Supplementary Information

Enantioselective interactions of aminonitrile dimers

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Atomic coordinates of aminonitriles optimized at the B3LYP-D3/6-311++G** are provided in the XYZ file format and in Å units.

Table S1. Calculated interaction energies (E_{inter}/kcal mol^{-1}) of Iva_AN dimers with the SMD solvation model[a]

	method	in water			
		Ala_AN	Aba_AN	Val_AN	Iva_AN
E_{inter}(LL)	B3LYP-D3//6-311++G**	-4.05	-5.25	-3.33	-4.06
E_{inter}(LD)	B3LYP-D3//6-311++G**	-4.08	-4.96	-3.40	-3.81
ΔE_{chir}[b]	B3LYP-D3//6-311++G**	0.03	-0.29	0.07	-0.25

[a] Geometry optimizations are performed at the B3LYP-D3//6-311++G** with the SMD solvation model [S1]. Zero-point vibrational energy (ZPE) and basis set superposition error (BSSE) corrections at the B3LYP-D3//6-311++G** method are included for all results. Solvation effects were accounted through the SMD solvation model.

[b] $\Delta E_{chir}=E_{inter}(LL) - E_{inter}(LD)$.

[S1] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, J. Phys. Chem. B, 2009, 113, 6378-96.

Table S2. Interaction energies (E_{inter}/kcal mol^{-1}) of Iva_AN dimers in the low-lying states calculated in the gas phase[a]

	B3LYP-D3//6-311++G**	DLPNO-CCSD(T)/aug-cc-pVTZ
Iva_AN_0 (LL)	**-9.24**	-8.32
Iva_AN_1 (LL)	-9.15	**-8.35**
Iva_AN_2 (LL)	-9.15	**-8.35**
Iva_AN_3 (LL)	-8.97	-8.34
Iva_AN_4 (LL)	-8.96	-8.33
Iva_AN_0 (LD)	**-9.09**	-8.34
Iva_AN_1 (LD)	-9.08	**-8.39**
Iva_AN_2(LD)	-8.90	-8.14

[a] Values in the bold font indicate the most stable conformation within each theoretical level and dimer. Zero-point vibrational energy (ZPE) at the B3LYP-D3//6-311++G** method and basis set superposition error (BSSE) corrections are included for all results.

Table S3. Interaction energies (E_{inter}/kcal mol^{-1}) of aminonitrile dimers in the most stable conformations.[a]

	method	in gas				in water			
		Ala_AN	Aba_AN	Val_AN	Iva_AN	Ala_AN	Aba_AN	Val_AN	Iva_AN
E_{inter}(LL)	B3LYP-D3//6-311++G**	-8.87	-9.27	-9.66	-9.24	-3.77	-4.55	-4.27	-4.39
	DLPNO-CCSD(T)/cc-pVTZ	-8.85	-8.99	-9.36	-7.29	-3.30	-3.72	-3.85	-3.93
	DLPNO-CCSD(T)/aug-cc-pVTZ	-8.25	-8.39	-8.88	-8.35	-1.98	-2.98	-2.42	-2.68
E_{inter}(LD)	B3LYP-D3//6-311++G**	-8.70	-8.72	-9.28	-9.09	-3.86	-4.16	-4.47	-4.23
	DLPNO-CCSD(T)/cc-pVTZ	-8.71	-8.77	-8.99	-7.33	-3.42	-3.87	-3.83	-3.85
	DLPNO-CCSD(T)/aug-cc-pVTZ	-8.14	-8.15	-8.70	-8.39	-2.09	-2.47	-2.62	-2.60
ΔE_{chir}[b]	B3LYP-D3//6-311++G**	–0.17	–0.55	–0.38	–0.15	0.09	-0.39	0.20	-0.17
	DLPNO-CCSD(T)/cc-pVTZ	-0.14	-0.22	-0.37	0.05	0.12	0.16	-0.02	-0.09
	DLPNO-CCSD(T)/aug-cc-pVTZ	-0.11	-0.24	-0.18	0.04	0.10	-0.51	0.20	-0.08

[a] Geometry optimizations are performed at the B3LYP-D3//6-311++G**. Zero-point vibrational energy (ZPE) at the B3LYP-D3//6-311++G** method and basis set superposition error (BSSE) corrections are included for all results. Detailed energy contributions are shown in Table S3. Solvation effects were accounted through the PCM.

[b] $\Delta E_{chir}=E_{inter}(LL) - E_{inter}(LD)$.

Table S4. Energy contributions (in Hartree unit[a]) at the different theoretical methods.[b]

			in gas				in water			
		method	Ala_AN	Aba_AN	Val_AN	Iva_AN	Ala_AN	Aba_AN	Val_AN	Iva_AN
Energy	Dimer (LL)	B3LYP-D3//6-311++G**	-454.814577	-533.41362	-612.014675	-612.019691	-454.827935	-533.426999	-612.027377	-612.032188
ZPE		B3LYP-D3//6-311++G**	0.184828	0.241906	0.297817	0.297337	0.184658	0.241228	0.29746	0.296932
BSSE		B3LYP-D3//6-311++G**	0.000654023261	0.000792133739	0.000840316664	0.00073304731	0.00082803996	0.000781968174	0.001011235255	0.000928991243
Energy		DLPNO-CCSD(T)/ cc-pVTZ	-454.082723204	-532.563725878	-611.047734106	-611.053174692	-454.10030208	-532.581018432	-611.065246667	-611.070562495
BSSE		DLPNO-CCSD(T)/ cc-pVTZ	0.00065402	0.00079213	0.00084032	0.00073305	0.00082804	0.00078197	0.00101124	0.00092899
Energy		DLPNO-CCSD(T)/ aug-cc-pVTZ	-454.119695577	-532.60739729	-611.097638857	-611.103555209	-454.137028523	-532.625471595	-611.114805452	-611.120974735
BSSE		DLPNO-CCSD(T)/ aug-cc-pVTZ	0.0017874	0.00239254	0.00253092	0.00253621	0.00160772	0.00235572	0.00217765	0.00258268
Energy	Dimer (LD)	B3LYP-D3//6-311++G**	-454.814309	-533.412717	-612.013956	-612.019389	-454.828159	-454.828159	-612.027699	-612.031895
ZPE		B3LYP-D3//6-311++G**	0.184792	0.241684	0.297701	0.297127	0.184682	0.241512	0.297515	0.296718
BSSE		B3LYP-D3//6-311++G**	0.000651535348	0.000761496026	0.000725734012	0.000692538803	0.000914172737	0.001015237144	0.001017102879	0.00090245038
Energy		DLPNO-CCSD(T)/ cc-pVTZ	-454.08246808	-532.563150386	-611.047032153	-611.0531911	-454.100523586	-532.581549684	-611.065270755	-611.070212929
BSSE		DLPNO-CCSD(T)/ cc-pVTZ	0.00065154	0.0007615	0.00072573	0.00069254	0.00091417	0.00101524	0.0010171	0.00090245
Energy		DLPNO-CCSD(T)/ aug-cc-pVTZ	-454.119405968	-532.606285436	-611.096918982	-611.103192981	-454.137358413	-532.624632475	-611.115465224	-611.120187605
BSSE		DLPNO-CCSD(T)/ aug-cc-pVTZ	0.00170554	0.00188284	0.00221633	0.00227336	0.00175132	0.00204947	0.00246122	0.00214182
Energy	Mono mer	B3LYP-D3//6-311++G**	-227.399893	-266.699028	-305.999217	-306.002113	-227.410547	-266.709483	-306.00978	-306.012128
ZPE		B3LYP-D3//6-311++G**	0.091534	0.12001	0.147921	0.147749	0.091555	0.119898	0.147887	0.147555
Energy		DLPNO-CCSD(T)/ cc-pVTZ	-227.033430905	-266.273758147	-305.515424707	-305.518531279	-227.046749308	-266.286831563	-305.528714128	-305.531236446
Energy		DLPNO-CCSD(T)/ aug-cc-pVTZ	-227.051501146	-266.29487238	-305.539491399	-305.542959831	-227.065355938	-266.308466866	-305.553543683	-305.556145949

