Electronic Supplementary Information

Bio-inspired design and computational prediction of scorpion-like SCS nickel pincer complexes for lactate racemization

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1. Computational details

All DFT calculations in this study were performed using the Gaussian 09 suite of ab initio programs[1] for the ωB97X-D[2] functional with all-electron 6-31+G(d,p) basis set for H, C, N, O, S, P, Cl, Br, [3] and the Stuttgart relativistic effective core potential basis set for Ni (ECP10MDF) and Pd (ECP28MWB).[4] All structures in this paper were optimized in water by using the integral equation formalism polarizable continuum model (IEFPCM)[5] with the SMD[6] atomic radii for solvent corrections. The ground states were confirmed as singlet through comparison with optimized high-spin analogs. An ultrafine integration grid (99,590) was used for numerical integrations. Thermal corrections were calculated within the harmonic potential approximation on optimized structures under T = 298.15 K and 1 atm pressure. Unless otherwise noted, the relative energies reported in the text are Gibbs free energies with the solvent effect corrections. The calculated structures were verified to have no imaginary frequency (IF) for all intermediates and only one IF for each transition state. All transition states were also confirmed to connect reactants and products by intrinsic reaction coordinate (IRC) calculations. The JIMP2 molecular visualizing and manipulating program was employed to draw the 3D molecular structures.[7]

2. Evaluation of density functionals

In order to examine the reliability of density functionals for this Ni system, we also calculated the relative free energies between **A + L-lactate** and $\mathbf{TS_{1A,2A}}$ using other six well recognized functionals with different Hartree-Fock exchanges and disperse corrections, including TPSS[8], B3LYP[9-10], B3LYP-D3(BJ)[11], M06[12], M06-2X[12] and *ω*B97X[2]. The calculated relative free energies are listed in Table S1. All structures were independently optimized using above six functionals with the same basis set described in computation details. We can see that the functionals without dispersion corrections, such as TPSS, B3LYP, and *ω*B97X, have much higher relative free energies. For example, the relative free energy obtained by using the *ω*B97X functional is 8.2 kcal/mol higher than the relative free energy obtained by using the *ω*B97X-D functional. Such a large difference clearly indicates the importance of dispersion correction for this nickel catalytic system. This is not unexpected because this catalytic system has some important non-covalent interactions in the reaction. The difference of relative free energies obtained by using the M06 and *ω*B97X-D functionals is only 0.9 kcal/mol. Therefore, we believe *ω*B97X-D is a suitable functional for the computational study of this Ni catalytic system.

Table S1. Relative free energies calculated by using different functionals.

Functionals	ΔG (Kcal/mol) **(A + L-lactate → $\mathbf{TS_{1A,2A}}$)**
TPSS	31.1
B3LYP	36.1
B3LYP-D3(BJ)	24.0
M06	27.8
M06-2X	27.8
*ω*B97X	35.1
*ω*B97X-D	26.9

3. Evaluation of Solvent effect

The relative free energies between **A** + **L-lactate** and **$TS_{1A,2A}$** calculated by using the ωB97X-D functional in water (ε = 78.3553), ethanol (ε = 24.852) and acetonitrile (ε = 35.688) are listed in Table S2. We can see the difference of relative free energies in those three solvents is less than 1.5 kcal/mol, which indicate a rather small influence of different solvent.

Table S2. Relative free energies calculated by using different solvent.

Solvent	ΔG (Kcal/mol) **(A + L-lactate → $TS_{1A,2A}$)**
Ethanol	26.8
Acetonitrile	28.3
Water	26.9

4. Absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all structures optimized in water.

A

G_{solv} = -2165.916837

Ni	2.32839157	-0.32851967	0.05250406
C	-0.99892877	2.04724963	-0.68382215
C	0.27279612	1.63024016	-0.34205017
C	0.02452064	-2.04002189	-0.88642256
C	0.62603874	0.26835578	-0.41060586
C	-0.37197256	-0.62078948	-0.84838314
C	-1.62632847	-0.15895349	-1.19600500
C	1.34740501	2.52854282	0.12135299
S	2.83487475	1.77981836	0.48483564
S	1.63033717	-2.37389569	-0.42561419
H	-1.34500674	3.07353407	-0.64108590
H	-2.43256676	-0.78964559	-1.55183475
N	1.17364931	3.82240703	0.25042757
Cl	4.37133898	-1.04505333	0.61127350
N	-0.80779245	-2.98803095	-1.24636321
C	-4.08086965	1.56604405	0.01144199
C	-3.31367895	1.59936906	-1.31809719
H	-3.28487314	2.60496044	-1.73705563
H	-3.76023516	0.92532704	-2.04906355
N	-1.91437596	1.15624807	-1.11574403
C	-3.95642771	0.24633637	0.70451289
N	-3.01940598	0.03036061	1.69925154
C	-4.60290185	-0.92760615	0.41428964
C	-3.10617939	-1.25412858	1.99132697
N	-4.04960545	-1.87089603	1.24378568
H	-5.37840108	-1.16785742	-0.29675420
H	-2.52125410	-1.77700481	2.73363643
H	-3.70912533	2.36098965	0.66437161
H	-5.12527690	1.78892754	-0.22405178
H	-4.30189414	-2.84851215	1.29201132
H	1.93044437	4.41553050	0.57205034
H	0.29513999	4.28193900	0.04333446
H	-0.51087251	-3.95732581	-1.26121993
H	-1.76532121	-2.79961850	-1.51837833

1A

G_{solv} = -2508.949578

Ni	-0.86720558	-2.31828217	-0.44134199
C	1.28055766	0.81945360	-2.10762169
C	0.89867619	-0.44100031	-1.69330470
C	-2.43149270	0.25137158	-0.19706545
C	-0.34747872	-0.64501692	-1.07027849
C	-1.17162603	0.48472530	-0.92286517
C	-0.77378727	1.71710243	-1.40139644
C	1.74279129	-1.64457599	-1.80423415
S	1.06292721	-3.08487083	-1.20228287
S	-2.73560260	-1.36031530	0.26513882
H	2.24221411	1.05562746	-2.54770346
H	-1.37598982	2.61636110	-1.36173284
N	2.94261218	-1.61289364	-2.33469287
C	1.43132779	3.95123913	-1.07038244
C	0.90814343	3.22800764	-2.31682310
H	1.69082283	3.12358154	-3.06712795
H	0.06602440	3.76234923	-2.75878085
N	0.43690607	1.86384382	-1.97762522
C	0.36106496	4.20018305	-0.05482915
N	0.06899283	3.30362651	0.95746898
C	-0.54328986	5.22955093	-0.02438113
C	-0.99261274	3.78960910	1.57600920
N	-1.39362943	4.95122017	1.01713343
H	-0.65442025	6.10742419	-0.64183330
H	-1.49064513	3.34616472	2.42596798
H	2.24875794	3.37147087	-0.63052656
H	1.84584595	4.90187509	-1.41727569
H	-2.16831979	5.52156693	1.32884464
C	1.38618080	-0.05382421	1.94088404
H	0.68032952	-0.53741291	1.25127242
C	1.71434230	-1.10286353	3.01622163
O	1.64334536	-0.78450671	4.23389374
O	2.05897458	-2.24054603	2.58041495
H	3.50419428	-2.45503153	-2.39035091
H	3.35617889	-0.76434457	-2.70150217
C	2.65343914	0.33225307	1.17729111
H	3.07022504	-0.53324279	0.65446839
H	2.42837102	1.10453945	0.43466413
H	3.40913546	0.72773203	1.86465567
O	0.77273430	1.07873215	2.53279414
H	0.62052423	1.76294892	1.84369682
N	-3.25332140	1.23065912	0.09847225
H	-4.10598033	1.05147041	0.61598595
H	-3.05316079	2.19644158	-0.13325108

Cl	-1.49284225	-4.32979758	0.30570273

$TS_{1A,2A}$

G_{solv} = -2508.913641

Ni	-0.60639187	-2.41647051	0.27548777
C	-0.67399523	0.76203439	-2.40248015
C	-0.43496381	-0.46655838	-1.85322789
C	-1.46571519	0.13293892	1.69044485
C	-0.53777509	-0.67294036	-0.42426416
C	-1.17191900	0.41056378	0.29086266
C	-1.44416291	1.59789647	-0.33041362
C	-0.02895656	-1.64735348	-2.60920970
S	-0.03987534	-3.12111553	-1.74642530
S	-1.34833689	-1.50679670	2.15699749
H	-0.55301875	0.99726885	-3.45362379
H	-1.92982016	2.43688918	0.15569510
N	0.32882809	-1.59838030	-3.87732301
C	0.12039051	3.91190202	-1.83678869
C	-1.16716155	3.15399740	-2.19085184
H	-1.26971650	3.07562357	-3.27308857
H	-2.04533362	3.66699235	-1.79461009
N	-1.14971894	1.78752868	-1.64205485
C	0.20345611	4.30959726	-0.39836330
N	0.68170800	3.50279889	0.62096015
C	-0.22410700	5.46571900	0.18722430
C	0.53105706	4.13707852	1.77647215
N	-0.00948324	5.33254533	1.53964564
H	-0.65737969	6.35465408	-0.24193898
H	0.80498869	3.75502295	2.74719302
H	0.99028873	3.31365653	-2.12367518
H	0.13320229	4.82319662	-2.44004988
H	-0.21985185	6.02439276	2.24845095
C	1.84061152	0.12188644	0.37947414
H	0.81779817	-0.53690848	0.02362137
C	2.56348845	-1.03575467	1.13175392
O	2.59060347	-0.98583929	2.39036562
O	3.07523514	-1.94823127	0.42374432
H	0.59100166	-2.44284215	-4.37087937
H	0.38080009	-0.73059859	-4.39500609
C	2.46633865	0.48301961	-0.96100045
H	2.52771124	-0.37503295	-1.63507784
H	1.88024888	1.27172142	-1.44202613
H	3.48014002	0.86445352	-0.79412913

O	1.43933542	1.12650214	1.12570393
H	1.03562490	2.46707934	0.61984716
N	-1.79658476	1.07538661	2.55316156
H	-1.98582543	0.84143997	3.51981789
H	-1.75663437	2.06016106	2.31951170
Cl	-0.57164754	-4.49306874	1.14530143

