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Supporting Information For

Deciphering the Mechanism of Copper Catalyzed N-arylation between Aryl halides and Nitriles: A DFT Study

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1. Test of DFT Methods

The reliability of B3LYP method was tested by,

1) Optimizing the geometries with the B3PW91 method. The optimized geometries were subjected to single point energy calculations in solution with the B3LYP method. The calculated activation energies were compared with the activation energies obtained by geometry optimizations and single point energy calculations with the B3LYP method (Table S1).

Table S1. Activation energies calculated by optimization with B3LYP/SP with B3LYP (B3LYP/B3LYP) and geometry optimization with B3PW91/SP with B3LYP (B3PW91/B3LYP).

Transition State	Activation Energy (kcal/mol)		Transition State	Activation Energy (kcal/mol)	
	B3LYP/B3LYP	B3PW91/B3LYP		B3LYP/B3LYP	B3PW91/B3LYP
Int1TS1	25.9	27.0	Int1TS2	24.8	24.8
Int1TS2-1	4.6	2.7	Int1TS2-2	1.2	5.9
Int2TS1	27.5	29.7	Int2TS2	23.8	23.7
Int1TS3	22.9	22.8	Int1TS4	6.9	7.0

2) The single point energy calculations in solution were repeated with the B3PW91, wB97XD and PBEh1PBE methods and the obtained activation energies were compared with the B3LYP method (Table S2).

Table S2. Activation energies of the important transition states calculated by four different DFT methods.

Transition State	Activation Energy (kcal/mol)			
	B3LYP	wB97XD	PBEh1PBE	B3PW91
Int1TS1	25.9	18.2	18.5	22.2
Int1TS2	24.8	24.8	23.6	23.2
Int1TS2-1	4.6	0.0	0.0	2.4
Int1TS2-2	1.2	0.0	0.0	0.0
Int1TS3	22.9	10.0	15.8	20.1
Int1TS4	6.9	4.4	6.1	6.3

2. Effect of solvent coordination on the activation energy barrier

The effect of potential coordination of H_2O molecules for the key intermediates and transition states was evaluated by optimizing the geometries with an added H_2O molecule in gas phase and calculating the single point energies in the solution. A comparison of activation energies of H_2O-coordinated geometries with the activation energies of geometries without H_2O is depicted in Fig. S1.

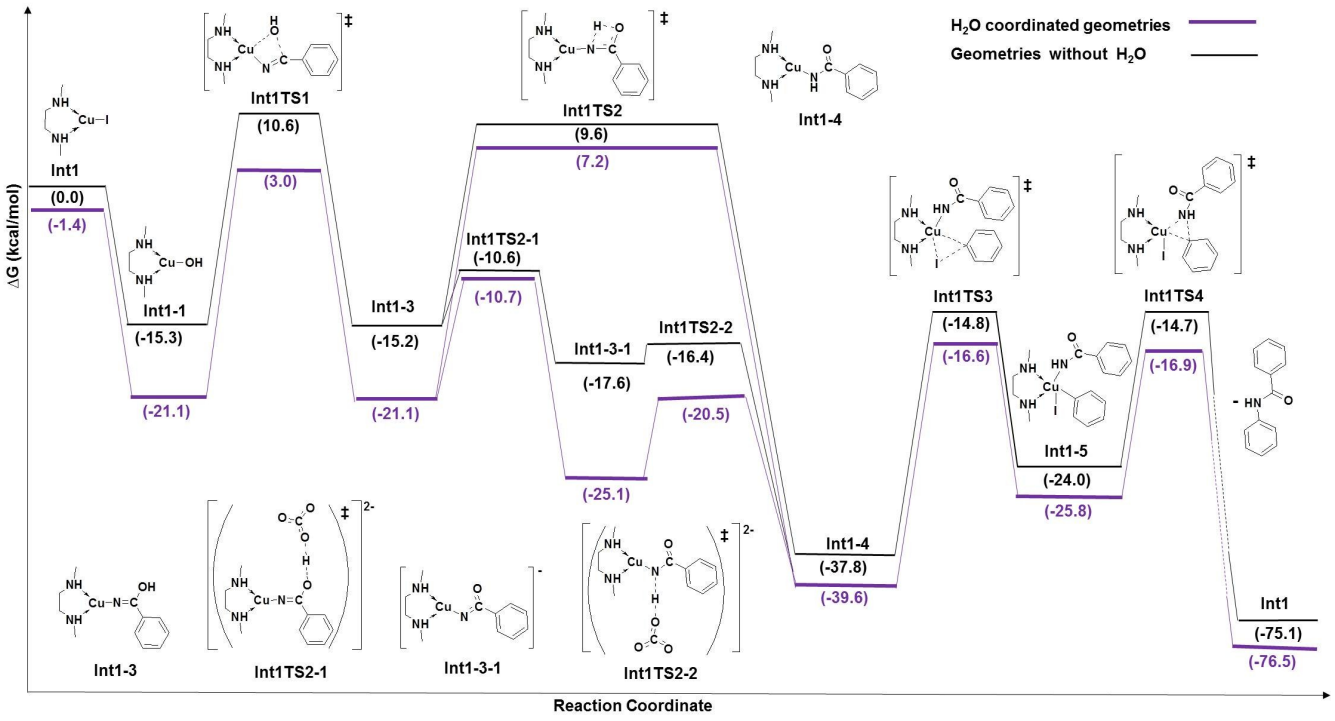

Fig. S1. Energy profile for the hydrolysis and C-N coupling reaction of benzonitrile.