[a] 1 Hartree = 627.5095 kcal mol^{-1}

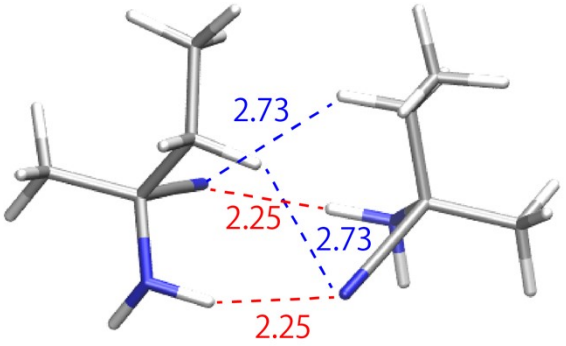
[b] ZPE: zero-point vibrational energy correction, BSSE: basis set superposition error calculated with the counterpoise method

Table S5. Energy contributions (in Hartree unit[a]) of Iva_AN in the gas phase at the different theoretical methods.[b]

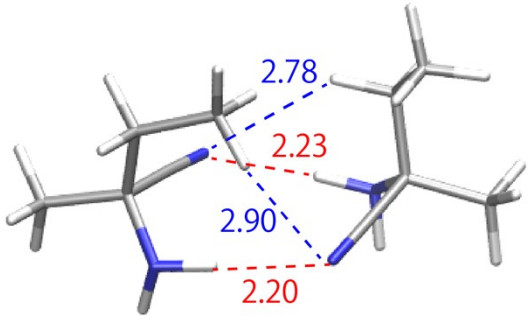
		Dimer (LL)				Dimer (LD)		
	method	Iva_AN_0	Iva_AN_1	Iva_AN_2	Iva_AN_3	Iva_AN_0	Iva_AN_1	Iva_AN_2
Energy	B3LYP-D3//6-311++G**	-612.317029091	-612.3167644	-612.3167644	-612.3162841	-612.3165252	-612.316516	-612.3162271
ZPE	B3LYP-D3//6-311++G**	0.297338	0.29722	0.29722	0.297034	0.297144	0.297127	0.297144
BSSE	B3LYP-D3//6-311++G**	0.00073304731	0.000728554328	0.000728558855	0.000722087183	0.00066424811	0.000692538803	0.000668095303
Energy (wZPE&BSSE)	B3LYP-D3//6-311++G**	-612.018958	-612.0188159	-612.0188159	-612.018528	-612.0187169	-612.0186965	-612.018415
Energy	DLPNO-CCSD(T)/ aug-cc-pVTZ	-611.103555209	-611.10342558	-611.103425783	-611.102899952	-454.10030208	-611.065246667	-611.070562495
BSSE	DLPNO-CCSD(T)/ aug-cc-pVTZ	0.00253621	0.002473269	0.002473221	0.002153446	0.002212824	0.002273357	0.002207407
Energy (wZPE&BSSE)	DLPNO-CCSD(T)/ aug-cc-pVTZ	-610.803681	-610.8037324	-610.8037325	-610.8037125	-610.8037253	-610.8037926	-610.8037238
		monomer						
Energy	B3LYP-D3//6-311++G**	-306.002113						
ZPE	B3LYP-D3//6-311++G**	0.147749						
Energy	DLPNO-CCSD(T)/ aug-cc-pVTZ	-305.5429598						

[a] 1 Hartree = 627.5095 kcal mol^{-1}

[b] ZPE: zero-point vibrational energy correction, BSSE: basis set superposition error calculated with the counterpoise method. Values in the bold font indicate the most stable conformation within each theoretical level and dimer.



Iva_AN_0(LL)



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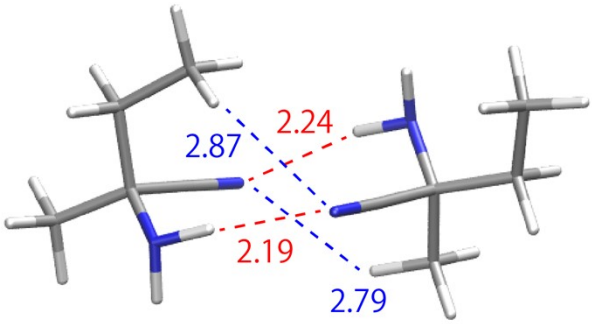
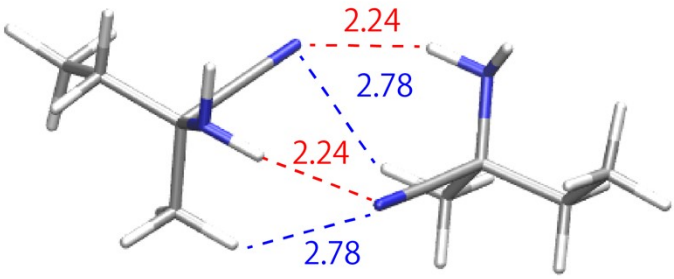


Iva_AN_2(LL)



Iva_AN_3(LL)

Figure S1. Molecular structures of the low-lying states of Iva_AN (LL) in the gas phase. The most stables of Iva_AN (LL) in the gas phase are Iva_AN_0(LL) and Iva_AN_2(LL) at the theoretical levels of B3LYP-D3//6-311++G** and DLPNO-CCSD(T)/aug-cc-pVTZ, respectively.