2A

G_{solv} = -2508.944305

Ni	-0.82416779	-2.60484635	-0.06148327
C	0.91416024	0.71360181	-1.74036040
C	0.83871637	-0.45713733	-1.05533636
C	-2.68542248	-0.21074560	0.21982901
C	-0.29177472	-0.76502838	-0.11835219
C	-1.41480471	0.20522450	-0.32163486
C	-1.27449472	1.33704111	-1.05136717
C	1.76555983	-1.53965296	-1.26993423
S	1.18553319	-3.09546984	-0.84781699
S	-2.85381168	-1.89304425	0.48349182
H	1.72222511	0.95428361	-2.42374962
H	-2.08651195	2.03372491	-1.23393864
N	2.98645033	-1.37321848	-1.76374940
C	0.52155233	4.04950765	-1.48824421
C	0.03309285	2.91760269	-2.40443145
H	0.73722549	2.78756943	-3.22808142
H	-0.94107143	3.17258800	-2.82792203
N	-0.09805012	1.64030566	-1.70337453
C	-0.36873131	4.24329665	-0.30768591
N	-0.20769378	3.54328049	0.87453861
C	-1.50844094	4.97699039	-0.15928382
C	-1.20819578	3.82162344	1.70187259
N	-2.00464907	4.69727443	1.09572601
H	-2.00202438	5.65748270	-0.83373999
H	-1.34327000	3.41929521	2.69302351
H	1.54116906	3.84011771	-1.15485338
H	0.54468284	4.97105859	-2.07506581
H	-2.83945309	5.09337083	1.51133836
C	2.50296489	1.09026329	1.34260229
H	0.06494112	-0.70397865	0.92443535
C	3.02594865	-0.32063452	1.76135624
O	2.25647886	-1.00816759	2.47259278
O	4.17573730	-0.62429752	1.35676453

H	3.59038709	-2.16936115	-1.91686319
H	3.38488209	-0.45279540	-1.89206883
C	3.35884176	1.93660731	0.46104120
H	3.58197863	1.40851510	-0.47093468
H	2.86230718	2.88471810	0.25156805
H	4.31692692	2.11861010	0.95897200
O	1.42111415	1.47024718	1.77173343
H	0.53293385	2.85577498	1.09319548
N	-3.65651513	0.64220801	0.52049595
H	-4.54913282	0.30878016	0.85898001
H	-3.51459713	1.64261869	0.47369970
Cl	-1.35598331	-4.81253042	0.32047839

3A

G_{solv} = -2167.102813

Ni	-0.27496656	-2.27626086	0.10277983
C	1.96062337	1.07549382	-0.79762262
C	1.60413014	-0.09592217	-0.21533756
C	-2.09774493	-0.02837683	-0.84561987
C	0.16981667	-0.41454473	0.10499484
C	-0.74598977	0.45690889	-0.70749066
C	-0.30919751	1.59880110	-1.29169868
C	2.55272124	-1.13887956	0.09420702
S	1.88117035	-2.69027286	0.36428557
S	-2.33123836	-1.67842426	-0.45460087
H	2.98741889	1.36769091	-0.99578475
H	-0.94565613	2.26799783	-1.86207952
N	3.86080824	-0.93410858	0.18385285
C	1.40452154	4.14488651	-0.15711818
C	1.38502133	3.36135174	-1.48599465
H	2.36924631	3.40262481	-1.95644187
H	0.65512924	3.79657312	-2.17093246
N	1.01984880	1.96295083	-1.26955053
C	0.18365932	3.86374608	0.65259659
N	0.14426906	2.84129829	1.58480319
C	-1.08965966	4.34572838	0.58027183
C	-1.09222864	2.68569792	2.04544089
N	-1.85250531	3.60055109	1.45376590
H	-1.51097039	5.13577506	-0.01949033
H	-1.41518729	1.96287546	2.77735015
H	2.28971884	3.86678730	0.42229846
H	1.46909827	5.21203523	-0.38089601
H	-2.84375805	3.71890118	1.62882880

H	4.49287777	-1.70361073	0.36001575
H	4.26552832	-0.01355391	0.07820360
H	0.92502798	2.24073794	1.83002988
H	-0.01103211	-0.22744003	1.18047710
Cl	-0.86735676	-4.47309604	0.43826930
N	-3.11478742	0.73669201	-1.22290967
H	-4.03806907	0.34289240	-1.34538399
H	-3.00162777	1.72577197	-1.39906912

4A

G_{solv} = -2508.950425

Ni	-0.44414647	-2.62208972	0.45372093
C	-1.18342031	0.56120077	-2.04743783
C	-0.62183821	-0.59573374	-1.61288982
C	-0.92881330	-0.09615880	2.09802633
C	-0.28166345	-0.82467609	-0.17488310
C	-0.90739375	0.21885021	0.69195950
C	-1.48908808	1.33091095	0.18159171
C	-0.39392030	-1.73094317	-2.47072844
S	-0.29084062	-3.24388198	-1.67061502
S	-0.76377675	-1.75836112	2.47754262
H	-1.42883761	0.75143836	-3.08724559
H	-1.97606643	2.08281660	0.79490696
N	-0.25934329	-1.63795952	-3.78740852
C	-1.01149662	3.91529489	-1.70973770
C	-2.09169012	2.82368535	-1.67449474
H	-2.48297825	2.66517626	-2.68058232
H	-2.92100759	3.13505493	-1.03438260
N	-1.58382638	1.54453067	-1.17479907
C	-0.48515141	4.22971265	-0.34893285
N	0.59369982	3.56880313	0.20877823
C	-0.97336107	5.05482688	0.62111537
C	0.75087738	3.95876023	1.46703785
N	-0.18482979	4.86796310	1.73513099
H	-1.80577967	5.73949979	0.61392162
H	1.50928690	3.61759842	2.15211400
H	-0.19370127	3.60323955	-2.36560722
H	-1.46077793	4.81599181	-2.13566352
H	-0.28228681	5.34436870	2.62364194
C	2.73764797	0.50769163	0.49248556
C	2.53149140	0.75865190	-1.03574376
O	1.93912914	1.82650431	-1.35108572

O	2.96697264	-0.11398715	-1.81773993
H	-0.14440914	-2.46767981	-4.35323083
H	-0.23386076	-0.74232288	-4.25592722
C	3.44177370	-0.74311232	0.91067237
H	4.47763212	-0.70577830	0.55486190
H	3.42832742	-0.83549618	1.99754055
H	2.97847025	-1.61960110	0.44861356
O	2.33402108	1.33992923	1.28912651
H	1.16997714	2.83515560	-0.27324955
H	0.81370944	-0.80860189	-0.05050729
N	-1.04358684	0.82937688	3.04194853
H	-1.09559535	0.57000207	4.01764861
H	-1.02950730	1.81587721	2.81767517
Cl	-0.30306567	-4.77556919	1.24377902

$TS_{4A,5A}$

G_{solv} = -2508.914085

Ni	0.59591914	-2.51901565	0.33047389
C	-1.96058779	0.60891719	1.32485168
C	-1.50305713	-0.60355702	0.88691900
C	2.18497291	0.02406367	0.81561120
C	-0.10791770	-0.79030005	0.54904955
C	0.76028388	0.28123153	0.97551986
C	0.24530726	1.44505063	1.47518444
C	-2.33432914	-1.78989265	0.70024059
S	-1.49136901	-3.25083173	0.42089246
S	2.61018296	-1.59311163	0.46287961
H	-3.00051796	0.83046845	1.53618732
H	0.85090018	2.27088481	1.83048257
N	-3.65063653	-1.76027823	0.75417792
C	-1.63512973	3.83292887	0.58801897
C	-1.60967087	2.98034882	1.86426808
H	-2.61853454	2.87831283	2.26348068
H	-0.97770849	3.43698409	2.62857750
N	-1.09401835	1.62597921	1.59568082
C	-0.27612622	4.21072438	0.09283318
N	0.50401613	3.43068784	-0.74545484
C	0.47000317	5.30976710	0.40539599
C	1.67829365	4.02352608	-0.91684645
N	1.67950072	5.16909245	-0.23593659
H	0.24112562	6.16445542	1.02122917
H	2.49412999	3.64809968	-1.51409573
H	-2.19304294	3.30772550	-0.19179551
H	-2.17651018	4.75186950	0.82686491

H	2.44769038	5.82845854	-0.21483622
C	-0.02720146	0.05237118	-1.95686105
C	-1.54370310	0.34507915	-2.13721364
O	-1.92272332	1.54102108	-2.02152934
O	-2.29934015	-0.64115195	-2.36468816
H	-4.18875850	-2.60832732	0.62629036
H	-4.16931633	-0.89733890	0.85368885
C	0.52447603	-1.02095732	-2.89216402
H	0.49489633	-0.65012599	-3.92377579
H	1.56402607	-1.23089012	-2.62605899
H	-0.04825589	-1.94934600	-2.83827658
O	0.75449022	1.09122637	-1.76748074
H	0.34674564	2.43658471	-1.14636485
H	-0.10887386	-0.58903771	-0.87633140
N	3.09545782	0.97203403	0.93035153
H	4.07762891	0.75944215	0.81047542
H	2.84659197	1.94688934	1.04654744
Cl	1.43162879	-4.57333869	-0.05981773

5A

G_{solv} = -2508.953478

Ni	-0.69561176	-2.46638070	-0.45856161
C	1.79839995	0.68042192	-1.52369736
C	1.33405055	-0.57344374	-1.17439094
C	-2.28904969	0.08664530	-0.69224423
C	-0.03481682	-0.78955529	-0.92815934
C	-0.88125742	0.32641889	-1.05186867
C	-0.38643146	1.54563012	-1.47055085
C	2.18671370	-1.76701527	-1.02454544
S	1.37404255	-3.22064215	-0.66102301
S	-2.69465594	-1.52322783	-0.30890188
H	2.84031567	0.92410709	-1.69509074
H	-0.99595624	2.41949421	-1.66562208
N	3.48833771	-1.72154427	-1.17707060
C	1.57300460	3.93231871	-0.77834451
C	1.45252045	3.05225028	-2.02760156
H	2.42345000	2.91646252	-2.50253878
H	0.76621833	3.49127432	-2.75310457
N	0.93429824	1.70149557	-1.69747396
C	0.25285057	4.22665088	-0.13828267
N	-0.28327267	3.42496421	0.85215827
C	-0.64918987	5.20246897	-0.47565519
C	-1.48627890	3.91126533	1.09626180
N	-1.74851189	4.98505682	0.31854752

H	-0.60737586	6.00540867	-1.19540731
H	-2.19083084	3.53064026	1.82145009
H	2.24466679	3.45223268	-0.06063183
H	2.04444340	4.86291296	-1.10711216
H	-2.59279379	5.54120553	0.33948931
C	0.36284705	-0.20936019	2.42076671
C	1.84153802	0.09888274	2.12774088
O	2.15178264	1.27789247	1.80701170
O	2.64601807	-0.87128773	2.21770004
H	4.04938768	-2.55794800	-1.06354313
H	3.98402268	-0.86275160	-1.38181163
C	0.17058977	-0.75637285	3.82983812
H	0.51968313	-0.03303271	4.57459086
H	-0.89053921	-0.95581171	4.00684740
H	0.72110563	-1.69114755	3.95977104
O	-0.47848710	0.91960510	2.25485965
H	-0.04548733	1.59700427	1.69722548
H	0.06785929	-0.98889192	1.70073778
N	-3.16977838	1.05786163	-0.64368163
H	-4.12880143	0.87142820	-0.37413374
H	-2.92226057	2.02504905	-0.81681973
Cl	-1.48559569	-4.47851814	0.11380578