3. Cartesian coordinates of relevant stationary points

Int1

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	0.23016200	-0.08591400	-0.02397400
C	3.11216900	-0.62483300	0.19850000
C	3.04299500	0.86711700	-0.13443200
H	4.06226000	-1.04719400	-0.16468500
H	3.09277300	-0.76542200	1.28652800

H	3.93289500	1.37934900	0.26554500
H	3.05827700	1.00384600	-1.22334700
N	1.94117500	-1.32926300	-0.35663200
N	1.78380500	1.44047500	0.36294900
C	1.50298900	2.79542700	-0.13916500
H	1.36889000	2.75465300	-1.22391100
H	0.56801300	3.14775500	0.30213800
H	2.30855900	3.51034500	0.09036900
C	1.82654600	-2.72599300	0.10419300
H	1.64184300	-2.73404500	1.18182000
H	0.97196900	-3.19326000	-0.38957000
H	2.73444200	-3.31269700	-0.10392300
H	2.02171100	-1.33665500	-1.37415200
I	-2.21196200	-0.01957100	0.00844600
H	1.81460700	1.47328800	1.38203600

Sum of electronic and zero-point Energies= -477.808492
Sum of electronic and thermal Energies= -477.796869
Sum of electronic and thermal Enthalpies= -477.795925
Sum of electronic and thermal Free Energies= -477.849871

Int2

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	0.22789500	-0.54843600	-0.08528600
C	2.90414400	1.08975700	-0.23987800
C	3.08112700	-0.36672000	0.19706500
H	3.80484100	1.67320000	0.05151200
H	2.83256100	1.12472400	-1.33546400
H	4.05551200	-0.70895500	-0.22312900
H	3.25092600	-0.36478200	1.30960100
N	1.67606600	1.66117600	0.29812800
N	2.00504800	-1.21361400	-0.22251800
C	2.29869700	-2.59031700	0.08330000
H	2.42947700	-2.80584000	1.17259200
H	1.49483200	-3.24391500	-0.27555900
H	3.24261100	-2.93801300	-0.39865100
C	1.43566900	3.04500300	-0.06156900
H	1.31340500	3.11857800	-1.14910300
H	0.50138100	3.38394200	0.39856200
H	2.24813100	3.74468800	0.22956800
H	1.65529800	1.54441700	1.30910500
I	-2.21742500	0.02221400	0.01851900

Sum of electronic and zero-point Energies= -477.253074

Sum of electronic and thermal Energies= -477.241423
Sum of electronic and thermal Enthalpies= -477.240479
Sum of electronic and thermal Free Energies= -477.294341

Int1-1

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	0.75963700	0.81688200	0.05458400
C	-1.60014700	-1.42106900	-0.03395900
C	-0.19236700	-1.88136700	-0.41514400
H	-2.32839400	-2.04949300	-0.58226700
H	-1.76786900	-1.62304300	1.03406400
H	-0.10203000	-2.96335100	-0.23172500
H	-0.00927600	-1.71481100	-1.48291000
N	-1.76547500	0.00630400	-0.24268300
N	0.85946700	-1.14412200	0.33308000
C	2.20497600	-1.70967800	0.07812900
H	2.46730500	-1.54920100	-0.97014000
H	2.93666900	-1.19008900	0.69949800
H	2.23872400	-2.78807300	0.29414900
C	-2.99949900	0.57021600	0.29342000
H	-3.01079400	0.44685900	1.38234900
H	-3.01811000	1.64204700	0.07954200
H	-3.91907500	0.10953800	-0.11094400
H	-1.67529000	0.23951600	-1.22928000
O	0.71671100	2.58846300	-0.21619500
H	1.62866400	2.91881000	-0.23235500
H	0.66059800	-1.25987100	1.32917200

Sum of electronic and zero-point Energies= -542.160634
Sum of electronic and thermal Energies= -542.148925
Sum of electronic and thermal Enthalpies= -542.147981
Sum of electronic and thermal Free Energies= -542.199953

Int1-2

Charge 1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.69683500	-0.00000700	-0.00000800
N	-0.53365300	-0.00000600	-0.00001400
C	-3.12082900	-0.00000500	-0.00000300
C	-3.81712400	1.16638200	0.37384100

C	-3.81713000	-1.16639000	-0.37384400
C	-5.20786900	1.15674900	0.37129900
H	-3.26867100	2.05807000	0.65960300
C	-5.20787500	-1.15675100	-0.37129500
H	-3.26868200	-2.05808000	-0.65960900
C	-5.90083900	0.00000000	0.00000400
H	-5.75250200	2.05060500	0.65817600
H	-5.75251300	-2.05060600	-0.65817000
H	-6.98670800	0.00000200	0.00000600
Cu	1.33517500	-0.00000500	0.00000200
C	4.12075800	0.72812200	-0.23031900
C	4.12078000	-0.72809700	0.23028100
H	5.02930000	1.23660500	0.11984700
H	4.12323300	0.77788900	-1.32594500
H	5.02931900	-1.23656300	-0.11991500
H	4.12329300	-0.77786500	1.32590700
N	2.89161000	1.41133400	0.24219300
N	2.89162700	-1.41133200	-0.24218700
C	2.71114800	-2.75084700	0.36685600
H	2.53517000	-2.63822300	1.43980000
H	1.83899200	-3.23281900	-0.08025600
H	3.59068000	-3.39117100	0.21874400
C	2.71109800	2.75085900	-0.36681900
H	2.53510200	2.63825400	-1.43976200
H	1.83894300	3.23280700	0.08032000
H	3.59062200	3.39119400	-0.21871000
H	2.97778600	1.54288300	1.25189500
H	2.97778300	-1.54290000	-1.25188900

Sum of electronic and zero-point Energies= -790.588249
Sum of electronic and thermal Energies= -790.571341
Sum of electronic and thermal Enthalpies= -790.570396
Sum of electronic and thermal Free Energies= -790.636707

Int1TS1

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.24310400	-0.32500300	0.11879800
N	0.38494200	-0.75075300	0.85690700
C	2.70609000	-0.14952600	0.09854100
C	3.44668300	-0.79407800	1.10618900
C	3.38253400	0.63645500	-0.84616500
C	4.83161300	-0.66141800	1.15905600
H	2.91227100	-1.39340600	1.83656700