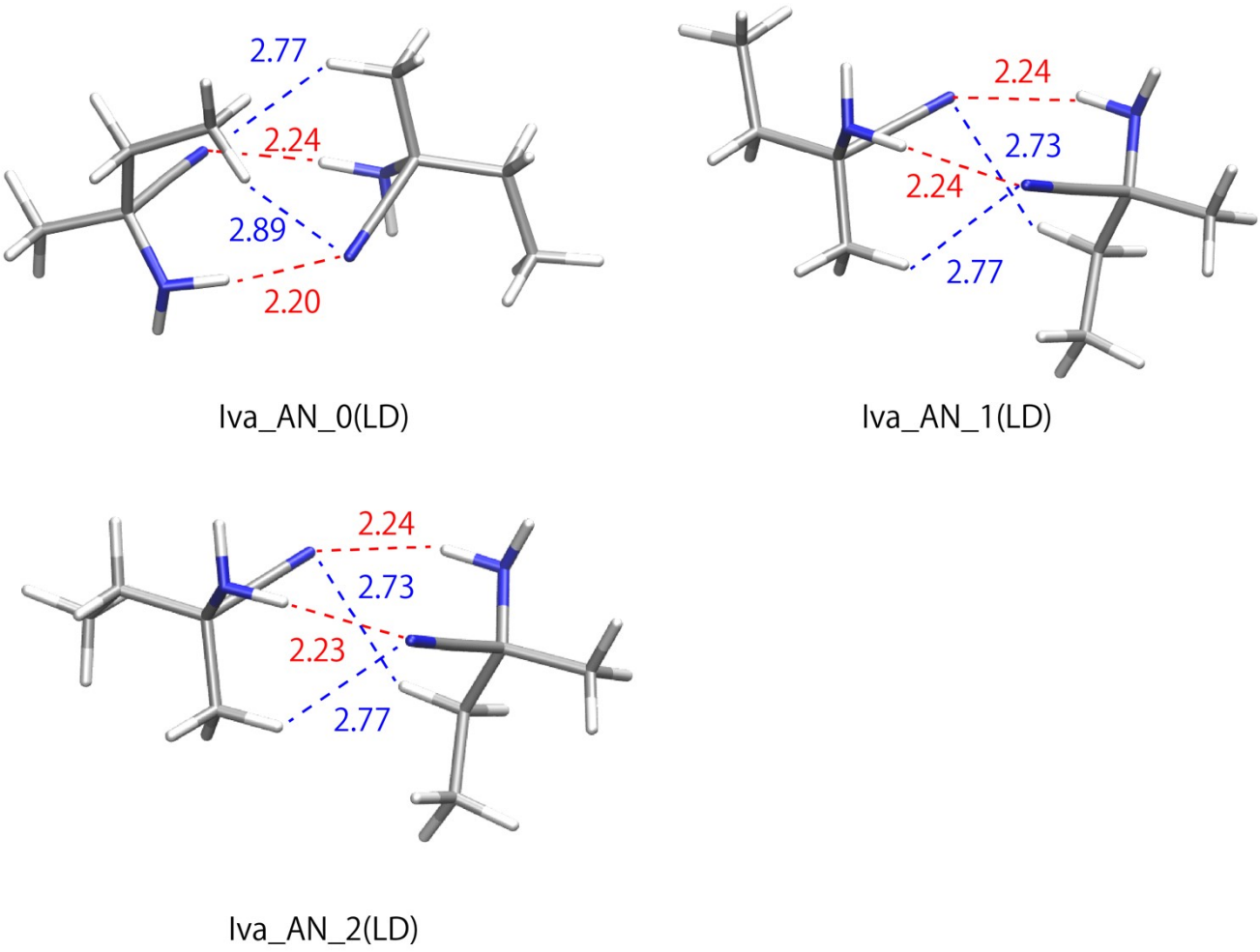


Figure S2. Molecular structures of the low-lying states of Iva_AN (LD) in the gas phase. The most stables of Iva_AN (LD) in the gas phase are Iva_AN_0(LD) and Iva_AN_1(LD) at the theoretical levels of B3LYP-D3//6-311++G** and DLPNO-CCSD(T)/aug-cc-pVTZ, respectively.

All the B3LYP-D3/6-311++G** optimized structures of aminonitriles in the lowest conformation are given in the xyz file format. In the second comment lines, total energies with the ZPE correction are given in Hartree units. Atomic coordinates after the comment lines are given in Å units.