L-lactate

G_{solv} = -343.03961

O	1.26101311	1.17798253	0.20825878
H	1.77945474	0.43063880	-0.13948299
C	-0.04688727	-0.85690136	0.04457971
O	-1.10924906	-1.50306286	0.24559840
O	1.02724701	-1.32410951	-0.43274308
C	-0.04151580	0.63845367	0.40957343
H	-0.28891064	0.71311104	1.47608496
C	-1.06939197	1.41825413	-0.40331026
H	-2.08036205	1.06048294	-0.19063861
H	-1.01958320	2.47980702	-0.14403809
H	-0.87591707	1.31064023	-1.47589525

Pyruvate

G_{solv} = -341.844773

C	-0.01714075	0.65777085	-0.26595406
C	0.14874749	1.66114483	0.83068513
H	0.20288493	2.66901766	0.41657607
H	-0.69687016	1.58807501	1.52231998
H	1.05149941	1.43806007	1.40805392

O	-0.17937475	0.97826041	-1.43403702
C	0.00276868	-0.85567057	0.11561665
O	0.19910240	-1.66496657	-0.82317124
O	-0.19019848	-1.12262177	1.32857873

D-lactate

G_{solv} = -343.03961

C	-0.04023328	0.63891938	-0.41012033
H	-0.28443510	0.71411302	-1.47731801
C	-1.07038277	1.41609745	0.40155230
H	-1.01839596	2.47883930	0.14730875
H	-2.08107839	1.06095067	0.18338429
H	-0.87995854	1.30267318	1.47413102
O	1.26131060	1.17919693	-0.20447083
H	1.77909809	0.43364532	0.14749089
C	-0.04654252	-0.85614746	-0.04537552
O	1.02801135	-1.32680577	0.42812608
O	-1.11085678	-1.50032087	-0.24257221

B

G_{solv} = -1838.260892

Ni	0.29539746	-2.33161206	-0.04891797
C	-1.96074531	1.09178801	0.73866392
C	-1.59712315	-0.19895893	0.39533966
C	2.08324933	-0.09430039	1.04464629
C	-0.25485880	-0.60476829	0.48015146
C	0.65936340	0.33350062	0.95496246
C	0.26154555	1.60710494	1.30071616
C	-2.52752899	-1.22800154	-0.09865956
S	-1.83238942	-2.73431913	-0.52083574
S	2.34488801	-1.74909739	0.50478956
H	-2.96824774	1.48702274	0.66865077
H	0.94858782	2.36200386	1.66490792
N	-3.81430312	-1.02745265	-0.21462736
C	-1.37937193	4.07900646	-0.03944928
C	-1.40474444	3.39073925	1.33412372
H	-2.39589142	3.43423988	1.78616309
H	-0.68204606	3.83769442	2.01627294
N	-1.03508191	1.96315397	1.18611234
C	-0.11530197	3.79777437	-0.78903990
N	-0.05385334	2.80782495	-1.75333471
C	1.13540679	4.32180018	-0.58283147
C	1.21493305	2.74413820	-2.11223225
N	1.96829074	3.63918660	-1.43420738

H	1.49490024	5.09092081	0.08328312
H	1.63223738	2.08056611	-2.85536735
H	-2.23365587	3.73659243	-0.63058032
H	-1.50640742	5.14992092	0.14112452
H	2.96390174	3.77898459	-1.53995364
O	2.98141729	0.63056168	1.44803802
C	0.86382254	-4.00203426	-0.59330832
O	1.22234710	-5.02221795	-0.93116669
H	-4.42409566	-1.76024968	-0.56205252
H	-4.25774747	-0.15036583	0.03292534

$TS_{4B,5B}$

G_{solv} = -2181.256709

Ni	0.55989035	-2.60656219	0.30659652
C	-1.90397813	0.61847784	1.31825432
C	-1.47974540	-0.61409102	0.89057754
C	2.24507951	-0.12532198	1.03561763
C	-0.08407270	-0.84599794	0.60390625
C	0.80092173	0.16890608	1.08581054
C	0.32574600	1.36243139	1.54394093
C	-2.34705729	-1.75816303	0.65499288
S	-1.55634871	-3.25455269	0.36057563
S	2.59128088	-1.78382973	0.54836251
H	-2.94274698	0.87915706	1.48752853
H	0.97625024	2.15926485	1.88839096
N	-3.65962873	-1.69504070	0.67431793
C	-1.57693761	3.80490556	0.61061569
C	-1.49438877	2.96511850	1.89067108
H	-2.48281195	2.87970205	2.34223935
H	-0.81903414	3.41953814	2.61760431
N	-1.01149221	1.60012740	1.61535780
C	-0.25026461	4.22912106	0.06969455
N	0.56657831	3.45072898	-0.73403631
C	0.41264672	5.40403955	0.27443278
C	1.67997292	4.12315558	-0.99650735
N	1.60914159	5.31195391	-0.39911106
H	0.13154271	6.28327651	0.83119380
H	2.50582174	3.76984942	-1.59344157
H	-2.14278190	3.25885467	-0.14956173
H	-2.13955203	4.70890117	0.85728507
H	2.32563866	6.02588006	-0.44455700
C	0.10763571	0.03248523	-1.89984321
C	-1.40329860	0.32208331	-2.13464410
O	-1.79242825	1.51525242	-2.02511208

O	-2.14557339	-0.66605042	-2.39563462
H	-4.22037847	-2.52225969	0.50787903
H	-4.15694001	-0.82111450	0.79098542
C	0.69972498	-1.02051571	-2.83471268
H	0.71417094	-0.62686936	-3.85809532
H	1.72711604	-1.23584863	-2.52890985
H	0.12616548	-1.95010378	-2.82502804
O	0.87848329	1.07057358	-1.66480561
H	0.45322269	2.43292848	-1.08215462
H	-0.01598342	-0.62211477	-0.83756108
O	3.12909904	0.68311499	1.31118547
C	1.20855403	-4.26921611	-0.10980424
O	1.62404834	-5.29040039	-0.38128621

C

G_{solv} = -4964.423596

Pd	1.55006322	0.12473933	1.02138132
C	-0.65663344	-0.50546694	-2.51212845
C	0.40613908	-0.36236015	-1.63462533
C	-1.38701714	-0.67678933	1.64488189
C	0.15890827	-0.36602687	-0.23970922
C	-1.15253829	-0.66169215	0.20071589
C	-2.16182600	-0.82445877	-0.73482719
C	1.78545763	-0.12895373	-2.06588422
S	2.88202420	0.27126709	-0.87412938
S	-0.11165817	-0.20151271	2.61046733
H	-0.56951898	-0.40544483	-3.58823929
H	-3.20164900	-0.98353731	-0.47581986
C	-3.47613073	0.81214702	-3.17587885
C	-3.04160306	-0.65022843	-3.00014666
H	-2.72067420	-1.08827225	-3.94511553
H	-3.84720198	-1.25530861	-2.58461143
N	-1.90318996	-0.73280013	-2.05440738
C	-3.71865197	1.49381106	-1.86638107
N	-2.73232615	2.23134556	-1.23560496
C	-4.82226358	1.40847030	-1.05663597
C	-3.24167757	2.57247628	-0.06643690
N	-4.50147616	2.10364812	0.08223164
H	-5.77645638	0.92121461	-1.18580192
H	-2.74857754	3.16091305	0.69342447
H	-2.70751256	1.35228523	-3.73630341
H	-4.38461522	0.79679952	-3.78439061
H	-5.09397140	2.23535688	0.89050584
Br	3.32488384	0.77654667	2.63544999

P	2.25094579	-0.18039047	-3.82598216
P	-3.02137519	-1.07706200	2.34370976
C	-2.68275777	-1.24359064	4.13535889
H	-3.59912568	-1.62832882	4.59305625
H	-1.86379538	-1.94036564	4.33882649
H	-2.46449124	-0.27158048	4.58374579
C	-3.17954124	-2.84796610	1.83864715
H	-4.06202251	-3.24060667	2.35147377
H	-3.33742015	-2.95039422	0.76361915
H	-2.30081821	-3.42368254	2.14044649
C	4.08043409	-0.11907166	-3.78144584
H	4.50473159	-0.87833586	-3.11731783
H	4.42512141	-0.30731444	-4.80277715
H	4.42881878	0.87306135	-3.48477049
C	1.94762215	-1.96619817	-4.19876436
H	2.47151117	-2.60998954	-3.48747006
H	0.88151412	-2.20090929	-4.19452311
H	2.33431872	-2.14695077	-5.20554285

4C

G_{solv} = -5307.471411

Pd	-0.26404293	-2.14867208	0.83072995
C	-1.41929890	0.68317050	-2.06758347
C	-0.83222656	-0.43193457	-1.53182781
C	-0.51964867	0.74424960	2.05932218
C	-0.26841890	-0.39033222	-0.14838111
C	-0.72863015	0.79242850	0.64642786
C	-1.34405537	1.83411836	0.01060922
C	-0.75631370	-1.66958665	-2.23012640
S	-0.53158405	-3.05213812	-1.28585321
S	-0.27537512	-0.80107071	2.70908929
H	-1.80609382	0.72025058	-3.08015300
H	-1.69165309	2.71914758	0.52149150
C	-1.12961794	4.00291213	-2.37316401
C	-2.21287271	3.00243143	-1.95249025
H	-2.78133306	2.68591419	-2.82700236
H	-2.90330647	3.46116443	-1.24203008
N	-1.64441219	1.80100430	-1.32149973
C	-0.38702367	4.58668197	-1.21664035
N	0.73844436	3.99874238	-0.66811171
C	-0.65697491	5.68483619	-0.45417143
C	1.13693256	4.70087808	0.38511362
N	0.31054286	5.73603532	0.52538040
H	-1.44076699	6.42124540	-0.52696033