C	4.77060800	0.77029300	-0.78572700
H	2.80450400	1.14370400	-1.60920900
C	5.49982100	0.12139400	0.21214800
H	5.39249600	-1.16857500	1.94018500
H	5.28299900	1.38552600	-1.52123900
H	6.58115100	0.22484200	0.25426200
Cu	-1.20729400	-0.22932100	-0.59276900
C	-4.02208200	-0.02563800	0.02313800
C	-3.37257100	0.66885700	1.22904900
H	-4.96874300	-0.49838100	0.32880900
H	-4.25393500	0.72129400	-0.74347200
H	-4.11501100	1.34089800	1.69201100
H	-3.10436800	-0.08090900	1.98065500
N	-3.10526500	-1.01839300	-0.58745700
N	-2.15440500	1.36986800	0.82486900
C	-2.34096200	2.75666000	0.40173000
H	-1.36904300	3.18157100	0.13701400
H	-2.97075200	2.79279800	-0.49378300
H	-2.81035600	3.38977400	1.17447500
C	-3.12583500	-2.33059100	0.09572200
H	-2.50782600	-3.03289200	-0.46775100
H	-2.68941100	-2.23389000	1.09183300
H	-4.14783600	-2.73081700	0.18469000
H	0.89268700	-0.29758700	-2.08122500
O	0.61600500	0.31920400	-1.38042500
H	-1.44395600	1.30644200	1.54776000
H	-3.39229700	-1.16318700	-1.55299100

Sum of electronic and zero-point Energies= -866.525809
Sum of electronic and thermal Energies= -866.507644
Sum of electronic and thermal Enthalpies= -866.506700
Sum of electronic and thermal Free Energies= -866.574787

Int1-3

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.60786900	0.94317600	-1.09122400
N	0.36133900	0.84042800	-1.20849800
C	2.57410300	0.18567500	-0.22106100
C	2.11378000	-0.75782600	0.70762900
C	3.95897000	0.40307000	-0.31493600
C	3.00058900	-1.46555000	1.51614000
H	1.04195700	-0.92673600	0.78208900
C	4.84992200	-0.30624600	0.49231500

H	4.33012800	1.13037500	-1.02675200
C	4.37652900	-1.24331900	1.41194400
H	2.61891700	-2.19179500	2.23050900
H	5.91823100	-0.12447300	0.40144000
H	5.07073600	-1.79431400	2.04175000
Cu	-1.02665800	-0.12874000	-0.55036100
C	-3.84223200	-0.57242100	0.07420400
C	-3.63223300	0.44255500	1.19819000
H	-4.66208800	-1.25742300	0.34002000
H	-4.13251800	-0.06083100	-0.85121500
H	-4.59915300	0.93212800	1.41734600
H	-3.34071100	-0.08770100	2.11583900
N	-2.59949400	-1.33184800	-0.21383400
N	-2.55950100	1.36741800	0.86385900
C	-2.10021500	2.20671400	1.96808300
H	-1.67791200	1.57074600	2.75374700
H	-1.30339900	2.86133300	1.60531200
H	-2.89462400	2.82708500	2.41876100
C	-2.80424200	-2.33856200	-1.28148200
H	-3.01064100	-1.82416100	-2.22304700
H	-1.89003000	-2.92272500	-1.40266300
H	-3.64323600	-3.01154500	-1.05028400
H	-2.34527300	-1.83609800	0.63793600
H	1.60603000	2.29849400	-2.37847200
O	2.31037500	1.88530500	-1.84717000
H	-2.82977200	1.95307200	0.07600800

Sum of electronic and zero-point Energies= -866.556344
Sum of electronic and thermal Energies= -866.538164
Sum of electronic and thermal Enthalpies= -866.537220
Sum of electronic and thermal Free Energies= -866.607416

Int1TS2

Charge 0
Spin multiplicity 1

Atomic Type	X	Y	Z
	Coordinates (Angstroms)		
C	-1.57591400	-1.40172000	-0.34345900
N	-0.28224900	-1.25716000	-0.32048200
C	-2.67263900	-0.44878400	-0.03371100
C	-2.42719100	0.81366700	0.52455500
C	-3.99748000	-0.82549000	-0.30271000
C	-3.48001500	1.68426100	0.80133100
H	-1.40111300	1.09652300	0.74320200
C	-5.05089500	0.04730300	-0.03018000
H	-4.17847200	-1.80740900	-0.72585300

C	-4.79594500	1.30460000	0.52195100
H	-3.27652900	2.65904200	1.23843100
H	-6.07240200	-0.25532600	-0.24639100
H	-5.61716500	1.98374400	0.73727000
Cu	0.97770900	0.05208300	-0.10101700
C	3.61252300	1.25798900	-0.41666500
C	4.11915600	0.03095800	0.34261300
H	4.29780600	2.10487400	-0.25910100
H	3.58741900	1.05460000	-1.49377900
H	5.17327700	-0.14925500	0.06309600
H	4.11861300	0.24548000	1.42049800
N	2.23194400	1.61971300	-0.00586600
N	3.24051800	-1.10809000	0.11906800
C	3.44663600	-2.23845000	1.02246400
H	3.23369900	-1.92192400	2.04931000
H	2.73696200	-3.02870800	0.76466800
H	4.46963700	-2.65205800	0.99480300
C	1.73885100	2.81524900	-0.72946000
H	1.63099400	2.57222000	-1.78915400
H	0.75736900	3.09188900	-0.33999000
H	2.42779600	3.66655400	-0.62593800
H	2.26217800	1.85396100	0.98868900
H	-0.60568200	-2.55998700	-0.71654900
O	-1.88032000	-2.63263700	-0.71451800
H	3.31061900	-1.42228100	-0.84697800

Sum of electronic and zero-point Energies= -866.521500
Sum of electronic and thermal Energies= -866.503553
Sum of electronic and thermal Enthalpies= -866.502608
Sum of electronic and thermal Free Energies=-866.571820

Int1TS2-1

Charge -2
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.90524700	-0.24113500	0.04742700
N	1.15526200	0.51217500	0.76454900
C	3.39969800	0.06880000	0.00594500
C	3.92012400	1.16409700	0.71754600
C	4.30309000	-0.72178100	-0.72683900
C	5.28147100	1.46135100	0.69877300
H	3.19734900	1.75393000	1.27624300
C	5.67053200	-0.42923400	-0.74624100
H	3.89420500	-1.56432300	-1.27460900
C	6.17243100	0.66424100	-0.03475300