22
Energy(ZPE): -454.814577 in gas Name: L-L Ala_AN_0
C -2.463734 0.373926 0.005525
N -2.615503 -0.676901 -0.995842
C -1.250290 1.207537 -0.196608
N -0.293105 1.825391 -0.381392
C -2.451831 -0.231593 1.416591
H -3.317697 1.054067 -0.081386
H -2.675751 -0.293519 -1.933011
H -1.822556 -1.314333 -0.962747
H -2.363463 0.545423 2.178809
H -1.614804 -0.924808 1.519508
H -3.381724 -0.781658 1.566571
C 2.463734 -0.373927 0.005514
N 2.615506 0.676924 -0.995825
C 1.250287 -1.207530 -0.196636
N 0.293099 -1.825378 -0.381427
C 2.451834 0.231555 1.416596
H 3.317694 -1.054070 -0.081416
H 2.675758 0.293567 -1.933004
H 1.822564 1.314359 -0.962715
H 1.614809 0.924772 1.519529
H 3.381728 0.781613 1.566591
H 2.363461 -0.545479 2.178794
22
Energy(ZPE): -454.814309 in gas Name: D-L Ala_AN_1
C -2.493338 -0.313109 -0.277299
N -2.410682 0.934905 -1.029568
C -1.265549 -1.143965 -0.377490
N -0.292259 -1.757479 -0.470026
C -2.807699 -0.024674 1.197903
H -3.303490 -0.914990 -0.702538
H -2.241973 0.767254 -2.015589
H -1.654684 1.513107 -0.669642
H -3.746890 0.527529 1.251367
H -2.898528 -0.950263 1.770138
H -2.015972 0.586301 1.635904
C 2.493343 0.313109 0.277278
N 2.410727 -0.934917 1.029529
C 1.265550 1.143956 0.377531
N 0.292261 1.757464 0.470114
C 2.807648 0.024703 -1.197942
H 3.303506 0.914992 0.702495
H 2.242054 -0.767285 2.015559
H 1.654723 -1.513121 0.669620
H 3.746841 -0.527490 -1.251453
H 2.015909 -0.586272 -1.635922
H 2.898445 0.950302 -1.770165
22
Energy(ZPE): -454.813873 in gas Name: L-L Ala_AN_2
C -2.381943 -0.074873 -0.286067
N -2.258065 -1.328838 0.448141
C -1.273317 0.877074 -0.018038
N -0.394737 1.588770 0.213802
C -3.731732 0.596988 0.000087
H -2.322014 -0.312653 -1.352926
H -1.395166 -1.807588 0.201572
H -2.259264 -1.165887 1.450249
H -3.819767 0.842494 1.061756
H -4.530138 -0.097678 -0.263793
H -3.846523 1.517908 -0.575220
C 2.679117 -0.152419 -0.135886
N 2.567163 1.087939 -0.897705
C 1.568958 -1.105466 -0.393849
N 0.686218 -1.817083 -0.609351
C 2.763936 0.153218 1.366605
H 3.596930 -0.662219 -0.447564
H 2.547295 0.912373 -1.896579
H 1.713476 1.580039 -0.643735
H 3.624863 0.799778 1.541702
H 2.874525 -0.763197 1.950015
H 1.861617 0.673984 1.693203
22
Energy(ZPE): -454.813448 in gas Name: D-L Ala_AN_3
C 2.516857 0.141274 0.327215
N 2.354360 1.424282 -0.346963
C 1.511018 -0.872317 -0.082854
N 0.712872 -1.632981 -0.423951
C 3.933578 -0.411259 0.119914
H 2.354382 0.309895 1.396603
H 1.436837 1.819013 -0.154591
H 2.453430 1.321723 -1.352239
H 4.074022 -1.353370 0.653676
H 4.124364 -0.586966 -0.942101
H 4.651805 0.323619 0.485692
C -2.516306 -0.141337 -0.327430
N -2.354966 -1.424289 0.347117
C -1.510900 0.872185 0.083892
N -0.713248 1.632914 0.426010
C -3.933221 0.411474 -0.122152
H -2.352381 -0.310123 -1.396569
H -1.437400 -1.819385 0.155722
H -2.455067 -1.321568 1.352271
H -4.125446 0.587320 0.939580
H -4.072758 1.353557 -0.656203
H -4.651066 -0.323319 -0.488848
28
Energy(ZPE): -533.413620 in gas Name: L-L Aba_AN_0
C 2.400002 -0.382365 0.143675
N 2.601329 -1.351265 -0.929843
C 1.324624 -0.775742 1.089172
N 0.472669 -1.105001 1.794772
C 2.115620 1.014377 -0.443748
C 1.953313 2.113192 0.607166
H 3.320894 -0.327551 0.735453
H 2.952737 1.236390 -1.110152
H 1.221999 0.944961 -1.069703
H 1.100425 1.922773 1.264182
H 1.791499 3.080345 0.125800
H 2.845514 2.198550 1.235093
H 1.749300 -1.454006 -1.477294
H 2.852876 -2.263472 -0.564457
C -2.401059 -0.379410 -0.143609
N -2.605835 -1.346907 0.930334
C -1.326003 -0.776044 -1.088226
N -0.474482 -1.107335 -1.793404
C -2.113520 1.017157 0.442939
C -1.947523 2.114634 -0.608796