H	1.98717525	4.48623437	1.01138457
H	-0.43036461	3.52041701	-3.06252528
H	-1.62777110	4.81193112	-2.91316526
H	0.38381504	6.43350436	1.25603751
C	2.87640803	1.00755069	0.00642668
C	2.56880149	0.98026078	-1.52254587
O	1.82810161	1.90274556	-1.96020602
O	3.09240961	0.06008593	-2.18581464
C	3.50535500	-0.20143257	0.62127176
H	4.54154614	-0.27499230	0.27154964
H	3.49132723	-0.11852791	1.70908622
H	2.99432060	-1.11354269	0.30055024
O	2.62129338	2.01836843	0.64089630
H	1.21115001	3.13391542	-1.03342715
H	0.83104812	-0.37310125	-0.21797930
Br	0.11428299	-4.37060486	2.05483071
P	-0.94007133	-1.74253124	-4.05775543
P	-0.20361757	2.19143999	3.14584672
C	-0.75332578	1.57592695	4.79140415
H	-0.06254067	0.82475684	5.17869881
H	-0.73764142	2.43287761	5.47208712
H	-1.76630847	1.16294574	4.76090124
C	-1.55352344	3.40453249	2.80523019
H	-1.33253836	4.02769614	1.93668153
H	-2.53198505	2.92900852	2.69262122
H	-1.58237065	4.06561786	3.67708109
C	0.60875163	-0.87008003	-4.55999173
H	1.49064444	-1.33775413	-4.11330892
H	0.68687933	-0.92019498	-5.65030137
H	0.56375083	0.18127220	-4.26521677
C	-0.49906489	-3.47971528	-4.45361329
H	0.46298350	-3.77533522	-4.02412942
H	-1.27854941	-4.16665728	-4.11462959
H	-0.43664820	-3.55144922	-5.54414818

$TS_{4C,5C}$

G_{solv} = -5307.422573

Pd	-0.19297788	-2.00852712	0.97012163
C	-1.33567376	0.67176703	-2.09461720
C	-0.88687543	-0.45608832	-1.44765589
C	-0.53832431	0.91232862	2.05311094
C	-0.49691274	-0.36699095	-0.05593928
C	-0.80496561	0.86723005	0.62917141
C	-1.28284841	1.93226879	-0.09913478

C	-0.77195930	-1.75188508	-2.08610822
S	-0.42342464	-3.05140425	-1.08593389
S	-0.19065879	-0.56511747	2.78254756
H	-1.62640970	0.69036723	-3.13790182
H	-1.53120128	2.88875423	0.33489669
C	-0.51933333	3.84460147	-2.51139891
C	-1.80450755	3.07365512	-2.18602046
H	-2.30999738	2.78165866	-3.10580999
H	-2.48877362	3.67717396	-1.58747795
N	-1.50689905	1.84013191	-1.42931333
C	0.09822123	4.51649602	-1.32726357
N	0.96981418	3.91013609	-0.43733277
C	-0.10753830	5.78563378	-0.86951294
C	1.26472719	4.77257220	0.52726475
N	0.63338785	5.92074760	0.28191003
H	-0.70816051	6.58856083	-1.26556733
H	1.91907852	4.58587750	1.36376982
H	0.19857506	3.17279680	-2.99021825
H	-0.78788406	4.61742990	-3.23588742
H	0.69370442	6.74925638	0.86069474
C	2.09334085	0.45048390	-0.28902519
C	2.23441582	0.36819360	-1.83602196
O	2.01971797	1.41776318	-2.49925426
O	2.52601549	-0.75871805	-2.32571836
C	3.05752089	-0.45630774	0.47641243
H	4.08603350	-0.10974979	0.32077172
H	2.83038887	-0.40124806	1.54471953
H	2.98679590	-1.49807772	0.15651312
O	1.95716197	1.66159618	0.22887585
H	1.33819019	2.88165602	-0.37647323
H	1.03526705	-0.14413983	-0.19393474
Br	0.25769683	-4.09849834	2.27933507
P	-1.19055510	-2.00925505	-3.84861226
P	-0.31552896	2.43099344	3.04424924
C	-0.76188509	1.86965120	4.73622566
H	-0.00414621	1.19190291	5.13373969
H	-0.77775904	2.76322622	5.36751356
H	-1.74482614	1.39031085	4.76730195
C	-1.74348472	3.53230408	2.65039899
H	-1.51313070	4.20126976	1.81782797
H	-2.66889697	2.98343424	2.45796151
H	-1.88331286	4.15637174	3.53846089
C	0.11366856	-1.04727804	-4.73317306
H	1.11319098	-1.39762005	-4.46581908

H	-0.05454909	-1.20517257	-5.80269019
H	0.03716421	0.02260805	-4.53067577
C	-0.63461199	-3.72657161	-4.17023881
H	0.40581539	-3.88966033	-3.87326924
H	-1.28238895	-4.44910750	-3.66852959
H	-0.72370682	-3.88454246	-5.24952940

D

G_{solv} = -2149.446244

Ni	-0.32178720	-2.45310401	0.09785505
C	2.00965836	0.93766467	-0.70546117
C	1.59261466	-0.34919343	-0.34526613
C	-2.07543845	-0.18932159	-0.84583186
C	0.23834445	-0.72607002	-0.39219914
C	-0.67575885	0.24973979	-0.82698280
C	-0.25821230	1.53304033	-1.20047454
C	2.50565308	-1.40519059	0.10661351
S	1.80548090	-2.91447080	0.49938023
S	-2.38661715	-1.79755078	-0.35630275
H	3.05666294	1.22703412	-0.65619695
H	-0.96828100	2.28303518	-1.53948881
N	3.80365249	-1.21051450	0.20732802
Cl	-0.99397612	-4.52764949	0.68552085
N	-3.05486347	0.60933847	-1.21388922
C	1.61442273	4.17857454	-0.18852357
C	1.53091437	3.29803100	-1.45466476
H	2.51467989	3.27932152	-1.93442426
H	0.82895570	3.75318814	-2.16078773
C	0.31565183	4.26163561	0.55403056
N	0.13026923	3.66228724	1.78686437
C	-0.85662951	4.84710095	0.14754064
C	-1.13169152	3.88845914	2.10632248
N	-1.76625707	4.59956492	1.14840896
H	-1.11924065	5.39808627	-0.74250247
H	-1.62484171	3.56595099	3.01136971
H	2.37557881	3.77172985	0.48510123
H	1.94766342	5.17792500	-0.48767755
H	-2.73303047	4.89323085	1.16908573
H	4.41923492	-1.95146989	0.51964309
H	4.23202861	-0.32298392	-0.02529241
H	-4.01453917	0.28615855	-1.21591916
H	-2.88939523	1.56539385	-1.50204359
C	1.08892636	1.89185719	-1.13925108

$TS_{1D,2D}$

G_{solv} = -2492.415415

Ni	-0.49757478	-2.44803638	0.28969511
C	-0.64276862	0.73260070	-2.45680651
C	-0.37959232	-0.51218898	-1.87500291
C	-1.51864036	0.08356573	1.62533463
C	-0.43937378	-0.68951220	-0.42504796
C	-1.17024068	0.37517768	0.26693913
C	-1.46039596	1.57678781	-0.36866604
C	-0.02513673	-1.68348043	-2.61255998
S	0.00494798	-3.16916291	-1.74067718
S	-1.33876778	-1.54946049	2.13116493
H	-0.50241709	0.87855354	-3.52674363
H	-1.97497975	2.37135411	0.17027503
N	0.26471148	-1.67135679	-3.91591893
C	0.00185293	4.04186833	-1.94757433
C	-1.24002796	3.18628137	-2.30423131
H	-1.31268602	3.13053159	-3.39502948
H	-2.13358936	3.70386568	-1.93709590
C	0.12880616	4.26559666	-0.47600316
N	0.79048292	3.40126619	0.37974246
C	-0.43792425	5.22490258	0.31101331
C	0.62000887	3.80457730	1.63239953
N	-0.11604501	4.91516952	1.61479260
H	-1.03951511	6.08245046	0.05677357
H	1.01062703	3.31908732	2.51114702
H	0.90525193	3.55117529	-2.32301702
H	-0.07767709	5.01569951	-2.43874844
H	-0.38397289	5.44314960	2.43600578
C	2.07768674	0.04076652	0.06476788
H	0.77651182	-0.57157059	-0.02211408
C	2.08589800	-0.00979161	1.61383704
O	1.65596285	1.01352130	2.21006330
O	2.52492134	-1.05693544	2.16544639
H	0.48951725	-2.52741722	-4.40237343
H	0.31516955	-0.80838750	-4.43917377
C	2.84663781	-1.03454535	-0.67200325
H	2.70003760	-2.02400513	-0.23938262
H	2.53794737	-1.04747743	-1.72176500
H	3.91424510	-0.78430124	-0.63680562
O	2.02904480	1.20116605	-0.49102391
H	1.27981759	2.49750032	0.11040807
Cl	-0.32067511	-4.52984113	1.22459459
C	-1.14237238	1.80384688	-1.71596056

N	-1.96374265	1.00742191	2.47859106
H	-2.18108243	0.76075563	3.43392931
H	-1.93230180	1.99108926	2.24738551

E

G_{solv} = -2122.909062

Pd	2.17892770	-0.26605645	0.04286300
C	-1.27920849	2.05037709	-0.70008896
C	0.00663782	1.67179894	-0.36693968
C	-0.18843667	-2.02646650	-0.91675684
C	0.38700407	0.31215346	-0.43568252
C	-0.59238346	-0.60851187	-0.86715240
C	-1.85873244	-0.16886988	-1.20209221
C	1.04186562	2.62121781	0.08686817
S	2.57689906	1.98258049	0.47292736
S	1.41717001	-2.40057765	-0.47567018
H	-1.65069838	3.06729402	-0.65731009
H	-2.65592172	-0.81512505	-1.54960699
N	0.80330267	3.90761843	0.19779240
Cl	4.38945907	-0.97985014	0.63438381
N	-1.02161061	-2.97421071	-1.27922216
C	-4.32971496	1.49807395	0.04742892
C	-3.59111268	1.54642163	-1.29789612
H	-3.59484535	2.55102089	-1.72011981
H	-4.03476313	0.85923142	-2.01822443
N	-2.17739253	1.13825592	-1.12039960
C	-4.15259963	0.18604775	0.74365800
N	-3.18801454	0.00282674	1.71838430
C	-4.77062621	-1.00785964	0.47342180
C	-3.23078062	-1.28195827	2.01869829
N	-4.17225124	-1.92990830	1.29540569
H	-5.55443253	-1.27435381	-0.21889118
H	-2.61430230	-1.78349010	2.75014421
H	-3.96712029	2.30644476	0.68897538
H	-5.38465034	1.69002631	-0.16733996
H	-4.39471439	-2.91420131	1.35370868
H	1.52964022	4.54115077	0.51301151
H	-0.09335197	4.32453299	-0.02109004
H	-0.71916396	-3.94171601	-1.30503914
H	-1.98196972	-2.79343274	-1.54507874