H	5.65832800	2.31928700	1.25835800
H	6.35116100	-1.05856100	-1.32245800
H	7.23846700	0.89387400	-0.04984300
Cu	-0.68615600	0.17363300	0.70917800
C	-3.80523100	0.16799200	0.78331700
C	-3.75404200	1.60083500	0.21812000
H	-4.70269100	0.03557000	1.41982100
H	-3.84883800	-0.55795100	-0.03926000
H	-4.68196800	2.14639100	0.47429700
H	-2.92988900	2.14931300	0.72678200
N	-2.59578500	-0.17686500	1.56823700
N	-3.59286700	1.57750700	-1.22723900
C	-3.17346400	2.85625100	-1.75671100
H	-2.26569400	3.27595500	-1.27268500
H	-2.95930100	2.75671500	-2.82832900
H	-3.97389400	3.61108500	-1.64689200
C	-2.66064800	-1.57697400	2.03132000
H	-2.70749100	-2.21679200	1.14459000
H	-1.75667500	-1.80934900	2.60083600
H	-3.55241200	-1.75870500	2.66581700
H	-2.54821800	0.43390700	2.38306100
H	0.51897400	-1.65865400	-0.77319100
O	1.63441400	-1.31068300	-0.71071000
H	-2.87084900	0.84813900	-1.43084100
C	-1.67537000	-1.59639900	-1.12922400
O	-1.52703900	-0.30107900	-1.30439000
O	-0.59464900	-2.30118800	-0.85948200
O	-2.81664400	-2.15369500	-1.15901400

Int1-3-1

Charge -1

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.08523800	-0.20331800	0.17335100
N	0.53617600	-1.35666300	-0.11745200
C	2.61441400	-0.14126400	0.06349200
C	3.37642900	-1.26054700	-0.30692900
C	3.29112800	1.05682600	0.33677700
C	4.76643400	-1.18543800	-0.40123900
H	2.83378100	-2.17791100	-0.51507100
C	4.68301400	1.13797400	0.24382900
H	2.68416600	1.91058800	0.62127400
C	5.43020500	0.01634600	-0.12590700
H	5.33953400	-2.06638500	-0.69077100

H	5.18868500	2.07921600	0.46040000
H	6.51558900	0.07597000	-0.19900600
Cu	-1.27044000	-1.15983500	0.06845300
C	-3.75986700	0.41681700	-0.35526200
C	-3.09559300	1.72136500	0.10389400
H	-4.84508600	0.48004600	-0.15606600
H	-3.61753200	0.30605200	-1.43448200
H	-3.79476400	2.52806300	-0.17005500
H	-3.06257400	1.72888400	1.21900700
N	-3.23429200	-0.80851300	0.30327800
N	-1.82412100	1.99980000	-0.52443200
C	-1.37340800	3.36003600	-0.27143100
H	-1.38555700	3.64912200	0.79945200
H	-0.34040000	3.44542000	-0.61802000
H	-1.99520200	4.08837600	-0.81688100
C	-4.05925200	-1.98984300	-0.01531900
H	-3.96159000	-2.21505400	-1.08060300
H	-3.69256900	-2.84915400	0.55126900
H	-5.12548900	-1.82300900	0.21394200
H	-3.27932800	-0.65260700	1.31262400
O	0.54346300	0.91616800	0.54802700
H	-1.06338800	1.38217000	-0.16764900

Int1TS2-2

Charge -2

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.93721300	1.53267300	0.16622600
N	0.66585200	1.23655000	0.00748800
C	3.01375300	0.40030500	0.13091600
C	2.74411800	-0.97599400	0.14236500
C	4.36432200	0.78982700	0.11957000
C	3.77256000	-1.92261800	0.13270600
H	1.69857800	-1.27975300	0.14874000
C	5.39963200	-0.14736800	0.09502200
H	4.54759100	1.86040800	0.13881700
C	5.11101400	-1.51629900	0.10297900
H	3.52926900	-2.98675600	0.14871200
H	6.43869900	0.18739600	0.07502600
H	5.91483700	-2.25372700	0.09097500
Cu	-0.48013400	-0.13340400	-0.46821300
C	-2.78023400	-2.12111500	-0.45151500
C	-2.55073300	-2.20288700	1.06695500
H	-3.18385400	-3.07504800	-0.84289300

H	-3.50571700	-1.32818700	-0.64717000
H	-3.09581200	-3.07318900	1.47856900
H	-1.47275800	-2.40671200	1.24486600
N	-1.55369600	-1.75841600	-1.19563500
N	-3.01145100	-0.98834700	1.71932600
C	-2.41230900	-0.78329900	3.02316800
H	-1.30457400	-0.80721100	3.01695900
H	-2.72079500	0.19349200	3.41186900
H	-2.75672000	-1.55376900	3.73579700
C	-1.85726000	-1.44898400	-2.60148900
H	-2.41980700	-0.51220600	-2.61362100
H	-0.92039600	-1.30366500	-3.14701200
H	-2.44677700	-2.24915200	-3.09203100
H	-0.90322500	-2.54052300	-1.15814300
O	2.45029000	2.67655300	0.36414100
H	-2.80589100	-0.18266700	1.09455200
H	-0.35542000	2.14275900	0.01974500
C	-2.46722400	2.16921100	-0.26056300
O	-2.40800700	0.84400300	-0.38865800
O	-1.33082500	2.80974200	-0.01424600
O	-3.54488200	2.79070200	-0.36647000

Int1-4

Charge 0

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.50927800	1.85043500	-0.24510900
N	0.21390200	1.62043700	-0.58804700
C	2.40922400	0.63796800	-0.10041700
C	2.25830700	-0.53103000	-0.86053600
C	3.48029500	0.72089300	0.79901800
C	3.14206100	-1.60242000	-0.70333000
H	1.46035200	-0.58323600	-1.59530700
C	4.35111000	-0.35458300	0.97378900
H	3.61376100	1.64798100	1.34753000
C	4.18374400	-1.52237400	0.22423100
H	3.02707800	-2.49410300	-1.31619500
H	5.16866700	-0.27911500	1.68679300
H	4.86943900	-2.35682900	0.35005900
Cu	-0.85726800	0.16346400	-0.16830400
C	-3.06705200	-1.73939500	0.08839800
C	-3.84018200	-0.49340000	0.51910100
H	-3.48770800	-2.63089800	0.57767500
H	-3.16434000	-1.88737300	-0.99397700