H -3.321317 -0.322542 -0.736173
H -1.220617 0.945997 1.069668
H -2.950678 1.241954 1.108368
H -1.094785 1.921359 -1.265179
H -1.783338 3.081730 -0.128104
H -2.839078 2.201973 -1.237358
H -1.755277 -1.450692 1.479765
H -2.858649 -2.259009 0.565633
28
Energy(ZPE): -533.412968 in gas Name: L-L Aba_AN_1
C -2.209100 -0.648440 -0.381140
N -2.460914 -1.119468 0.976944
C -1.005481 -1.257834 -0.999610
N -0.052236 -1.732900 -1.444370
C -2.084697 0.890824 -0.418636
C -3.383922 1.586930 -0.012143
H -3.059248 -0.941851 -1.007661
H -1.270160 1.179587 0.252015
H -1.789932 1.192913 -1.428570
H -4.195578 1.339347 -0.703590
H -3.254926 2.672070 -0.022531
H -3.689830 1.282941 0.989559
H -2.638049 -2.117505 0.998555
H -1.661497 -0.923143 1.575912
C 2.534861 -0.093641 0.349464
N 2.889575 -1.376491 -0.250241
C 1.366576 -0.179623 1.262215
N 0.445775 -0.278889 1.950913
C 2.279955 0.959150 -0.747581
C 1.976959 2.357935 -0.208733
H 3.377372 0.244208 0.963703
H 1.461210 0.603422 -1.379270
H 3.179022 0.969656 -1.368691
H 2.791912 2.726568 0.421912
H 1.848272 3.064574 -1.031812
H 1.060797 2.372366 0.387970
H 2.112373 -1.737051 -0.800034
H 3.121963 -2.065677 0.456794
28
Energy(ZPE): -533.412717 in gas Name: L-D Aba_AN_2
C 2.349009 0.779553 -0.514780
N 1.852251 2.077954 -0.067395
C 1.303351 -0.053721 -1.160832
N 0.461774 -0.679282 -1.643202
C 2.986391 0.017249 0.663545
C 3.624450 -1.314999 0.267464
H 3.118721 0.949133 -1.276427
H 3.732864 0.692482 1.089380
H 2.218004 -0.133504 1.427347
H 4.091155 -1.787305 1.134889
H 2.885411 -2.013648 -0.134227
H 4.400009 -1.174250 -0.491978
H 1.465847 2.614496 -0.836630
H 1.122886 1.951880 0.630910
C -2.348292 -0.779718 0.514627
N -1.850773 -2.077551 0.066571
C -1.302788 0.054290 1.160061
N -0.461360 0.680301 1.642106
C -2.987284 -0.017560 -0.662952
C -3.626368 1.313858 -0.265738
H -3.117286 -0.950108 1.276811
H -2.219604 0.134248 -1.427249
H -3.733428 -0.693350 -1.088481
H -4.401301 1.171851 0.494117
H -4.094211 1.786250 -1.132515
H -2.887749 2.012968 0.135899
H -1.121934 -1.950792 -0.632154
H -1.463443 -2.614019 0.835381
28
Energy(ZPE): -533.412600 in gas Name: D-L Aba_AN_3
C 2.124004 0.325623 0.381440
N 2.149443 1.749967 0.695228
C 1.225329 -0.003330 -0.753778
N 0.520914 -0.216903 -1.642905
C 3.544024 -0.208029 0.113974
C 3.607943 -1.721068 -0.102137
H 1.713379 -0.195486 1.253002
H 4.144590 0.086459 0.978123
H 3.956658 0.317217 -0.754638
H 3.211912 -2.259365 0.764568
H 3.033762 -2.028420 -0.980294
H 4.640903 -2.044057 -0.250067
H 2.447819 2.295525 -0.107082
H 1.226660 2.068904 0.979516
C -2.715403 0.316135 -0.276131
N -2.560103 0.637085 -1.692175
C -1.738785 1.023942 0.590710
N -0.956354 1.584660 1.227550
C -2.621956 -1.206785 -0.058698
C -2.865667 -1.642894 1.386794
H -3.707941 0.651631 0.045774
H -1.639183 -1.541594 -0.403123
H -3.362694 -1.651902 -0.727674
H -2.823911 -2.731366 1.469592
H -2.116095 -1.228096 2.066370
H -3.850782 -1.320344 1.738191
H -2.675132 1.630327 -1.863000
H -1.634182 0.365337 -2.016197
34
Energy(ZPE): -612.014675 in gas Name: L-L Val_AN_0
C 2.428248 -0.718003 0.174528
N 2.480441 -1.463481 -1.080692
C 1.319237 -1.169490 1.050751
N 0.434587 -1.543819 1.690393
C 2.329716 0.810765 -0.079429
C 2.229339 1.593380 1.235444
C 3.527808 1.284637 -0.909772
H 3.356697 -0.907733 0.726802
H 1.414633 0.971748 -0.661022
H 1.355268 1.307140 1.824300
H 2.158292 2.664557 1.031118
H 3.120609 1.432435 1.851737
H 3.606880 0.733934 -1.846537
H 4.461416 1.145079 -0.353249
H 3.429784 2.350059 -1.134560
H 1.608379 -1.350685 -1.593925
H 2.626772 -2.453289 -0.916472
C -2.651749 -0.644786 -0.314904
N -2.595229 -1.639927 0.752715
C -1.462356 -0.684183 -1.203510
N -0.511409 -0.736122 -1.855295
C -2.873474 0.787254 0.240444
C -3.168322 1.780682 -0.889774
C -1.707430 1.266358 1.111661

H -3.512602 -0.884359 -0.948042
H -3.762922 0.689873 0.871308
H -3.405932 2.764424 -0.477417
H -2.303968 1.898529 -1.550793
H -4.018460 1.459018 -1.498974
H -0.794473 1.371275 0.518222
H -1.498582 0.580430 1.934301
H -1.938297 2.244498 1.541411
H -1.715969 -1.594707 1.263353
H -2.672356 -2.578481 0.375961
34
Energy(ZPE): -612.014057 in gas Name: L-L Val_AN_1
C 2.488698 -0.535328 0.543871
N 2.643587 -1.722501 -0.292966
C 1.282901 -0.608941 1.405520
N 0.326055 -0.705015 2.043596
C 2.464121 0.760688 -0.311119
C 3.752439 0.873158 -1.133930
C 2.260186 2.005260 0.561362
H 3.350176 -0.475556 1.220103
H 1.616243 0.664566 -0.999340
H 3.711173 1.757600 -1.775253
H 4.621974 0.978106 -0.475349
H 3.905284 -0.006546 -1.758266
H 3.082247 2.116155 1.276921
H 2.241610 2.902619 -0.061983
H 1.325036 1.970617 1.124578
H 2.743062 -2.560297 0.269420
H 1.831149 -1.837517 -0.895718
C -2.521254 -0.762735 -0.454793
N -2.591684 -1.220634 0.929678
C -1.248716 -1.133853 -1.122208
N -0.237664 -1.422809 -1.597923
C -2.763941 0.768050 -0.585834
C -1.706076 1.588720 0.161274
C -4.181179 1.114817 -0.117131
H -3.316361 -1.266470 -1.014732
H -2.684195 0.998304 -1.655385
H -1.881583 2.656224 0.006342
H -0.696844 1.360723 -0.188821
H -1.741923 1.396938 1.236479
H -4.370040 2.183905 -0.245253
H -4.308633 0.862363 0.937002
H -4.936998 0.568810 -0.690037
H -2.677256 -2.229683 0.974893
H -1.759251 -0.963167 1.455632
34
Energy(ZPE): -612.013956 in gas Name: L-D Val_AN_2
C -1.904159 -0.304148 -0.541041
N -2.128228 -1.655732 -1.045260
C -1.218715 -0.283227 0.774632
N -0.681955 -0.297193 1.796260
C -3.208899 0.531204 -0.495881
C -4.253461 -0.071722 0.450150
C -2.916853 1.995853 -0.148106
H -1.217395 0.184894 -1.239045
H -3.595017 0.478233 -1.519021
H -4.525262 -1.089236 0.158921
H -5.168030 0.526523 0.434488
H -3.886812 -0.091093 1.481646
H -2.533770 2.093964 0.872221
H -3.829431 2.592889 -0.218872
H -2.178772 2.430344 -0.829191
H -1.238297 -2.086980 -1.279270
H -2.595546 -2.237713 -0.358964
C 2.822028 -0.647244 0.369653
N 2.461475 -0.873320 1.766830
C 1.830240 -1.208301 -0.583269
N 1.026665 -1.642381 -1.288815
C 3.078267 0.854534 0.073689
C 3.679756 1.048813 -1.323418
C 1.825314 1.716048 0.265645
H 3.760075 -1.179298 0.178988
H 3.818886 1.147858 0.824772
H 2.971054 0.758607 -2.105339
H 3.936972 2.098884 -1.482808
H 4.590661 0.457393 -1.456764
H 1.403728 1.613992 1.266662
H 2.069557 2.770113 0.110878
H 1.049770 1.445479 -0.458046
H 1.512452 -0.565350 1.966149
H 2.508359 -1.859982 1.997157
34
Energy(ZPE): -612.013905 in gas Name: D-L Val_AN_3
C -2.426595 0.528535 -0.943661
N -1.801103 1.845791 -0.860953
C -1.438777 -0.575269 -1.049705
N -0.638476 -1.404406 -1.110570
C -3.400320 0.277970 0.238490
C -2.683906 0.248002 1.593235
C -4.225831 -0.994895 0.015101
H -3.017824 0.497717 -1.865057
H -4.069025 1.144691 0.216801
H -3.413786 0.130884 2.398506
H -2.120080 1.162652 1.782717
H -1.986908 -0.594108 1.648664
H -4.761154 -0.967230 -0.938920
H -4.966274 -1.110525 0.810468
H -3.591146 -1.886503 0.021250
H -1.324877 2.075472 -1.726537
H -1.108967 1.885083 -0.115851
C 2.426713 -0.528468 0.943771
N 1.801191 -1.845700 0.861091
C 1.438917 0.575355 1.049822
N 0.638685 1.404562 1.110631
C 3.400346 -0.277965 -0.238463
C 4.225420 0.995259 -0.015508
C 2.683868 -0.248694 -1.593188
H 3.017983 -0.497619 1.865138
H 4.069326 -1.144466 -0.216506
H 4.760819 0.968067 0.938484
H 4.965767 1.110917 -0.810960
H 3.590420 1.886643 -0.021878
H 3.413680 -0.131737 -2.398544
H 2.120236 -1.163552 -1.782264
H 1.986678 0.593236 -1.648920
H 1.324969 -2.075359 1.726681
H 1.109068 -1.884980 0.115976
34
Energy(ZPE): -612.019691 in gas Name: L-L Iva_AN_0
C -2.453320 -0.332754 0.139457
N -2.442792 -1.286783 1.251178
C -1.481671 -0.726253 -0.919461
N -0.713607 -1.051894 -1.717371