$TS_{1E,2E}$

G_{solv} = -2465.902409

Pd	0.24874954	-2.34558948	0.52032513

C	-2.37015012	0.96477032	0.73963535
C	-1.85807653	-0.26157795	0.42136553
C	1.75307916	0.27442775	1.31666248
C	-0.43005035	-0.49689423	0.47137523
C	0.33713005	0.55116230	1.10672396
C	-0.25598230	1.73343125	1.45557704
C	-2.67556916	-1.38591690	-0.02682084
S	-1.93761084	-2.92780470	-0.06457169
S	2.25683671	-1.35651106	1.19682535
H	-3.42200482	1.21709613	0.66891113
H	0.26811610	2.54579875	1.94740994
N	-3.93277831	-1.23198280	-0.39312150
C	-1.81283967	4.12320916	0.05687096
C	-2.10374651	3.32478216	1.33580714
H	-3.17914194	3.25426460	1.49808402
H	-1.64990848	3.79844813	2.20798968
N	-1.57593705	1.95312773	1.23431868
C	-0.37879174	4.51835513	-0.08750048
N	0.61107066	3.72061615	-0.63698290
C	0.23295905	5.66048484	0.34121127
C	1.77577044	4.34675916	-0.52794056
N	1.57225457	5.52802194	0.05585454
H	-0.16969435	6.53886204	0.81916331
H	2.72971403	3.96868232	-0.86008042
H	-2.14656354	3.55317306	-0.81558549
H	-2.41166942	5.03622609	0.10389227
H	2.29424318	6.21102666	0.24967351
C	0.29473286	0.38002976	-1.91193077
H	-0.03824428	-0.29578538	-0.91421745
C	1.02713068	-0.76111457	-2.67914404
O	2.28166563	-0.69054811	-2.77272348
O	0.30888407	-1.68793616	-3.14917816
H	-4.48466942	-2.02779647	-0.68879104
H	-4.37891440	-0.32416125	-0.43028738
C	-1.05738843	0.76196839	-2.50073881
H	-1.72768056	-0.09723035	-2.58507970
H	-1.53324235	1.52357448	-1.87505100
H	-0.90978985	1.18602579	-3.50052590
O	1.05454460	1.37293984	-1.50006434
H	0.58437678	2.69635594	-1.02729428
N	2.61746600	1.23431313	1.58486698
H	3.59629695	1.01971701	1.72857233
H	2.36167815	2.21328817	1.54021131
Cl	1.09367502	-4.60935143	0.54566159

A1

G_{solv} = -2322.984061

Ni	2.19566496	-1.06541651	0.13735866
C	-0.34212551	2.10395459	-0.67013616
C	0.78722457	1.37518882	-0.34523892
C	-0.50057547	-2.12097584	-0.62979368
C	0.72380165	-0.03565137	-0.31787085
C	-0.50124255	-0.64057787	-0.66137520
C	-1.55838998	0.13644277	-1.09958663
C	2.08787524	1.94538172	0.08395741
S	3.16330200	0.79926653	0.79120779
S	1.06644752	-2.83101851	-0.56763188
H	-0.41940573	3.18018822	-0.61501718
H	-2.48501365	-0.25482945	-1.49591427
N	2.44912620	3.20343245	-0.06265291
Cl	3.98524666	-2.30378751	0.68920696
N	-1.59069205	-2.85873624	-0.61543807
C	-3.45112779	2.65410497	-0.15908788
C	-2.65488501	2.29583252	-1.41524900
H	-2.30259246	3.19352824	-1.92374815
H	-3.25793569	1.71350847	-2.11205960
N	-1.46346897	1.47975350	-1.08385794
C	-3.96700512	1.46692047	0.59366813
N	-3.38078043	1.01934433	1.76322722
C	-5.03650267	0.66772513	0.27732134
C	-4.09546940	-0.02613588	2.13865633
N	-5.10926148	-0.26966813	1.27727635
H	-5.73951863	0.69377743	-0.54125124
H	-3.92404103	-0.62874449	3.01831415
H	-2.82953640	3.26575336	0.50177364
H	-4.28304504	3.28042744	-0.49490359
H	-5.78348636	-1.01965626	1.34821300
C	1.77428890	4.18250389	-0.92334931
H	1.28739228	3.68851581	-1.76266078
H	1.05972579	4.77646068	-0.34833941
H	2.54053348	4.84502606	-1.32496917
C	3.69293033	3.68527446	0.54731522
H	3.80630003	3.27746108	1.55182984
H	4.55304678	3.39937989	-0.06563619
H	3.63978950	4.77110350	0.61011546
C	-2.92928565	-2.35748226	-0.27652849
H	-2.85428875	-1.45028810	0.31881306
H	-3.52518563	-2.18886479	-1.17636258
H	-3.41577868	-3.11987984	0.33279983

C	-1.50178717	-4.31573888	-0.74046966
H	-0.76074959	-4.58810750	-1.49158816
H	-1.23390974	-4.76323039	0.22139018
H	-2.47691396	-4.68693255	-1.05385241

$TS_{1A1,2A1}$

G_{solv} = -2665.982353

Ni	-0.46501344	-2.42428341	0.70941001
C	-1.26973856	0.51893353	-2.04472072
C	-0.72553273	-0.60794492	-1.50123725
C	-0.96501952	0.20274482	2.16522581
C	-0.53025945	-0.71311677	-0.06876998
C	-1.01934409	0.40364541	0.71068120
C	-1.55669944	1.50034297	0.08910564
C	-0.38286059	-1.81490129	-2.26572991
S	-0.31874991	-3.25566860	-1.32622917
S	-0.80849549	-1.44523900	2.64691771
H	-1.48638989	0.64344685	-3.09732706
H	-1.97817075	2.34934356	0.61000903
N	-0.12445658	-1.83471765	-3.56268355
C	-0.73321528	3.60108653	-2.32741712
C	-1.99733004	2.83237094	-1.92248302
H	-2.58337664	2.59664391	-2.81179620
H	-2.61788227	3.41901342	-1.24398236
N	-1.66032506	1.56255314	-1.26097644
C	-0.01273334	4.26363285	-1.19884643
N	0.85683537	3.63687667	-0.32023276
C	-0.06171049	5.57560839	-0.82684955
C	1.30160325	4.53161689	0.55434411
N	0.76265754	5.71453162	0.26615846
H	-0.60097243	6.40733956	-1.25041014
H	1.98369085	4.33349208	1.36593200
H	-0.05712076	2.93306281	-2.87128401
H	-1.04074103	4.38533392	-3.02379331
H	0.95166153	6.57298492	0.76886543
C	1.92899495	0.19708782	0.09096536
H	0.89868929	-0.51332076	0.07269739
C	2.77723342	-0.73754377	1.00117658
O	3.00613405	-0.35554909	2.18089147
O	3.16884043	-1.82959197	0.49837132
C	2.34205539	0.19941021	-1.37448782
H	2.32908859	-0.79899996	-1.81880949
H	1.66295142	0.84907446	-1.93541437
H	3.35532739	0.60695226	-1.46595325

O	1.62589379	1.37467091	0.59721385
H	1.11942843	2.59366693	-0.17027934
N	-1.01895872	1.16338411	3.07309259
Cl	-0.28584614	-4.46470645	1.66066065
C	0.21191068	-0.65619584	-4.36894537
H	-0.64543433	-0.32964985	-4.96300052
H	0.56800936	0.15735646	-3.74096782
H	1.01877595	-0.94327639	-5.04459608
C	0.04541324	-3.10698279	-4.26586660
H	1.05913227	-3.49355012	-4.12015819
H	-0.67847114	-3.83914454	-3.90829890
H	-0.12511882	-2.93258694	-5.32803172
C	-0.84496060	2.59033853	2.78928410
H	-0.26558759	2.72452084	1.88040025
H	-1.81108672	3.09582993	2.70919970
H	-0.28389076	3.02725594	3.61594127
C	-1.10488926	0.83084223	4.49717597
H	-1.80513351	0.01016257	4.65560786
H	-0.12077303	0.54922451	4.88482025
H	-1.46563756	1.70980201	5.02995021

A2

G_{solv} = -1805.537126

Ni	0.54384700	2.49059543	0.15229765
C	-2.03296071	-0.64286681	-0.70978086
C	-1.53850230	0.58925751	-0.32920166
C	2.11937333	0.10697519	-0.81325397
C	-0.15434629	0.85059003	-0.36500056
C	0.67509128	-0.19439818	-0.81171932
C	0.13691955	-1.40593949	-1.19851882
C	-2.37166989	1.71189766	0.14607839
S	-1.53810391	3.13841836	0.56067764
S	2.55693159	1.67197010	-0.30469850
H	-3.08044949	-0.92103030	-0.69426565
H	0.71771925	-2.24507232	-1.56304103
N	-3.67684817	1.61936394	0.24787567
N	3.01454676	-0.78050765	-1.17862402
C	-1.77295587	-3.76475622	-0.08067479
C	-1.72839694	-2.96711436	-1.39185145
H	-2.72138408	-2.86140156	-1.82821852
H	-1.07181572	-3.44193005	-2.12091960
N	-1.19645695	-1.60591285	-1.14854919
C	-0.46146524	-3.74639872	0.63847581
N	-0.20208968	-2.85002704	1.65990844

C	0.67177087	-4.46364295	0.35273941
C	1.06794405	-3.03009388	1.97194559
N	1.63411684	-3.99512718	1.21206054
H	0.87291108	-5.23660873	-0.37304627
H	1.61469823	-2.49948227	2.73750284
H	-2.55324050	-3.35438967	0.56683071
H	-2.06163533	-4.78596534	-0.34478030
H	2.59154303	-4.31384289	1.27089455
H	-4.22576455	2.40498470	0.57836738
H	-4.18776736	0.77779324	0.01047191
H	4.00201189	-0.55137066	-1.16892224
H	2.76544507	-1.71530859	-1.47910944
F	1.23678631	4.11835042	0.67156760

$TS_{1A2,2A2}$

G_{solv} = -2148.532304

Ni	-0.65754030	-2.58587778	0.38743049
C	-0.62666040	0.50113911	-2.37811538
C	-0.38764053	-0.70070305	-1.77649254
C	-1.56672267	-0.00165766	1.70284581
C	-0.54502574	-0.86222623	-0.34557653
C	-1.21593153	0.23968491	0.30829139
C	-1.46818277	1.40590298	-0.36074001
C	0.06237765	-1.89809093	-2.48056089
S	0.00666157	-3.35467307	-1.59387726
S	-1.46462215	-1.62487736	2.22547524
H	-0.48239867	0.69501997	-3.43512866
H	-1.96731909	2.26239462	0.07944022
N	0.49369927	-1.86603418	-3.72647397
C	0.14680338	3.64710646	-1.98220968
C	-1.15330486	2.88741013	-2.28034547
H	-1.27263482	2.75941306	-3.35632979
H	-2.02149234	3.42613006	-1.89660368
N	-1.13812116	1.54843798	-1.67053492
C	0.24304975	4.14367366	-0.57653575
N	0.67440966	3.39183613	0.50376076
C	-0.11785288	5.36369517	-0.08320722
C	0.56583569	4.12238640	1.60610524
N	0.09159475	5.32348742	1.27602014
H	-0.49945348	6.24011575	-0.58151867
H	0.82139790	3.80261856	2.60387700
H	1.00551260	3.01458060	-2.22805522
H	0.17530012	4.51463116	-2.64637117
H	-0.07461842	6.08016517	1.92813532