H	-4.91997300	-0.67388100	0.37095900
H	-3.69754100	-0.32828600	1.59582000
N	-1.61982200	-1.60982000	0.38651600
N	-3.34322800	0.68764900	-0.17968500
C	-3.84710000	1.95616000	0.34942500
H	-3.47433100	2.09444500	1.36969600
H	-3.46016200	2.77663000	-0.26095800
H	-4.94833000	2.02114300	0.37141000
C	-0.84402800	-2.77280300	-0.10711600
H	-0.90637500	-2.80372700	-1.19787100
H	0.20378600	-2.65076800	0.17353600
H	-1.22995300	-3.71979400	0.29769800
H	-1.51679900	-1.58658800	1.40321100
H	-0.24435000	2.52707000	-0.67389000
O	1.99605400	2.97294300	-0.05141000
H	-3.57078800	0.61875700	-1.17031300

Sum of electronic and zero-point Energies= -866.588359
Sum of electronic and thermal Energies= -866.570389
Sum of electronic and thermal Enthalpies= -866.569445
Sum of electronic and thermal Free Energies= -866.637645

Int2-1

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	1.13644000	-0.55654900	-0.07316600
C	-1.94677800	0.92686900	-0.22293200
C	-0.69816000	1.63787800	0.31700800
H	-2.82398000	1.39349300	0.27767400
H	-2.04240900	1.14066800	-1.29881900
H	-0.87704000	2.71967900	0.12120300
H	-0.73130000	1.55384600	1.43739600
N	-1.94529100	-0.51791700	-0.03034500
N	0.55430700	1.23282700	-0.26063300
C	1.56231100	2.22285200	0.04705700
H	1.77270000	2.35942700	1.13792200
H	2.51585200	1.96077300	-0.42748300
H	1.27812300	3.23471000	-0.32457500
C	-3.25613300	-1.11889100	0.04666300
H	-3.77330200	-1.01440700	-0.91850300
H	-3.16046700	-2.19163600	0.25306300
H	-3.92898400	-0.67764000	0.81659100
H	-1.36020800	-0.77888100	0.75877600

O	1.69928500	-2.28817800	0.05301600
H	2.34942500	-2.27129200	0.77451900

Sum of electronic and zero-point Energies= -541.593194
Sum of electronic and thermal Energies= -541.581359
Sum of electronic and thermal Enthalpies= -541.580415
Sum of electronic and thermal Free Energies= -541.632494

Int2-2

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.61023200	-0.24969000	-0.02975100
N	-0.45000600	-0.35938100	-0.03936700
C	-3.02837100	-0.13023000	-0.00790500
C	-3.62767100	1.11188600	0.28267800
C	-3.83235600	-1.25717300	-0.27369400
C	-5.01467200	1.21716200	0.30566700
H	-3.00218700	1.97504300	0.48635900
C	-5.21786600	-1.13405800	-0.24661500
H	-3.36350300	-2.21014600	-0.49657500
C	-5.81144500	0.09867300	0.04206400
H	-5.47608100	2.17433900	0.53002700
H	-5.83695800	-2.00255200	-0.45109700
H	-6.89375200	0.18761800	0.06169900
Cu	1.37406400	-0.54152800	-0.02697400
C	3.73194100	1.26835800	-0.33841700
C	4.15556600	-0.10639100	0.18024000
H	4.52127600	2.01322000	-0.12699000
H	3.60549500	1.21688900	-1.42714500
H	5.09561700	-0.37627700	-0.34201900
H	4.44482800	-0.00444700	1.25412400
N	2.43622400	1.66753300	0.23004200
N	3.13316000	-1.09616200	-0.03348300
C	3.61375800	-2.43508300	0.21363100
H	3.93544600	-2.60231800	1.26384300
H	2.83212200	-3.16988600	-0.00598600
H	4.49042100	-2.68592800	-0.41762700
C	1.96655100	2.96560800	-0.24970700
H	1.77068500	2.90207100	-1.32571100
H	1.02814500	3.22687000	0.25094300
H	2.68863000	3.78574400	-0.08701100
H	2.52511500	1.69577100	1.24590300

Sum of electronic and zero-point Energies= -790.142725

Sum of electronic and thermal Energies= -790.125876
Sum of electronic and thermal Enthalpies= -790.124932
Sum of electronic and thermal Free Energies= -790.190546

Int2TS1

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.42657600	-0.81591900	-0.00853500
N	-0.88446200	-1.81065700	0.42541600
C	-2.80955000	-0.28070000	0.00732000
C	-3.74174900	-0.91593100	0.84959900
C	-3.24968300	0.79773100	-0.77745200
C	-5.06243700	-0.48054300	0.91404600
H	-3.39031400	-1.75652700	1.44047100
C	-4.57710300	1.22941000	-0.71658400
H	-2.53772200	1.27637000	-1.43985400
C	-5.48954300	0.59772100	0.13029400
H	-5.76494200	-0.98325400	1.57645300
H	-4.89899000	2.06448500	-1.33641200
H	-6.52199400	0.93804100	0.17910900
Cu	1.24679200	-0.74635800	-0.38986500
C	3.57900800	1.43126600	-0.08109300
C	3.95909600	-0.00544200	0.29376600
H	4.44181600	2.08531800	0.16933200
H	3.42626400	1.49399700	-1.16700500
H	5.00859300	-0.14795800	-0.06266400
H	4.05946300	-0.02406100	1.41675900
N	2.36313500	1.90785300	0.58751300
N	3.09986200	-1.02716500	-0.21799500
C	3.59063500	-2.32233400	0.17770600
H	3.63655700	-2.47751000	1.28444100
H	2.95440600	-3.11665800	-0.22850500
H	4.62822100	-2.51133400	-0.18776100
C	2.23512200	3.35398700	0.58017600
H	2.09057100	3.70357400	-0.45034700
H	1.35339700	3.65529600	1.15885300
H	3.11587300	3.89720800	0.98580400
H	2.36406000	1.55994400	1.54456600
H	-0.35305900	1.04072600	-0.33535600
O	-0.48278000	0.24012800	-0.87772500