C -3.861260 -0.309619 -0.481223
C -2.043281 1.053455 0.699580
C -1.937905 2.181354 -0.328327
H -3.913213 0.365349 -1.336380
H -4.570708 0.014994 0.282257
H -4.147629 -1.307997 -0.821241
H -1.087443 0.930965 1.215401
H -2.784566 1.296085 1.465965
H -1.599544 3.098874 0.158727
H -2.898917 2.396315 -0.801678
H -1.220201 1.942657 -1.117971
H -1.514880 -1.351619 1.665148
H -2.712319 -2.214530 0.939549
C 2.453407 -0.332624 -0.139475
N 2.443025 -1.286594 -1.251229
C 1.481934 -0.726435 0.919488
N 0.713863 -1.051965 1.717438
C 3.861385 -0.309202 0.481106
C 2.042993 1.053504 -0.699540
C 1.937385 2.181351 0.328402
H 4.570707 0.015582 -0.282418
H 4.147994 -1.307525 0.821084
H 3.913252 0.365758 1.336273
H 1.087144 0.930779 -1.215293
H 2.784150 1.296353 -1.465981
H 1.598760 3.098793 -0.158614
H 1.219788 1.942457 1.118083
H 2.898369 2.396552 0.801701
H 2.712733 -2.214300 -0.939631
H 1.515099 -1.351560 -1.665138

34

Energy(ZPE): -612.019389 in gas Name: D-L Iva_AN_1

C -2.345967 0.055690 0.426794
N -2.265887 -1.338951 0.865220
C -1.406149 0.330323 -0.697922
N -0.669370 0.513546 -1.567382
C -1.951518 0.960357 1.608718
C -3.783760 0.386433 -0.042873
C -4.292499 -0.450495 -1.218814
H -1.990658 2.014087 1.324653
H -0.943379 0.723268 1.952576
H -2.649499 0.780702 2.428437
H -4.428275 0.238829 0.828362
H -3.820456 1.449230 -0.302538
H -3.641585 -0.353565 -2.092437
H -5.292089 -0.120898 -1.511922
H -4.366762 -1.509721 -0.958883
H -2.461672 -1.979739 0.103907
H -1.332668 -1.548726 1.213241
C 2.802127 -0.314055 -0.187007
N 2.386603 -0.336701 -1.590485
C 1.736376 -0.854348 0.704710
N 0.885316 -1.272906 1.362782
C 4.052995 -1.196931 -0.025978
C 3.122082 1.138710 0.245098
C 1.950243 2.118667 0.163161
H 4.405424 -1.194261 1.007202
H 4.838206 -0.807222 -0.676454
H 3.841748 -2.230024 -0.313670
H 3.934660 1.471285 -0.407204
H 3.511672 1.111266 1.268048
H 1.564279 2.207121 -0.853873
H 1.124092 1.809141 0.808375
H 2.271340 3.112243 0.485433
H 2.288590 -1.291953 -1.919869
H 1.486807 0.117914 -1.729648

34

Energy(ZPE): -612.019250 in gas Name: L-L Iva_AN_2

C -2.818610 -0.143106 0.133567
N -2.459531 0.090946 1.533156
C -1.761500 -0.914513 -0.580594
N -0.916216 -1.498809 -1.106666
C -4.123173 -0.958683 0.085807
C -3.013352 1.211156 -0.593430
C -1.773323 2.105550 -0.650494
H -4.433986 -1.143092 -0.944281
H -3.999187 -1.923335 0.584580
H -4.902624 -0.396294 0.603202
H -3.368532 1.004267 -1.608283
H -3.820168 1.722402 -0.060448
H -1.419693 2.375570 0.346014
H -0.949852 1.612684 -1.174350
H -2.004281 3.030329 -1.184871
H -1.538435 0.513904 1.624278
H -2.436332 -0.783257 2.048705
C 2.402431 -0.520645 -0.027417
N 2.055400 -0.385604 -1.443887
C 1.417275 0.179811 0.845338
N 0.639877 0.736388 1.492015
C 2.382395 -2.016441 0.336836
C 3.805274 0.078429 0.236820
C 3.948946 1.565799 -0.093832
H 2.640580 -2.165301 1.387423
H 3.110411 -2.534002 -0.290638
H 1.394747 -2.442016 0.150898
H 4.055304 -0.092322 1.288760
H 4.503762 -0.508582 -0.366281
H 3.232300 2.173009 0.466606
H 3.805630 1.758073 -1.160403
H 4.951781 1.914704 0.163591
H 1.984390 0.587700 -1.719773
H 1.159289 -0.829028 -1.632668

