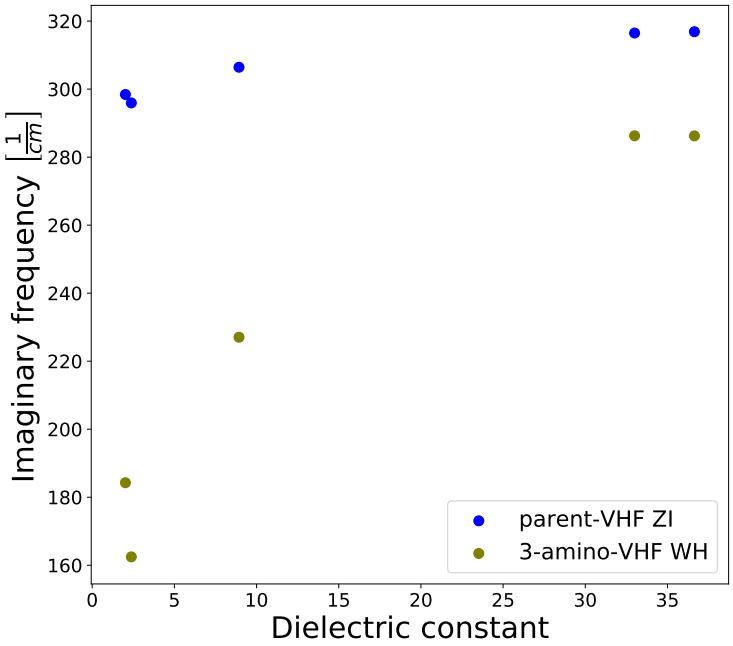

Figure 2: Imaginary frequency as a function of the dielectric constant for the DHA/VHF systems.

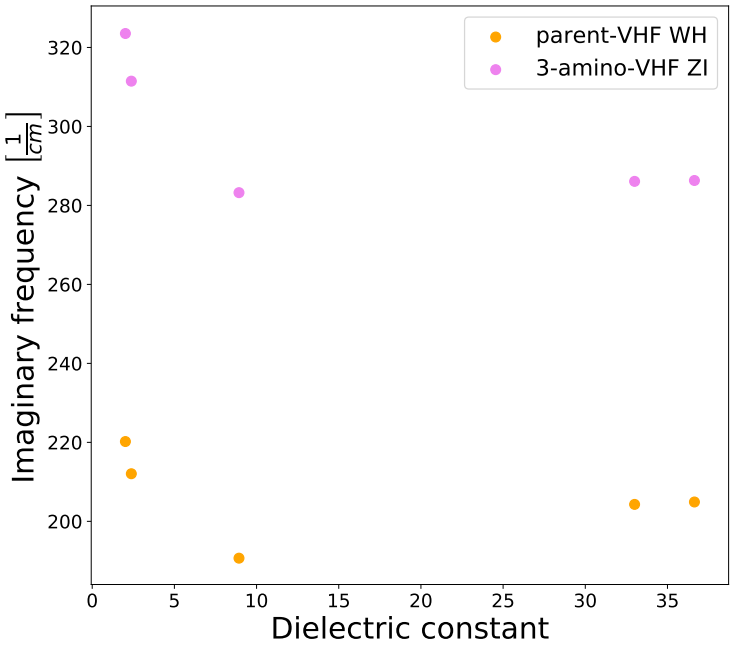

Figure 3: Imaginary frequency as a function of the dielectric constant for the DHA/VHF systems.

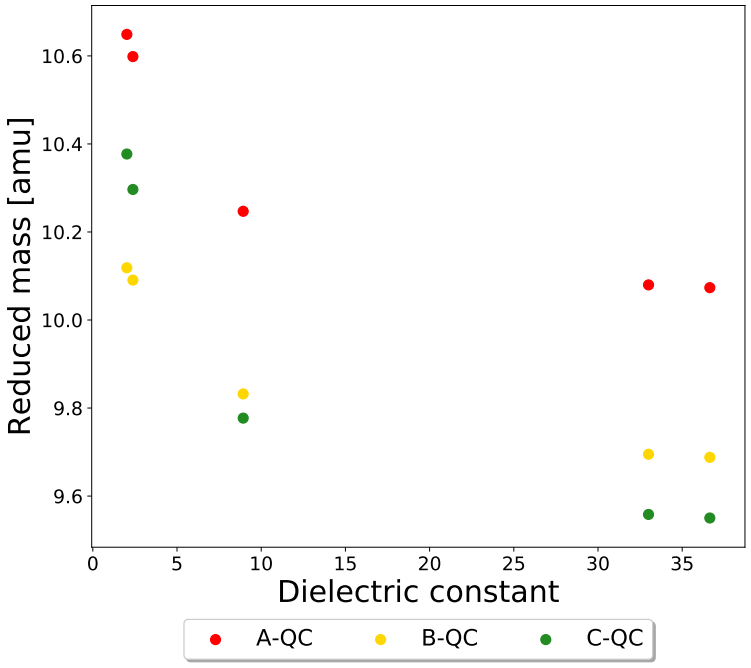

Figure 4: Reduced mass as a function of the dielectric constant for the NBD/QC systems.