Sum of electronic and zero-point Energies= -865.956091
Sum of electronic and thermal Energies= -865.937773

Sum of electronic and thermal Enthalpies= -865.936828
Sum of electronic and thermal Free Energies= -866.006826

Int2-3

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.65221000	-1.65122100	-0.42735800
N	-0.41840600	-1.84125800	-0.45026200
C	-2.43968100	-0.43397500	-0.03597200
C	-1.77362800	0.77161900	0.23877100
C	-3.84038100	-0.46376200	0.08097700
C	-2.48689500	1.90485500	0.62699300
H	-0.69180700	0.80240300	0.13384000
C	-4.55235500	0.67234900	0.47244900
H	-4.36196800	-1.38927200	-0.13418300
C	-3.87990300	1.86405700	0.74909700
H	-1.95173500	2.82933300	0.83816900
H	-5.63669300	0.62502200	0.56149700
H	-4.43279100	2.75067700	1.05437900
Cu	1.22604200	-1.11072200	-0.08045900
C	2.92737800	1.73462000	-0.55385400
C	3.50574100	0.69733000	0.41285300
H	3.58851100	2.62950800	-0.53495900
H	2.96230900	1.32788100	-1.57335100
H	4.60912900	0.71586100	0.25253700
H	3.38227800	1.11667700	1.45059800
N	1.54517900	2.10035400	-0.25395900
N	3.00821000	-0.63621600	0.26359000
C	3.79181400	-1.53982800	1.07030200
H	3.73137400	-1.34817500	2.17004200
H	3.47192000	-2.57653900	0.91146300
H	4.87861000	-1.49019500	0.82424200
C	1.07593600	3.24741300	-1.00838400
H	1.04604600	2.99164700	-2.07505200
H	0.05453200	3.50308500	-0.70422500
H	1.70887900	4.15574500	-0.90750300
H	1.46223500	2.27593600	0.74574700
H	-1.93023000	-3.40489000	-0.99697300
O	-2.55569900	-2.68558300	-0.79422200

Sum of electronic and zero-point Energies= -865.999304
Sum of electronic and thermal Energies= -865.981199
Sum of electronic and thermal Enthalpies= -865.980255

Sum of electronic and thermal Free Energies= -866.048685

Int2TS2

Charge -1

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.65887900	-1.62067000	-0.51291500
N	-0.38883800	-1.85310900	-0.55407900
C	-2.41003600	-0.43192900	-0.03142300
C	-1.75379400	0.74730300	0.35545000
C	-3.81117300	-0.48610700	0.04485500
C	-2.48832700	1.83999600	0.81704900
H	-0.67075500	0.79905100	0.27502200
C	-4.54232600	0.60852200	0.50866700
H	-4.30408100	-1.40148000	-0.26516600
C	-3.88324500	1.77688400	0.89860200
H	-1.96843900	2.74828400	1.11649400
H	-5.62784700	0.55005300	0.56522600
H	-4.45084300	2.63216400	1.26067000
Cu	1.23684100	-1.10884500	-0.06719000
C	2.85020200	1.69611200	-0.66545700
C	3.46613400	0.77039900	0.38684700
H	3.50758900	2.58657400	-0.77545000
H	2.84154700	1.17837500	-1.63359200
H	4.56684300	0.78242100	0.20366000
H	3.35909300	1.29224800	1.37908000
N	1.47951300	2.09263300	-0.34726600
N	2.97305500	-0.57199400	0.39069000
C	3.72278400	-1.36533300	1.33131000
H	3.62847700	-1.02907000	2.39342300
H	3.39945000	-2.41247100	1.29995900
H	4.81771600	-1.35411700	1.11768900
C	0.95026200	3.10897800	-1.23860300
H	0.86926900	2.69476500	-2.25110500
H	-0.05849900	3.39579000	-0.92013300
H	1.57044500	4.02851000	-1.30816900
H	1.45390200	2.42318800	0.61599700
H	-1.11708300	-2.96657000	-1.05229200
O	-2.34761200	-2.66610700	-0.98306300

Sum of electronic and zero-point Energies= -865.968312

Sum of electronic and thermal Energies= -865.950464

Sum of electronic and thermal Enthalpies= -865.949520

Sum of electronic and thermal Free Energies= -866.017383

Int2-4

Charge -1

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.74389100	-1.49635600	-0.77121300
N	0.44650000	-1.27222200	-1.04035200
C	2.54380700	-0.40623700	-0.06384400
C	2.03188900	0.83455500	0.34006000
C	3.89401800	-0.68302900	0.19822800
C	2.84552000	1.76875300	0.98595100
H	0.98677500	1.06670100	0.14647200
C	4.70997700	0.24614100	0.84263200
H	4.26962000	-1.64925400	-0.12247500
C	4.18818100	1.48013800	1.24081300
H	2.42573000	2.72589800	1.28957300
H	5.75508500	0.00900100	1.03558200
H	4.82109400	2.20900800	1.74418300
Cu	-0.90406500	0.01992200	-0.80036800
C	-3.85816700	-0.03430800	0.69972800
C	-3.19100000	1.31342800	0.41153100
H	-4.63831300	0.12871300	1.47639700
H	-4.37335000	-0.37927400	-0.20790600
H	-4.02352800	2.02575400	0.21339100
H	-2.74858200	1.67617900	1.37953500
N	-2.91046300	-1.06687000	1.10204900
N	-2.26471900	1.31025600	-0.68492900
C	-1.91957600	2.66762000	-1.03854300
H	-1.39674000	3.24066800	-0.23331200
H	-1.26236400	2.68190400	-1.91622000
H	-2.81861500	3.27365700	-1.29330900
C	-3.53226200	-2.25779800	1.64597800
H	-4.12194300	-2.75251200	0.86294600
H	-2.75993700	-2.96282400	1.97395100
H	-4.21891400	-2.07150900	2.50027700
H	-2.24000200	-0.67873600	1.76180000
H	0.10079400	-2.11490000	-1.50003200
O	2.35302100	-2.55022600	-1.06068500