34

Energy(ZPE): -612.019084 in gas Name: D-L Iva_AN_3

C -2.616416 -0.176146 -0.330533
N -2.459252 -0.695802 -1.691090
C -1.708963 -0.874380 0.623182
N -0.987952 -1.426696 1.335739
C -4.067795 -0.409684 0.124569
C -2.248739 1.329726 -0.351526
C -2.302050 2.044431 0.999983
H -4.318321 -1.472463 0.078343
H -4.228793 -0.069798 1.148333
H -4.733139 0.134347 -0.548438
H -2.937522 1.794223 -1.062643
H -1.246633 1.419492 -0.779579
H -1.635154 1.577610 1.730271
H -3.310126 2.051107 1.421509
H -1.988964 3.084780 0.884160
H -1.500753 -0.581783 -2.014809
H -2.690204 -1.683311 -1.734912
C 2.295203 -0.309295 0.342476
N 2.178481 -1.599248 1.026478
C 1.402685 -0.246514 -0.849165

N 0.700112 -0.228676 -1.765027
C 1.869575 0.798424 1.323762
C 3.760879 -0.137516 -0.128664
C 4.070655 1.161461 -0.875051
H 2.561696 0.796608 2.167936
H 1.878546 1.780622 0.849219
H 0.863616 0.602459 1.697803
H 4.375538 -0.223744 0.771692
H 4.012013 -0.993473 -0.765073
H 5.112855 1.165473 -1.202753
H 3.443194 1.275095 -1.763318
H 3.923361 2.038910 -0.240961
H 1.221062 -1.762661 1.331441
H 2.447805 -2.363586 0.414883
22
Energy(ZPE): -454.828159 in water Name: D-L Ala_AN
C -1.607576 -0.039386 -0.020687
N -0.954530 1.207144 -0.436260
C -2.971991 0.180881 0.513498
N -4.033719 0.379336 0.921109
C -1.644728 -1.042924 -1.180180
H -1.020151 -0.468068 0.795768
H -0.904182 1.870544 0.331348
H -1.474848 1.652970 -1.187257
H -2.109979 -1.979318 -0.868744
H -0.622433 -1.246898 -1.499190
H -2.206296 -0.635863 -2.024378
C 2.603857 0.047625 -0.088365
N 1.996736 0.572609 -1.311228
C 1.859773 -1.113866 0.462846
N 1.240204 -2.002349 0.863808
C 2.715429 1.144870 0.979763
H 3.606422 -0.318875 -0.327491
H 2.008526 -0.123810 -2.050059
H 1.021690 0.832151 -1.135404
H 1.726911 1.536921 1.228589
H 3.179787 0.762119 1.890440
H 3.325132 1.957748 0.583121
22
Energy(ZPE): -454.827945 in water Name: L-L Ala_AN
C 1.784836 0.021661 0.059737
N 1.164609 -1.155774 -0.558142
C 3.184881 0.227040 -0.380083
N 4.275132 0.361862 -0.735039
C 1.713105 -0.067774 1.589612
H 1.224842 0.902028 -0.266612
H 1.677024 -2.001000 -0.320629
H 1.157501 -1.079541 -1.571017
H 2.238614 -0.955390 1.949846
H 2.158119 0.814523 2.052229
H 0.666175 -0.132113 1.887919
C -2.422506 -0.201475 -0.441088
N -1.842282 -1.324017 0.294622
C -1.724372 1.079846 -0.163021
N -1.147083 2.050381 0.079590
C -3.922777 -0.059263 -0.154025
H -2.282303 -0.391365 -1.509710
H -1.958582 -1.189711 1.295392
H -0.840392 -1.395160 0.097274
H -4.421400 -0.988991 -0.431588
H -4.357426 0.762235 -0.726220
H -4.093814 0.127106 0.909107
28
Energy(ZPE): -533.426999 in water Name: L-L Aba_AN
C 2.391714 -0.352985 0.045461
N 2.510579 -1.276910 -1.083376
C 1.424821 -0.827971 1.066613
N 0.650034 -1.218972 1.828233
C 2.004483 1.057308 -0.441601
C 1.944987 2.106514 0.668990
H 3.362460 -0.295366 0.547911
H 2.752854 1.335045 -1.187640
H 1.045220 0.992521 -0.962652
H 1.692071 3.083841 0.252644
H 1.189552 1.862160 1.420743
H 2.908779 2.195408 1.178386
H 2.842698 -2.186242 -0.777587
H 1.603846 -1.411260 -1.525940
C -2.391648 -0.353154 -0.045526
N -2.510480 -1.277184 1.083266
C -1.424669 -0.827941 -1.066646
N -0.649776 -1.218789 -1.828237
C -2.004593 1.057143 0.441663
C -1.945326 2.106457 -0.668842
H -3.362399 -0.295636 -0.547970
H -2.752964 1.334701 1.187766
H -1.045289 0.992441 0.962653
H -1.189817 1.862340 -1.420598
H -1.692663 3.083811 -0.252408
H -2.909131 2.195159 -1.178248
H -2.842631 -2.186480 0.777374
H -1.603699 -1.411670 1.525698
28
Energy(ZPE): -533.426610 in water Name: D-L Aba_AN
C -1.647069 -0.436203 0.052572
N -0.925624 -1.242705 1.043922
C -2.840190 -1.132553 -0.481921
N -3.767026 -1.698430 -0.873875
C -2.031347 0.933852 0.641956
C -2.681248 1.875814 -0.371820
H -0.977313 -0.269163 -0.796203
H -2.691730 0.775617 1.500823
H -1.105548 1.371389 1.021731
H -2.892859 2.841985 0.091364
H -2.015634 2.046991 -1.221806
H -3.625575 1.474225 -0.749544
H -0.642890 -2.137299 0.654485
H -1.516801 -1.437635 1.847645
C 2.406427 0.414201 0.549596
N 1.715635 0.265423 1.830602
C 1.593784 1.153666 -0.449386
N 0.921316 1.716666 -1.200957
C 2.816193 -0.962091 -0.010847
C 3.618048 -0.891455 -1.311098
H 3.311518 1.009900 0.706885
H 1.912685 -1.563794 -0.150206
H 3.403884 -1.444678 0.774001
H 4.524787 -0.293004 -1.182342
H 3.033727 -0.449330 -2.122775
H 3.918977 -1.892990 -1.626246
H 0.824982 -0.221500 1.694662
H 1.520097 1.171224 2.245370
34
Energy(ZPE): -612.027702 in water Name: D-L Val_AN