C	1.78858407	-0.02620901	0.52126505
H	0.77620536	-0.70216968	0.14803030
C	2.45205858	-1.14151241	1.38517931
O	2.44999324	-0.98911928	2.63588049
O	2.94973024	-2.12547186	0.76927798
H	0.79078387	-2.71453767	-4.19190268
H	0.57596019	-1.00225870	-4.24719171
C	2.48954424	0.23753157	-0.80463634
H	2.58269646	-0.66727477	-1.41070860
H	1.93710979	0.99137505	-1.37400889
H	3.49500654	0.62713666	-0.60828432
O	1.35945482	1.02663129	1.17656839
H	0.99185231	2.35089022	0.57547710
N	-1.93666518	0.96327404	2.52415487
H	-2.16663917	0.75646359	3.48814809
H	-1.89359706	1.94023506	2.26168266
F	-0.71162380	-4.29218462	1.13375406

A3

G_{solv} = -1706.248229

Ni	-0.78285925	-2.63180462	0.25999726
C	2.00217311	0.31663336	-0.72135313
C	1.42871837	-0.86973402	-0.30898204
C	-2.19271601	-0.16900899	-0.74270920
C	0.03150534	-1.03289902	-0.31942257
C	-0.73349790	0.05287921	-0.77622902
C	-0.12410446	1.21702660	-1.19828818
C	2.17183158	-2.04975118	0.18032537
S	1.22984015	-3.40007540	0.65451403
S	-2.71661654	-1.70203132	-0.18826601
H	3.06592441	0.52627338	-0.72427914
H	-0.65165633	2.08671154	-1.57269432
N	3.48225289	-2.06797962	0.25205408
N	-3.04262248	0.76103401	-1.11091094
C	1.96172122	3.46490792	-0.16178050
C	1.84118664	2.64090750	-1.45165346
H	2.81780256	2.45938808	-1.90008379
H	1.20728299	3.14356070	-2.18226032
N	1.22270272	1.32514712	-1.17006941
C	0.66400782	3.55512937	0.57678918
N	0.36131470	2.70698568	1.62700506
C	-0.42256694	4.33989853	0.28735190
C	-0.88832673	2.98163202	1.95222482
N	-1.40027010	3.96192769	1.17366605

H	-0.58296891	5.10448950	-0.45722018
H	-1.45699748	2.51086338	2.74060922
H	2.72208769	3.01727761	0.48476119
H	2.31588455	4.45722588	-0.45498624
H	-2.33270924	4.34681918	1.23759897
H	3.96943703	-2.88977800	0.59097963
H	4.05624305	-1.28010916	-0.02258965
H	-4.04135268	0.59111008	-1.07734860
H	-2.74290528	1.67264350	-1.43598433
H	-1.44082740	-3.91777081	0.73375303

$TS_{1A3,2A3}$

G_{solv} = -2049.241070

Ni	-0.79296076	-2.66687698	0.61176281
C	-0.57315695	0.21993528	-2.39061160
C	-0.39911112	-0.94455434	-1.69837274
C	-1.58080539	0.04880004	1.70377723
C	-0.56392382	-0.98481518	-0.25966997
C	-1.19735247	0.18661572	0.30442707
C	-1.40053620	1.30630920	-0.45085060
C	-0.03216956	-2.22746991	-2.29151836
S	-0.17575466	-3.60264880	-1.27462172
S	-1.57352967	-1.54872681	2.33279380
H	-0.41672169	0.33343809	-3.45771204
H	-1.88412065	2.20701441	-0.08758619
N	0.39073206	-2.34405572	-3.53611474
C	0.31040160	3.39693510	-2.11412918
C	-0.98080328	2.63781520	-2.45363987
H	-1.02948217	2.44691540	-3.52579471
H	-1.86006674	3.21680677	-2.16447883
N	-1.03831059	1.34030717	-1.76290126
C	0.33420546	3.94008607	-0.72174872
N	0.73919407	3.23268133	0.39811417
C	-0.09122493	5.15896670	-0.27943077
C	0.54707223	3.98456404	1.47416155
N	0.05137619	5.16067776	1.08911842
H	-0.47890543	6.00817973	-0.81854744
H	0.76150499	3.69794224	2.49158002
H	1.17481633	2.75040677	-2.29180230
H	0.38090153	4.23999767	-2.80620713
H	-0.17510852	5.92617843	1.71200400
C	1.78879934	-0.18868294	0.55658976
H	0.73735388	-0.85342258	0.22217264
C	2.41999185	-1.29857304	1.44913567

O	2.38235506	-1.13295931	2.69773127
O	2.93013709	-2.29143821	0.85739367
H	0.62141263	-3.25267185	-3.91845739
H	0.52372565	-1.54315121	-4.13981147
C	2.47863755	0.00599093	-0.78530425
H	2.52408159	-0.91746545	-1.36770984
H	1.94957559	0.76719032	-1.36602144
H	3.50307110	0.35644933	-0.61460798
O	1.40367255	0.89807933	1.18101535
H	1.06108978	2.19647093	0.51882356
N	-1.91064081	1.08186999	2.45768807
H	-2.16454446	0.94856052	3.42845470
H	-1.81350364	2.03650982	2.13327494
H	-0.93954885	-4.01213958	1.32496879

A4

G_{solv} = -2244.452391

Ni	1.82743710	-0.00034591	1.12321310
C	-0.82906755	-0.63162256	-1.97782328
C	0.36306709	-0.46742695	-1.29546339
C	-0.71825759	-1.21013750	2.18990817
C	0.38602572	-0.59210607	0.10903484
C	-0.78119238	-1.08149913	0.72391686
C	-1.92150505	-1.32441692	-0.01562660
C	1.62589626	0.01816657	-1.89713549
S	2.74267919	0.67721334	-0.76323835
S	0.73648115	-0.70734936	2.91856592
H	-0.97299272	-0.38855956	-3.02252570
H	-2.85425778	-1.69244092	0.39303967
N	1.91448791	-0.05198151	-3.17864207
Cl	3.55067549	0.74856039	2.34242047
N	-1.72745869	-1.67186770	2.89112683
C	-3.74756847	0.49843844	-1.95364778
C	-3.24421072	-0.95557948	-2.02343767
H	-3.11437680	-1.28709108	-3.05375880
H	-3.92739045	-1.63570992	-1.51531340
N	-1.93611039	-1.05990979	-1.33731160
C	-3.59792383	1.07829752	-0.58221972
N	-2.50140570	1.85161649	-0.24705264
C	-4.35387549	0.83710223	0.53738110
C	-2.59956074	2.05876776	1.05270078
N	-3.70472026	1.47230887	1.56700125
H	-5.26264335	0.27470717	0.68715967
H	-1.91250321	2.63185128	1.65804997

H	-3.18404218	1.10920434	-2.66468480
H	-4.79293514	0.48952735	-2.27365302
H	-3.99565389	1.50170766	2.53474784
C	1.20146716	-0.88147201	-4.15727400
H	0.68755494	-1.70731471	-3.66944126
H	0.50138502	-0.27778530	-4.73966512
H	1.94945343	-1.30178641	-4.83014800
C	3.11657612	0.60073549	-3.70332823
H	3.25113234	1.57784968	-3.23951003
H	3.99717000	-0.02133568	-3.51709123
H	2.98695411	0.73245307	-4.77693245
H	-1.66786811	-1.73794835	3.90105326
H	-2.59804683	-1.96564227	2.46455172

$TS_{1A4,2A4}$

G_{solv} = -2587.446919

Ni	-0.64882464	-2.21157133	0.89851118
C	-1.03523732	0.62205826	-2.08933827
C	-0.64287740	-0.51635471	-1.44554728
C	-1.19429045	0.50907020	2.11731843
C	-0.59347379	-0.56126551	0.00115123
C	-1.12615765	0.60368268	0.66609283
C	-1.51807467	1.70542987	-0.04277408
C	-0.30019714	-1.78547296	-2.09981349
S	-0.45075545	-3.16794571	-1.08046942
S	-1.00685297	-1.05870121	2.76692731
H	-1.10902067	0.71831186	-3.16414670
H	-1.93400404	2.59971304	0.40960066
N	0.11646577	-1.89718374	-3.34830203
C	-0.21781856	3.77455284	-2.04566379
C	-1.55002065	3.01140981	-2.10131087
H	-1.81893557	2.80189042	-3.13671356
H	-2.35480932	3.58837039	-1.64242156
N	-1.44383010	1.72490568	-1.39508711
C	0.09258708	4.33819324	-0.69566918
N	0.71875238	3.64892002	0.33095687
C	-0.23186015	5.56708440	-0.19821386
C	0.75493203	4.42323267	1.40757068
N	0.18993237	5.59336753	1.11107102
H	-0.72166541	6.40778814	-0.66231391
H	1.17778943	4.15543231	2.36271747
H	0.59142288	3.12127522	-2.38668918
H	-0.29065168	4.60719016	-2.74992344
H	0.10255357	6.37194672	1.75267259

C	1.86530524	0.25389923	0.42259204
H	0.80757428	-0.41287148	0.27139005
C	2.64924145	-0.82624487	1.22337045
O	2.92904964	-0.57827626	2.42651041
O	2.94812409	-1.88924641	0.60827025
C	2.34348337	0.43174807	-1.01216246
H	2.34440824	-0.50757005	-1.57067830
H	1.69921860	1.15283696	-1.52594492
H	3.36373230	0.83204079	-1.00404206
O	1.56893172	1.36011428	1.07079563
H	1.07276414	2.61908546	0.41552242
N	-1.38322138	1.56581488	2.88550394
Cl	-0.60149719	-4.18908042	1.97977144
C	0.62548489	-0.78279386	-4.15589100
H	-0.13054889	-0.43408153	-4.86406028
H	0.95527826	0.03662216	-3.52049935
H	1.48772946	-1.15094432	-4.71344697
C	0.29568527	-3.21564081	-3.95816593
H	1.25459650	-3.64853941	-3.65625712
H	-0.51464377	-3.88390328	-3.66706876
H	0.27956983	-3.09340964	-5.04093006
H	-1.42445409	1.47071217	3.89230943
H	-1.37943341	2.50578419	2.50828807