Sum of electronic and zero-point Energies= -866.038481

Sum of electronic and thermal Energies= -866.020509

Sum of electronic and thermal Enthalpies= -866.019565

Sum of electronic and thermal Free Energies= -866.089062

Int1TS3

Charge 0

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.91988900	1.84178500	0.04834000
N	0.67544600	1.58412200	-0.42468900
C	3.04583500	1.01851600	-0.55273300
C	2.90600800	0.31781800	-1.76185100
C	4.28581300	0.99450100	0.10348100
C	3.97706700	-0.40746900	-2.28905200
H	1.95542300	0.36571600	-2.28294800
C	5.35391800	0.26432500	-0.41846500
H	4.38801900	1.57480400	1.01520100
C	5.20157000	-0.44078400	-1.61590400
H	3.86086400	-0.93667100	-3.23197000
H	6.30854700	0.25206200	0.10187000
H	6.03537900	-1.00383600	-2.02786000
Cu	-0.28114900	-0.09663700	0.13621700
C	1.28992900	-1.75680200	2.08802800
C	1.09318300	-0.43879300	2.83311100
H	2.21821600	-2.24093500	2.43202400
H	0.46588200	-2.44678500	2.31386900
H	1.20024700	-0.61157700	3.91744400
H	1.87469500	0.27313800	2.54383000
N	1.30610700	-1.53629100	0.63194200
N	-0.19921500	0.17361800	2.49017700
C	-0.30485000	1.55582200	2.99043800
H	0.46073900	2.16624100	2.50177700
H	-1.28761500	1.95802200	2.73076800
H	-0.17339100	1.62013700	4.08298300
C	1.40863300	-2.78850300	-0.13020800
H	0.47622000	-3.35363500	-0.03498700
H	1.56479900	-2.55117400	-1.18499400
H	2.23986900	-3.42025400	0.21799300
H	2.11639000	-0.95956100	0.40029700
H	0.07267200	2.31826700	-0.04423300
O	2.21435100	2.69231000	0.91329100
H	-0.94308200	-0.39029300	2.90179800
C	-2.69283500	2.43775700	-2.01466200
C	-2.15642600	1.16820100	-1.80524900
C	-2.25194100	0.59393500	-0.53003600
C	-2.95355200	1.23622100	0.49899800
C	-3.48297300	2.50888000	0.26902200
C	-3.35314100	3.11318800	-0.98296400
H	-2.59200400	2.89937800	-2.99321600
H	-1.64311500	0.65014300	-2.60695900

H	-3.08469400	0.75478200	1.46175100
H	-4.01069400	3.01763100	1.07163100
H	-3.77512100	4.09818300	-1.15943600
I	-2.25439300	-1.72889700	-0.42730200

Sum of electronic and zero-point Energies= -1109.506322
Sum of electronic and thermal Energies= -1109.481545
Sum of electronic and thermal Enthalpies= -1109.480601
Sum of electronic and thermal Free Energies= -1109.564625

Int1-5

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.04091100	1.29370500	1.16846000
N	0.73549900	1.37334500	0.77708300
C	3.06643200	1.03476500	0.09142000
C	2.81390900	1.30550000	-1.26286700
C	4.33296400	0.56315300	0.46970800
C	3.80554600	1.08957600	-2.22178700
H	1.84808500	1.71159500	-1.54640100
C	5.31823100	0.33520500	-0.49020900
H	4.52553600	0.39799600	1.52527800
C	5.05597000	0.59726300	-1.83826300
H	3.60730100	1.31670000	-3.26615300
H	6.29428300	-0.03519600	-0.18792500
H	5.82715100	0.42937800	-2.58553000
Cu	-0.37090300	-0.06530000	0.04370800
C	0.96425300	-2.60144600	0.89353400
C	0.75934100	-2.01712200	2.28770900
H	1.83704900	-3.27134200	0.89723700
H	0.09347300	-3.19189000	0.58826200
H	0.74714300	-2.84076400	3.02283800
H	1.60908000	-1.37419900	2.54868300
N	1.15031400	-1.53062000	-0.11240800
N	-0.44817400	-1.18909200	2.34345700
C	-0.53509900	-0.42359300	3.59365900
H	0.29098900	0.29386300	3.62728300
H	-1.47737400	0.13138400	3.61793300
H	-0.48378400	-1.05778100	4.49451100
C	1.41771700	-2.07849700	-1.46062800
H	0.52483600	-2.58549200	-1.82988900
H	1.66706700	-1.25680100	-2.13490300
H	2.25712000	-2.78699300	-1.43607800
H	1.97613500	-0.99266500	0.15287700

H	0.19759300	1.70874300	1.57575100
O	2.41968400	1.48233800	2.33492300
H	-1.26812900	-1.78716100	2.24628200
C	-2.54832100	3.28526700	-1.23679900
C	-1.69775700	2.17513300	-1.20799500
C	-1.73948500	1.32694100	-0.10577600
C	-2.61420000	1.54524400	0.95199400
C	-3.45663200	2.66515700	0.91242300
C	-3.42476400	3.53398600	-0.17784500
H	-2.51783900	3.95543700	-2.09233700
H	-1.01817800	1.99159800	-2.03403100
H	-2.66726900	0.85872100	1.79016200
H	-4.14317300	2.84226700	1.73671700
H	-4.08284100	4.39796700	-0.20651500
I	-2.18232300	-1.53164600	-1.01336400

Sum of electronic and zero-point Energies= -1109.515140
Sum of electronic and thermal Energies= -1109.489975
Sum of electronic and thermal Enthalpies= -1109.489031
Sum of electronic and thermal Free Energies= -1109.573684