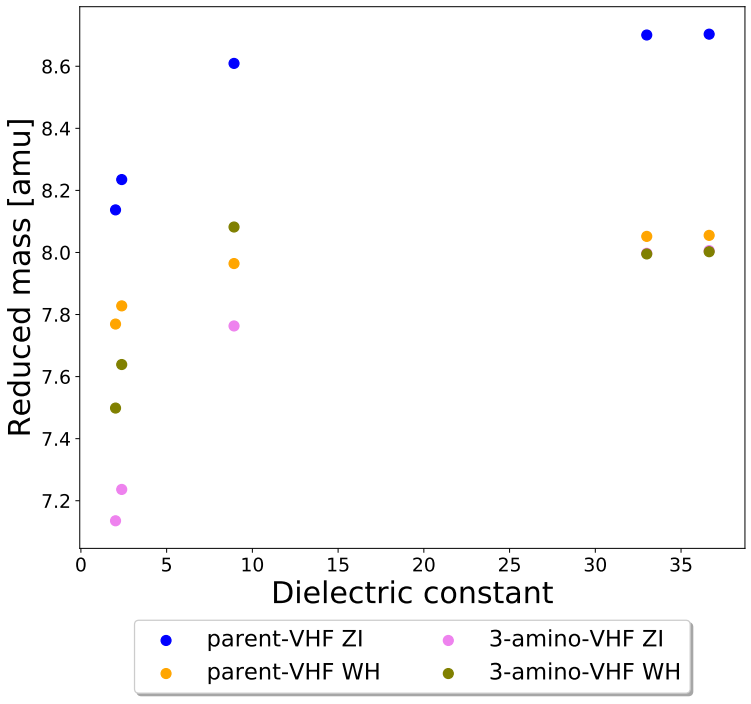

Figure 5: Reduced mass as a function of the dielectric constant for the DHA/VHF systems.

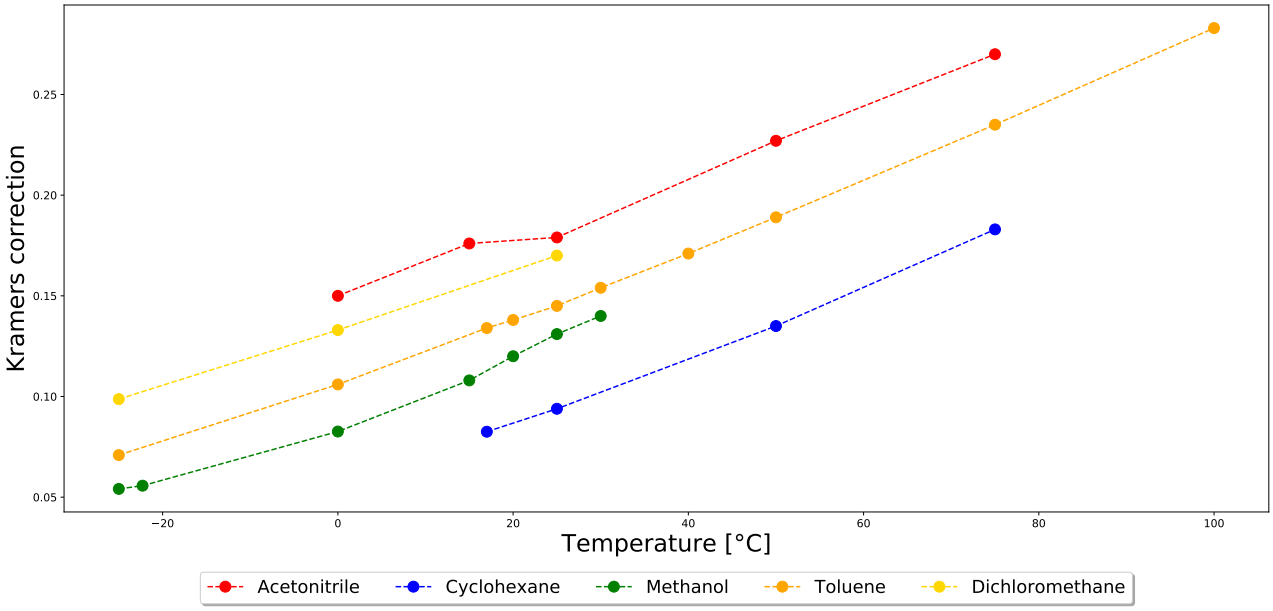

Figure 6: Kramers' correction as a function of the temperature for the A-QC system.