A5

G_{solv} = -2706.286050

Ni	0.14911358	0.14415180	1.80494180
C	1.12782092	-1.66378006	-1.79983692
C	1.19450435	-1.18047213	-0.50804205
C	-2.19397023	0.30447163	-0.09125484
C	0.08716927	-0.53161839	0.07261454
C	-1.06889836	-0.41708621	-0.72044866
C	-1.09710663	-0.93436150	-2.00076231
C	2.38960401	-1.27168676	0.35680412
S	2.23217259	-0.58320484	1.90926567
S	-1.93850719	0.81232488	1.51636690
H	1.94098006	-2.15523025	-2.32075613
H	-1.95441933	-0.89445488	-2.66145921
N	3.49522382	-1.85134390	-0.05214087
Cl	0.22597721	0.96194624	3.88711577
N	-3.30428919	0.55437209	-0.74683327
C	0.52157168	-0.72031907	-4.78320028
C	-0.00010667	-1.90157761	-3.95079201
H	0.62956687	-2.78277939	-4.07118542

H	-1.02311626	-2.15828456	-4.22575850
N	-0.01055996	-1.54745498	-2.51246818
C	-0.19076690	0.55619703	-4.46453622
N	0.32815737	1.47475839	-3.56948484
C	-1.44326684	0.95145566	-4.85933874
C	-0.60537342	2.39782977	-3.43087371
N	-1.68973600	2.12542652	-4.19207125
H	-2.16354773	0.50554542	-5.52798716
H	-0.54071017	3.27696685	-2.80675737
H	1.59333525	-0.59681567	-4.60261414
H	0.38938910	-0.99348303	-5.83380976
H	-2.52723664	2.68754621	-4.25795500
H	-3.41449582	0.20202495	-1.69074758
H	3.54943182	-2.20673043	-0.99973269
C	4.73952281	-1.91603526	0.71562304
H	4.51033236	-2.25348266	1.72953093
H	5.34718249	-2.68647105	0.23790972
C	5.48124804	-0.59586109	0.74746349
C	5.96064352	-0.09310168	1.95799193
C	5.71844481	0.11672212	-0.43202706
C	6.67195860	1.10658813	1.99237430
H	5.77076629	-0.63860243	2.87864796
C	6.42082045	1.31961440	-0.39787447
H	5.35519625	-0.26798386	-1.38156535
C	6.90051517	1.81711488	0.81491262
H	7.03776490	1.48898756	2.94049144
H	6.59754880	1.86686433	-1.31889503
H	7.44856443	2.75399905	0.84088208
C	-4.47220733	1.23807381	-0.19056310
H	-5.06689463	1.55976142	-1.04742082
H	-4.13509039	2.13431138	0.33666267
C	-5.29429674	0.35595062	0.72542190
C	-5.68523721	0.82328430	1.98111070
C	-5.69517785	-0.91894056	0.31382725
C	-6.47001181	0.02901869	2.81759331
H	-5.36949400	1.81014662	2.30881050
C	-6.47122483	-1.71677945	1.15186193
H	-5.40045235	-1.29206778	-0.66365053
C	-6.86159108	-1.24394786	2.40591142
H	-6.76710851	0.40255613	3.79283142
H	-6.77506143	-2.70635885	0.82420537
H	-7.46696913	-1.86604946	3.05809084

$TS_{1A5,2A5}$

G_{solv} = -3049.278611

Ni	1.98965727	-0.27761699	-0.32316355
C	-1.72706015	-2.02757226	-0.86556348
C	-0.50470343	-1.48067143	-1.13068033
C	0.27646599	0.12703204	2.15419381
C	0.14931181	-0.61805116	-0.17145359
C	-0.47386968	-0.59481757	1.13181169
C	-1.66773795	-1.22012428	1.35581687
C	0.23029653	-1.66022342	-2.38185977
S	1.86456147	-1.16551541	-2.35301186
S	1.91436824	0.43835288	1.77784077
H	-2.28683375	-2.63793074	-1.56530968
H	-2.15508516	-1.26300124	2.32422182
N	-0.34461671	-2.16558233	-3.45771979
C	-4.66490763	-1.11670294	0.26583204
C	-3.71180629	-2.28936193	0.53854987
H	-3.91391067	-3.10411677	-0.15658557
H	-3.83209940	-2.66383544	1.55648417
N	-2.30794995	-1.88666142	0.35916673
C	-4.62440361	-0.06515203	1.32653109
N	-3.70872743	0.97216474	1.36614101
C	-5.37616438	0.03642044	2.46099933
C	-3.88453191	1.66128355	2.48609908
N	-4.89427772	1.11713000	3.16404791
H	-6.19667918	-0.56393969	2.81928523
H	-3.31350001	2.52273736	2.79414931
H	-4.44066698	-0.68377749	-0.71391489
H	-5.67858356	-1.52298761	0.22533301
H	-5.24889404	1.46345151	4.04723365
C	-0.89099757	1.70825046	-0.83058162
H	-0.14661545	0.68831970	-0.64947036
C	0.25569040	2.73562720	-1.08254883
O	0.49788067	3.57378261	-0.17304559
O	0.86929876	2.65702244	-2.18380203
C	-1.65839631	1.31210970	-2.08392560
H	-0.99715570	0.95772417	-2.87819143
H	-2.38566399	0.52991422	-1.84559237
H	-2.20582919	2.18437415	-2.45952083
O	-1.59926124	1.89654329	0.25716634
H	-2.88094039	1.21546113	0.71223905
N	-0.29068748	0.53274538	3.27522403
Cl	4.17353057	0.22873471	-0.54892233
H	-1.28442802	0.37555640	3.39969483
H	-1.33988209	-2.35364152	-3.42767439

C	0.27519027	-2.23898662	-4.77855941
H	-0.32728052	-2.93900084	-5.36069559
H	1.27598251	-2.66566946	-4.68079958
C	0.33481921	-0.88936277	-5.46579769
C	1.51690879	-0.45998362	-6.07101731
C	-0.79519495	-0.06702852	-5.51413800
C	1.57236693	0.77549703	-6.71660984
H	2.40141128	-1.09008775	-6.02704432
C	-0.73895156	1.17145525	-6.14963663
H	-1.72248260	-0.38858693	-5.04668844
C	0.44569364	1.59575688	-6.75348251
H	2.49917633	1.10072872	-7.17942862
H	-1.62024998	1.80540881	-6.17341164
H	0.49002886	2.56175468	-7.24724396
C	0.40627630	1.20107004	4.36531155
H	-0.36786790	1.59843141	5.02513142
H	0.96175462	2.05374903	3.96289701
C	1.33921224	0.29535411	5.14434034
C	2.46141848	0.85126171	5.76340915
C	1.08666606	-1.07073403	5.28928684
C	3.31637804	0.05550267	6.52434417
H	2.66998155	1.91130819	5.64258211
C	1.94497403	-1.86914178	6.04491045
H	0.22349353	-1.51885403	4.80438664
C	3.06082408	-1.30862320	6.66638072
H	4.18663244	0.49990954	6.99801079
H	1.74136820	-2.93088468	6.14718146
H	3.72938583	-1.93099115	7.25339413

A6

G_{solv} = -2436.102235

Ni	0.08325910	-2.33197622	-0.04389795
C	-0.67120997	1.43153538	-1.62268597
C	-0.02720378	0.27840851	-1.21836408
C	-2.88990784	-1.80858376	-0.08548476
C	-0.75883338	-0.80414329	-0.69204608
C	-2.15779950	-0.66482359	-0.65758724
C	-2.76300209	0.49335073	-1.10482278
C	1.43770348	0.08651625	-1.24458909
S	2.00376067	-1.36798383	-0.55567039
S	-1.93240251	-3.12245439	0.42476708
H	-0.17414594	2.32548122	-1.98386532
H	-3.83231654	0.66390089	-1.11123153
N	2.23821393	0.97903245	-1.77967327

Cl	1.09935235	-4.16610259	0.73616761
N	-4.19666810	-1.81102945	0.03327557
C	-2.61264820	3.67687633	-0.53499030
C	-2.66978387	2.82082313	-1.80966004
H	-2.15774577	3.30480666	-2.64140627
H	-3.69940186	2.61307773	-2.09966550
N	-2.01636979	1.51384703	-1.57118585
C	-3.08803975	2.92809528	0.67027189
N	-2.20072652	2.31752470	1.53861357
C	-4.37527889	2.61930535	1.03029618
C	-2.95048108	1.65417826	2.39893942
N	-4.26748433	1.80717300	2.13201694
H	-5.32878523	2.89160218	0.60446391
H	-2.59220937	1.06172377	3.22801065
H	-1.58466976	4.01303873	-0.37152913
H	-3.22753937	4.56158708	-0.72202310
H	-5.02980879	1.40359153	2.65934883
H	-4.77484791	-1.03300486	-0.26055917
H	1.84090714	1.82652466	-2.16836022
C	3.70093268	0.92446061	-1.74746151
H	4.02427491	-0.08086497	-2.02782210
H	4.04561932	1.61376023	-2.51987861
C	4.25873614	1.31568172	-0.39520557
C	5.17086708	0.48827728	0.26109219
C	3.87574877	2.52213619	0.19995354
C	5.69692709	0.86105696	1.49881628
H	5.46628382	-0.45368004	-0.19319840
C	4.39425668	2.89172727	1.43858964
H	3.16838624	3.17422911	-0.30656663
C	5.30693309	2.06089622	2.09144153
H	6.40389059	0.20865506	2.00225846
H	4.08890060	3.82938749	1.89305325
H	5.71051348	2.34847230	3.05751724
H	-4.67553722	-2.60668206	0.43985163

$TS_{1A6,2A6}$

G_{solv} = -2779.096160

Ni	0.78127564	-2.17155672	-0.59069586
C	-0.72162682	1.49522166	-1.83410936
C	0.14182451	0.51865182	-1.42885439
C	-2.25644761	-2.18295807	-0.47096727
C	-0.34845006	-0.68443676	-0.78969973
C	-1.77603282	-0.88042639	-0.90777145
C	-2.58541545	0.11301272	-1.38597781