C -1.960901 -0.683551 -0.180608
N -1.332256 -1.318329 0.983216
C -3.418707 -0.943954 -0.247975
N -4.552910 -1.157950 -0.269842
C -1.658855 0.835492 -0.239922
C -2.196776 1.593693 0.978162
C -2.158735 1.447633 -1.552926
H -1.529319 -1.141680 -1.075263
H -0.568154 0.895547 -0.225085
H -3.287934 1.527880 1.037217
H -1.930387 2.650571 0.903772
H -1.776611 1.218589 1.914575
H -1.762639 0.911355 -2.420021
H -3.251479 1.431140 -1.611338
H -1.838238 2.489480 -1.625361
H -1.782353 -1.030077 1.846899
H -1.413676 -2.329380 0.930113
C 2.594158 -0.117307 0.883367
N 1.695787 -0.861230 1.765181
C 2.109545 1.258542 0.601344
N 1.700414 2.320130 0.402682
C 2.883505 -0.881714 -0.435257
C 1.619817 -1.119882 -1.269438
C 3.971693 -0.181530 -1.257823
H 3.548305 0.007326 1.404963
H 3.267110 -1.851460 -0.101831
H 0.859175 -1.665968 -0.708321
H 1.187207 -0.172752 -1.607802
H 1.863582 -1.707134 -2.157986
H 4.234875 -0.788872 -2.127081
H 3.628625 0.790910 -1.624853
H 4.879758 -0.022221 -0.669325
H 0.743028 -0.918377 1.397776
H 1.643409 -0.417756 2.676754

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Energy(ZPE): -612.027377 in water Name: L-L Val_AN

C 2.101054 -0.538505 -0.409007
N 1.390696 0.068484 -1.534321
C 1.458754 -0.231032 0.895219
N 0.921774 0.027552 1.884502
C 3.606766 -0.169733 -0.385575
C 4.358344 -0.971445 0.683820
C 3.841345 1.336429 -0.220950
H 2.028820 -1.624657 -0.524047
H 3.972481 -0.473795 -1.371772
H 4.036005 -0.690133 1.691331
H 5.431530 -0.778781 0.613970
H 4.199512 -2.046933 0.563790
H 3.448826 1.693919 0.736588
H 3.375904 1.916731 -1.021322
H 4.912326 1.552099 -0.242100
H 1.357157 1.078895 -1.441427
H 0.426264 -0.273585 -1.557564
C -2.055138 -0.591736 0.034763
N -1.459612 -1.158314 -1.181904
C -3.419199 -1.112064 0.287768
N -4.481977 -1.530790 0.455052
C -2.040581 0.959002 0.017827
C -2.844058 1.544648 -1.148247
C -2.501545 1.526743 1.364593
H -1.440320 -0.913702 0.879559
H -0.986358 1.216186 -0.119343
H -2.779705 2.635257 -1.133602
H -3.902055 1.272799 -1.075652
H -2.467675 1.209276 -2.117765
H -3.557588 1.306791 1.549604
H -1.913747 1.114832 2.188993
H -2.382743 2.612772 1.373293
H -1.333238 -2.161476 -1.087023
H -2.056007 -1.008851 -1.990092

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Energy(ZPE): -612.032411 in water Name: L-L Iva_AN

C -2.111553 -0.444173 -0.056424
N -1.345680 -0.175855 -1.284494
C -3.574953 -0.433961 -0.331586
N -4.705144 -0.422799 -0.568099
C -1.727996 -1.839907 0.467928
C -1.798133 0.631822 1.011607
C -2.109162 2.072186 0.601057
H -0.661128 -1.845061 0.695950
H -2.284890 -2.078290 1.375608
H -1.933896 -2.609152 -0.279844
H -2.355743 0.375438 1.916931
H -0.737672 0.526761 1.250660
H -3.161973 2.197545 0.332658
H -1.895445 2.748911 1.431316
H -1.497971 2.397529 -0.244100
H -1.543023 -0.879635 -1.991017
H -1.593078 0.722614 -1.687726
C 2.631412 -0.287828 -0.209602
N 1.729414 -0.863091 -1.211887
C 2.076723 -0.457117 1.164300
N 1.612339 -0.606783 2.211431
C 3.983512 -1.022224 -0.268833
C 2.836847 1.223053 -0.479742
C 1.566997 2.074194 -0.434170
H 4.682366 -0.615956 0.464464
H 3.856916 -2.089797 -0.074407
H 4.402693 -0.895920 -1.268819
H 3.564442 1.602682 0.243910
H 3.298244 1.290735 -1.469130
H 0.835351 1.748552 -1.176234
H 1.091954 2.034359 0.549727
H 1.809005 3.118845 -0.642319
H 0.777358 -0.495978 -1.145649
H 1.667814 -1.870757 -1.097847

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Energy(ZPE): -612.031895 in water Name: L-D Iva_AN

C -2.313155 0.036861 -0.494171
N -1.507165 -1.184090 -0.411295
C -1.947340 0.997545 0.586812
N -1.644679 1.717977 1.437495
C -2.038997 0.718766 -1.847223
C -3.819851 -0.296577 -0.361252
C -4.221478 -0.989398 0.942548
H -0.980629 0.964854 -1.950998
H -2.623263 1.635076 -1.948371
H -2.316579 0.028506 -2.645984
H -4.065571 -0.934250 -1.215278
H -4.385703 0.632790 -0.477217
H -3.963254 -0.383763 1.816117
H -5.301173 -1.154263 0.961173
H -3.741610 -1.965684 1.048533
H -0.515970 -0.985931 -0.574379

H	-1.590459	-1.623221	0.499819
C	2.365630	-0.479219	0.156826
N	1.536154	-0.701585	-1.038429
C	3.797785	-0.312593	-0.214709
N	4.902578	-0.186247	-0.525814
C	2.246332	-1.708290	1.075684
C	1.890033	0.792493	0.900372
C	1.917806	2.080207	0.075474
H	2.847316	-1.576901	1.976845
H	2.578557	-2.614203	0.563874
H	1.200420	-1.830489	1.362363
H	2.509253	0.909269	1.794388
H	0.870519	0.591495	1.237414
H	1.611038	2.924668	0.696098
H	2.919598	2.294264	-0.307964
H	1.227678	2.036510	-0.770733
H	1.805877	-1.560712	-1.509897
H	1.645144	0.050831	-1.711674a