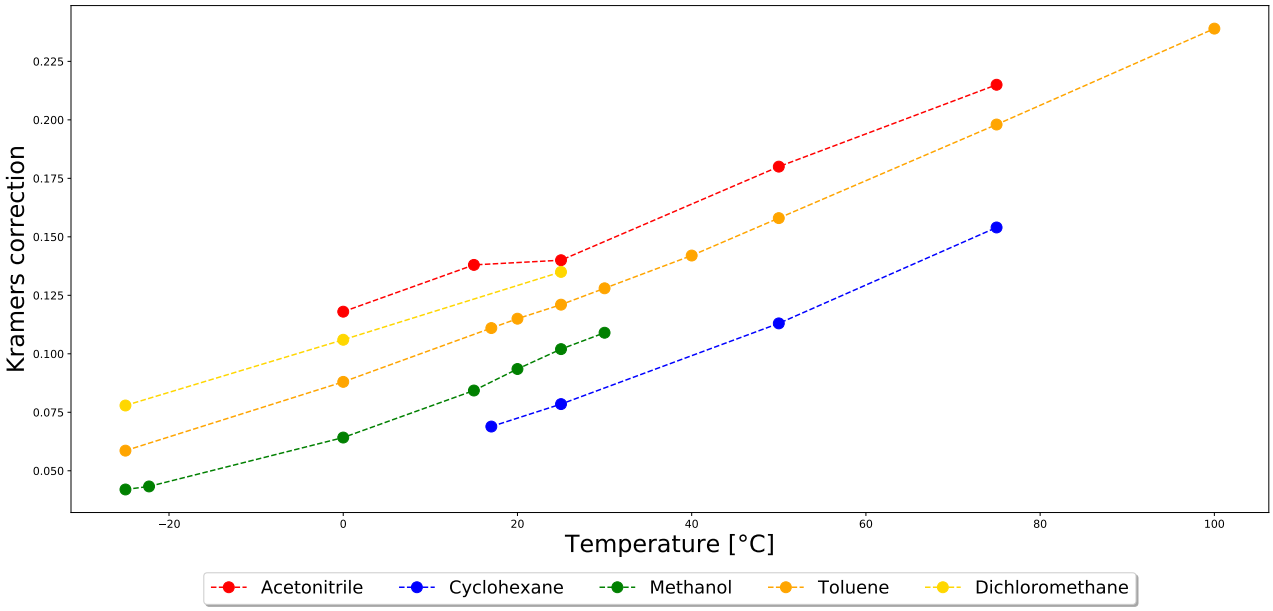

Figure 7: Kramers' correction as a function of the temperature for the C-QC system.