C	1.59829817	0.60118312	-1.53506383
S	2.44944189	-0.83078571	-1.16315045
S	-1.05107721	-3.36587976	-0.21376141
H	-0.41738889	2.45141422	-2.24489867
H	-3.65905316	0.01557036	-1.50160340
N	2.20981663	1.71200342	-1.90294200
C	-3.36589575	3.09764558	-0.67098592
C	-2.97280238	2.44369730	-2.00357545
H	-2.44954112	3.16431559	-2.63184968
H	-3.85393460	2.08833042	-2.54078130
N	-2.07050467	1.30106370	-1.79076259
C	-4.30921159	2.27266894	0.14381342
N	-3.92680020	1.28558794	1.03713700
C	-5.67368905	2.27084355	0.12228586
C	-5.01402202	0.70087386	1.52357040
N	-6.08600252	1.28384627	0.98758579
H	-6.37044464	2.88138247	-0.42888946
H	-5.03140147	-0.10854184	2.23611475
H	-2.46417292	3.33122505	-0.09702838
H	-3.86036276	4.04301224	-0.90812381
H	-7.04543009	1.03988350	1.20135211
C	-0.57702947	0.13352603	1.70638416
H	-0.21912610	-0.38851038	0.59917855
C	0.30542852	-0.76070746	2.63127972
O	-0.27199014	-1.67149599	3.28358683
O	1.54305729	-0.51134014	2.66291942
C	-0.07439629	1.56235740	1.55849028
H	0.95633291	1.60531301	1.19730862
H	-0.71819808	2.11446402	0.86726079
H	-0.11566734	2.05835373	2.53505141
O	-1.87550427	-0.02115211	1.82877103
H	-2.94192086	0.89728954	1.29287140
N	-3.53527422	-2.44511209	-0.27697372
Cl	2.15005016	-3.92407843	-0.23236805
H	-4.24925160	-1.72996087	-0.33931210
H	1.65410037	2.54605607	-2.04628123
C	3.65613436	1.90367282	-1.91376720
H	3.83819727	2.81569898	-2.48591698
H	4.12357072	1.07650229	-2.45421462
C	4.24683979	2.02469985	-0.52275636
C	5.48591934	1.44534676	-0.24325988
C	3.58019549	2.72924202	0.48350494
C	6.05374701	1.56805486	1.02471591
H	6.00331045	0.88572209	-1.01833963

C	4.14106030	2.84324599	1.75422787
H	2.61465933	3.18524162	0.28137373
C	5.38050834	2.26408847	2.02831015
H	7.01586481	1.10876600	1.23089592
H	3.60886156	3.38460091	2.53069748
H	5.81642862	2.35152751	3.01881378
H	-3.82860495	-3.36493075	0.02735733

A7

G_{solv} = -2896.169646

Ni	0.06765550	-1.67902836	-1.81256230
C	-1.12919864	1.92917396	-0.18810000
C	-0.60875066	0.98473599	-1.05565743
C	-0.49952022	-2.03043429	1.13574145
C	-0.44324770	-0.34969509	-0.62593642
C	-0.73519366	-0.64367548	0.72158485
C	-1.24486383	0.34677219	1.54759056
C	-0.24015360	1.25752393	-2.44813127
S	0.17034769	-0.08646105	-3.34273984
S	-0.05828740	-3.06554813	-0.09704727
H	-1.33757753	2.95798865	-0.45978896
H	-1.54610809	0.18851564	2.57510827
C	-0.65756294	3.47092555	2.48522855
C	-1.86906495	2.66255155	2.01204904
H	-2.58073265	3.29664927	1.48203381
H	-2.37772657	2.18031424	2.84633649
N	-1.44741412	1.59184653	1.07767754
C	0.40655527	2.64426553	3.13580244
N	1.41049941	2.02943544	2.40691367
C	0.56202069	2.36023362	4.46815968
C	2.14974424	1.39249099	3.29569504
N	1.68343877	1.57260526	4.55199747
H	-0.00301100	2.65500341	5.33913017
H	3.03040922	0.80454270	3.08290783
H	-0.23479681	4.01364322	1.63320099
H	-1.03892902	4.21468932	3.19044652
H	2.07770768	1.17698774	5.39440402
Cl	0.68919947	-3.26787467	-3.22966367
C	1.00413680	3.76831572	-2.18277492
H	0.72126878	3.89969020	-1.13647074
H	1.94089890	3.20829450	-2.24405444
H	1.14233292	4.75810786	-2.62667484
C	0.48072783	2.73761833	-4.78823112
H	1.46834900	2.27291363	-4.70870582

H	-0.15032865	2.15977052	-5.46773110
H	0.59378803	3.74349206	-5.20376388
C	0.40091342	-1.57311995	3.78738523
H	1.39078635	-1.57093109	3.32506284
H	0.04027752	-0.55043383	3.90631362
H	0.46812596	-2.02313358	4.78211436
C	0.03063312	-4.24910104	2.85891085
H	-0.53100822	-4.97598510	2.26781505
H	1.06546712	-4.20083232	2.50627622
H	0.02424230	-4.58474375	3.90029714
P	-0.32689134	2.92964328	-3.15607206
P	-0.78883295	-2.61193879	2.82916160

4A7

G_{solv} = -3239.222016

Ni	-0.28580579	-1.61696101	-2.08966142
C	-1.51433472	1.81348223	-0.13902969
C	-0.90450187	1.01594304	-1.06685876
C	-0.85361406	-2.21157947	0.85242089
C	-0.41680352	-0.33912299	-0.69172217
C	-0.95928265	-0.81498341	0.61169098
C	-1.56700157	0.06305499	1.47070629
C	-0.73015660	1.38321071	-2.43085996
S	-0.39822565	0.08875841	-3.46411926
S	-0.50679357	-3.13251968	-0.52350585
H	-1.87462407	2.81372188	-0.35267607
H	-1.96707307	-0.22427273	2.43714970
C	-1.26056429	3.11767970	2.79203434
C	-2.35727394	2.30233827	2.09837558
H	-3.03511658	2.97505222	1.57093959
H	-2.93630979	1.73239015	2.82635209
N	-1.80020362	1.35980245	1.11814205
C	-0.35393362	2.29576252	3.64697305
N	0.80717519	1.70463729	3.18167190
C	-0.46347248	1.94551252	4.96058544
C	1.38146488	1.02503742	4.16631107
N	0.63158161	1.16476772	5.25724887
H	-1.21160586	2.19070300	5.69680581
H	2.29849166	0.46328208	4.10066952
H	-0.67536061	3.65865124	2.04166548
H	-1.75707675	3.85944658	3.42260736
H	0.84203636	0.74566397	6.15499362
C	2.74101018	-0.08646203	0.51070966
C	2.45622060	1.34512800	-0.04910830

O	1.82273948	2.12835403	0.70990622
O	2.88744857	1.59523805	-1.19520372
C	3.38286137	-1.08599185	-0.39781026
H	4.39671099	-0.74879759	-0.64016609
H	3.42285386	-2.06116849	0.08944269
H	2.83498877	-1.15501561	-1.34256257
O	2.45405601	-0.33534383	1.67010444
H	1.19548989	1.76584410	2.20743330
H	0.68729579	-0.32478830	-0.64342443
C	-0.43122644	-4.65507777	2.29978739
H	0.59733210	-4.61501817	1.92853273
H	-0.43279582	-5.11327792	3.29382888
H	-1.03519216	-5.28118954	1.63893769
C	0.09734237	-2.15871674	3.53749347
H	1.09344360	-2.21168725	3.09049236
H	-0.18058134	-1.11694165	3.70758953
H	0.10734278	-2.66858901	4.50560995
C	0.33626840	4.00611385	-2.07623744
H	0.39204712	5.01989048	-2.48494061
H	0.05593482	4.07861439	-1.02301136
H	1.31551091	3.52822307	-2.16252325
C	-0.16696861	3.04730797	-4.69800504
H	0.84965498	2.64390376	-4.66448841
H	-0.77038734	2.46154833	-5.39543093
H	-0.13065648	4.07730525	-5.06625354
Cl	0.29641436	-3.11600328	-3.70990130
P	-0.95283602	3.09818246	-3.03904545
P	-1.17506757	-2.98542312	2.48442118

$TS_{4A7,5A7}$

G_{solv} = -3239.173311

Ni	-0.15747278	1.67489454	1.99973340
C	-1.44684964	-1.82000240	0.18313277
C	-0.93981750	-0.94348356	1.11190247
C	-0.79121005	2.19319743	-0.92817974
C	-0.59477588	0.39905683	0.71580413
C	-0.99602655	0.79614620	-0.60484707
C	-1.51579722	-0.13801634	-1.47410088
C	-0.71839153	-1.26427568	2.50795829
S	-0.29231761	0.03968318	3.46983175
S	-0.29781865	3.14378502	0.36356935
H	-1.71361623	-2.84677139	0.40152905
H	-1.83365395	0.08838940	-2.48451796
C	-0.83254629	-3.13610611	-2.66285751

C	-2.07247774	-2.44300565	-2.08815326
H	-2.70532292	-3.17410532	-1.58480676
H	-2.65779822	-1.95596909	-2.86876202
N	-1.70229352	-1.41996594	-1.08935815
C	-0.05907846	-2.32765058	-3.65341330
N	0.87113663	-1.34931390	-3.34226102
C	-0.10273986	-2.40417525	-5.01533142
C	1.35965457	-0.84874617	-4.46922175
N	0.78980631	-1.47505045	-5.49816991
H	-0.67921082	-3.04126881	-5.66644506
H	2.09908488	-0.06771661	-4.54569109
H	-0.18167710	-3.46258767	-1.84581785
H	-1.18364647	-4.03422292	-3.17721077
H	0.99510993	-1.29271320	-6.47289809
C	1.96477460	0.02488326	-0.16273509
C	2.18945374	-1.43259411	0.33878944
O	1.87659130	-2.37148357	-0.44100553
O	2.65010763	-1.57509013	1.50596064
C	2.96212971	1.03590283	0.40460123
H	3.97059187	0.79381944	0.04865697
H	2.70014677	2.03716404	0.05132026
H	2.96809515	1.03944627	1.49683918
O	1.71768048	0.16378858	-1.45603074
H	1.16018266	-0.90756885	-2.39186304
H	0.94702955	0.26225962	0.46806559
C	-0.35443147	4.55389690	-2.48810657
H	0.71079714	4.43235925	-2.26942712
H	-0.46735008	4.99644439	-3.48244133
H	-0.80619906	5.23427978	-1.76294216
C	-0.23121535	2.01730384	-3.75799714
H	0.79963991	1.89441070	-3.41935594
H	-0.67318881	1.04673887	-3.98837460
H	-0.24132083	2.61333995	-4.67561909
C	0.20234195	-3.97126927	2.36131905
H	0.15154790	-4.95642693	2.83448939
H	-0.01474641	-4.09228633	1.29867075
H	1.20598650	-3.55804063	2.48669899
C	-0.34053287	-2.81019443	4.89222160
H	0.69966514	-2.47052713	4.88095640
H	-0.93809400	-2.15463646	5.52997361
H	-0.37956335	-3.81904884	5.31459711
Cl	0.50710680	3.18645126	3.50828387
P	-1.05608644	-2.91649075	3.20756337
P	-1.24139710	2.94851845	-2.52562909

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