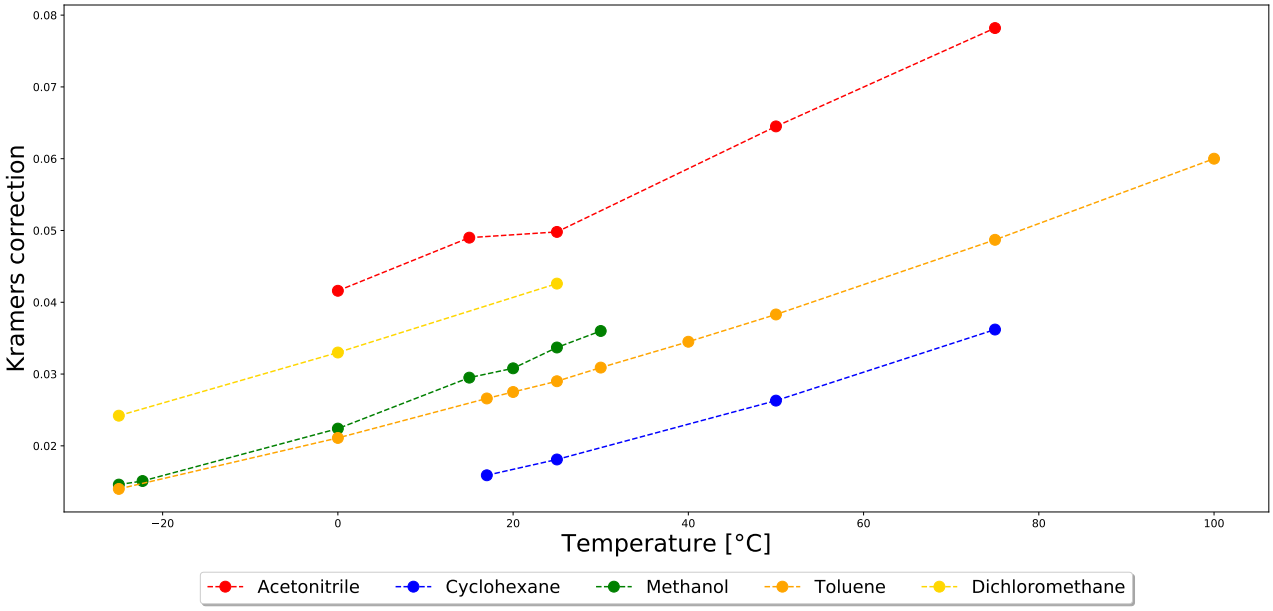

Figure 8: Kramers' correction as a function of the temperature for the parent-VHF ZI system.

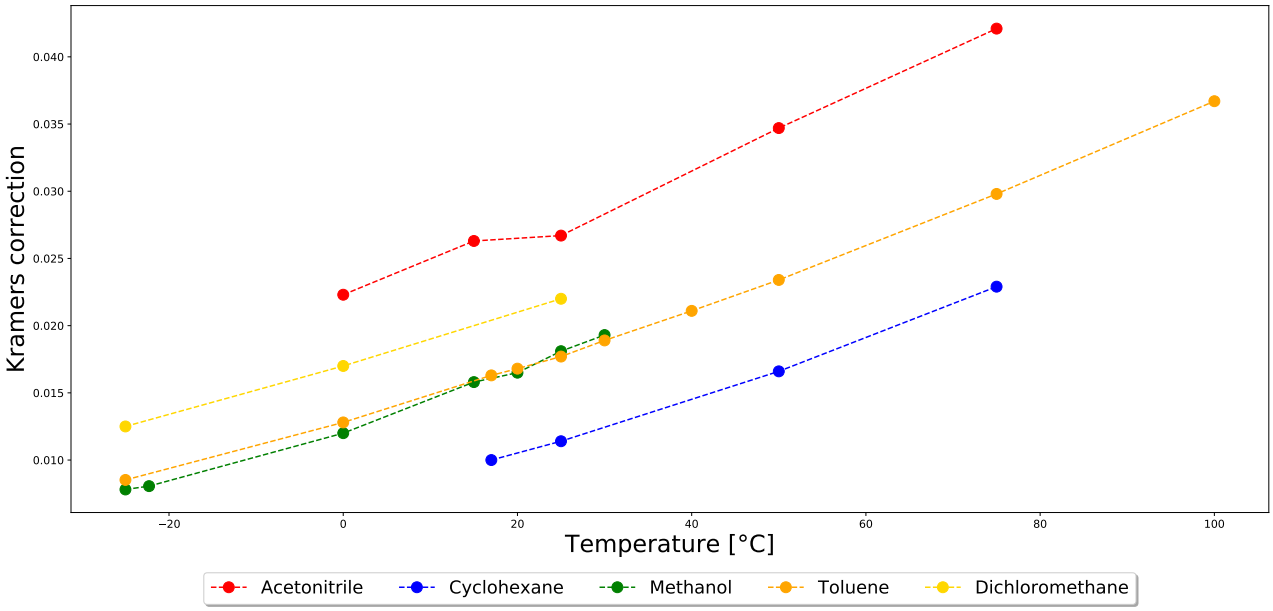

Figure 9: Kramers' correction as a function of the temperature for the parent-VHF WH system.

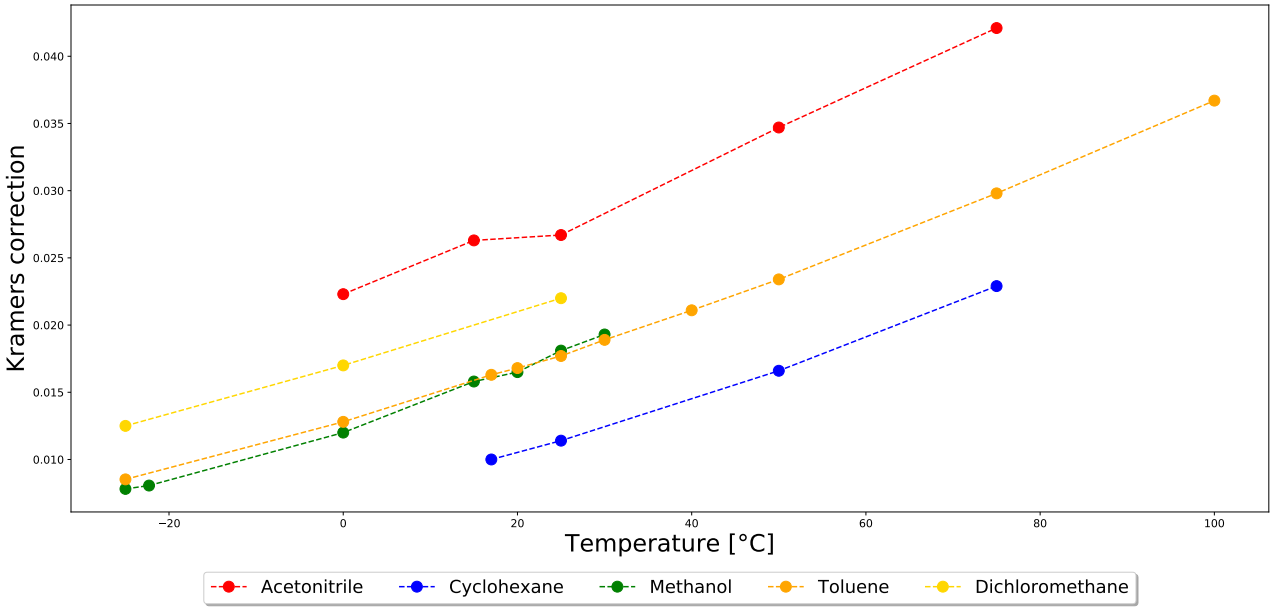

Figure 10: Kramers' correction as a function of the temperature for the 3-amino-VHF ZI system.

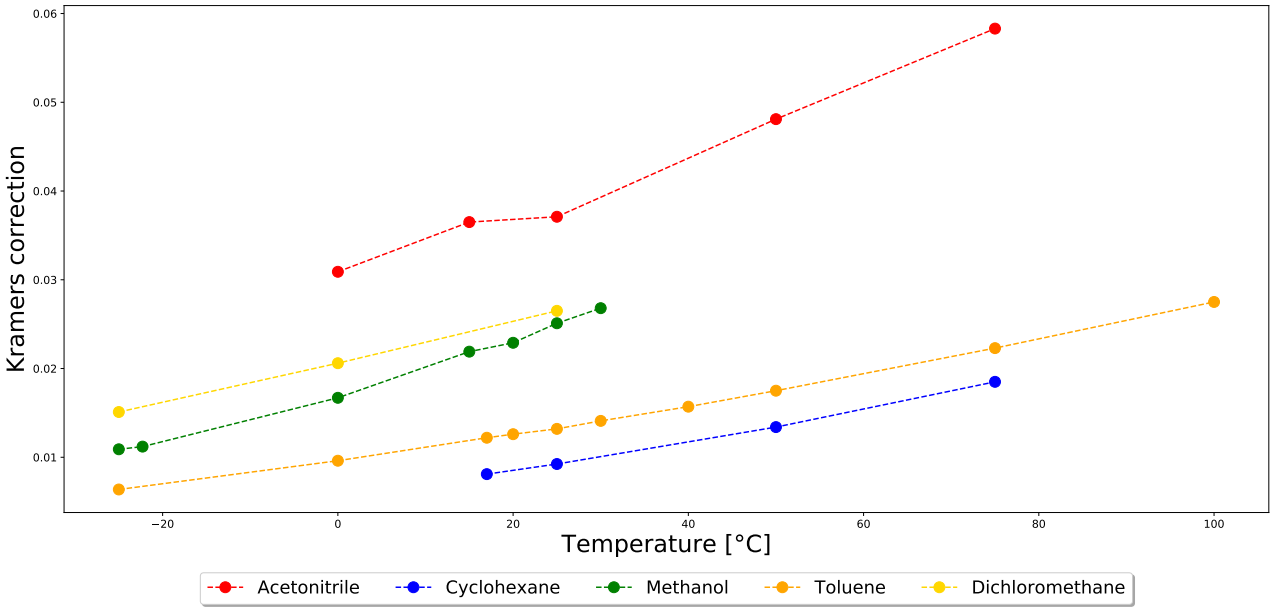

Figure 11: Kramers' correction as a function of the temperature for the 3-amino-VHF WH system.