Int1TS4

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.04752800	0.34422100	1.72689200
N	0.71459000	0.64792400	1.55657400
C	2.99549300	0.43145300	0.56648000
C	2.96966200	1.48888900	-0.35177800
C	4.01117400	-0.53317500	0.47226400
C	3.92212800	1.55951600	-1.37158900
H	2.22472700	2.26913300	-0.24754100
C	4.94742100	-0.47399400	-0.55906300
H	4.06034900	-1.31467500	1.22441900
C	4.90282700	0.57207700	-1.48611400
H	3.90419500	2.39264600	-2.06922200
H	5.72138600	-1.23330900	-0.63118900
H	5.63953400	0.62519200	-2.28311200
Cu	-0.50026700	-0.26550400	0.33965100
C	0.61234500	-2.56252400	-1.36838000
C	0.82107200	-2.97197700	0.08728400
H	1.33627100	-3.09223800	-2.00932400
H	-0.39060400	-2.86317200	-1.69337400
H	0.81321600	-4.07060100	0.16866700
H	1.80190800	-2.63063200	0.44035600

N	0.70413500	-1.10171800	-1.52384700
N	-0.20598700	-2.35573600	0.94139500
C	0.00162900	-2.60227100	2.37863100
H	0.89649200	-2.07340600	2.71770900
H	-0.86126600	-2.21869100	2.93024200
H	0.11298800	-3.67369900	2.60335000
C	0.30586100	-0.67126100	-2.87273500
H	-0.77308900	-0.80973600	-2.98527200
H	0.52874300	0.39132200	-2.99785700
H	0.82620900	-1.23106300	-3.66619700
H	1.67008300	-0.81909700	-1.35946300
H	0.26735700	0.67940300	2.47078800
O	2.46790500	0.00659400	2.83690300
H	-1.12221000	-2.71722800	0.67055600
C	-0.84668600	3.66125100	-0.95044900
C	-0.28095900	2.40410700	-0.70648700
C	-0.64853900	1.71832200	0.44954500
C	-1.50519900	2.28778400	1.39423600
C	-2.05565200	3.54232700	1.13440600
C	-1.72827900	4.23544700	-0.03534100
H	-0.58992600	4.18512100	-1.86776600
H	0.39159400	1.96381600	-1.43152700
H	-1.77897500	1.75352300	2.29883300
H	-2.74609200	3.97516500	1.85332300
H	-2.15532900	5.21509800	-0.22780000
I	-2.94968300	-0.79189500	-0.45885600

Sum of electronic and zero-point Energies= -1109.506150
Sum of electronic and thermal Energies= -1109.481457
Sum of electronic and thermal Enthalpies= -1109.480512
Sum of electronic and thermal Free Energies= -1109.563855

Int1.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	-0.22990000	0.21213300	-0.38854800
C	-3.06756800	-0.61749700	-0.23599500
C	-2.95361300	0.75966600	0.42188800
H	-3.86546000	-1.19421800	0.25954800
H	-3.36582400	-0.50050800	-1.28698700
H	-3.92698400	1.27397200	0.38547400
H	-2.68312300	0.64593100	1.47813300
N	-1.77174700	-1.30701300	-0.21220200
N	-1.88675100	1.55395000	-0.22162800
C	-1.61530100	2.82766400	0.47054500

H	-1.21517000	2.61422100	1.46514100
H	-0.85777200	3.38273500	-0.08719500
H	-2.51790200	3.44920300	0.57579800
C	-1.72809300	-2.51125700	-1.05150300
H	-1.86035700	-2.23429600	-2.10248900
H	-0.74709500	-2.98100100	-0.94527800
H	-2.50669100	-3.24418900	-0.78543300
H	-1.51805800	-1.56154800	0.75033000
I	2.20921200	0.07737700	-0.09123100
H	-2.17378400	1.76337500	-1.17860400
O	-0.25231600	-1.58262100	2.32229500
H	0.18136200	-2.42885600	2.51395500
H	0.45116500	-1.05669400	1.88961700

Sum of electronic and zero-point Energies= -554.212959
Sum of electronic and thermal Energies= -554.198004
Sum of electronic and thermal Enthalpies= -554.197060
Sum of electronic and thermal Free Energies= -554.258615

Int2.H_2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	0.24239400	0.52212200	-0.12069600
C	-2.54053500	-0.76896000	-1.17650400
C	-2.49748300	0.75993900	-1.07502300
H	-3.39413900	-1.01782300	-1.84295900
H	-1.63184300	-1.12795300	-1.68463300
H	-2.37798600	1.14004500	-2.11368600
H	-3.50598000	1.10390500	-0.75513000
N	-2.66404200	-1.43879400	0.11304100
N	-1.49467200	1.29704700	-0.17438400
C	-1.52458000	2.75092800	-0.23218600
H	-2.52175400	3.15027400	0.04728000
H	-0.79575600	3.17474600	0.46839800
H	-1.29704000	3.16292100	-1.23824100
C	-3.32451900	-2.72252200	0.05609500
H	-2.71869500	-3.43562000	-0.52119800
H	-3.43282700	-3.12988500	1.06863500
H	-4.33291600	-2.70457600	-0.41398800
H	-3.06947000	-0.82154300	0.81588100
I	2.55163700	-0.37038200	0.04671600
O	-2.58150900	0.62463900	2.27643900
H	-1.95740400	-0.06133700	2.56191300
H	-2.14460600	0.93433500	1.41556300

Sum of electronic and zero-point Energies= -553.665487
Sum of electronic and thermal Energies= -553.651319
Sum of electronic and thermal Enthalpies= -553.650374
Sum of electronic and thermal Free Energies= -553.710121

Int1-1.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu	-0.04568100	0.88706300	-0.30506000
C	0.68839000	-2.00635100	0.34291900
C	1.95366800	-1.15710100	0.21492500
H	0.96749700	-3.07448500	0.28276500
H	0.24175500	-1.85481200	1.33432100
H	2.73965400	-1.53280300	0.88734100
H	2.34240200	-1.21887500	-0.80876500
N	-0.29207900	-1.59683400	-0.65392900
N	1.67474900	0.27582100	0.49294500
C	2.85179300	1.13264300	0.22317900
H	3.05411800	1.13651200	-0.85060600
H	2.63059700	2.15472500	0.53660100
H	3.74672600	0.77345700	0.75275500
C	-1.64743100	-2.11052900	-0.43321700
H	-2.07701600	-1.60878500	0.43974500
H	-2.26067500	-1.84692200	-1.29947000
H	-1.68313900	-3.20535500	-0.29397000
H	0.03319700	-1.86342600	-1.58129000
O	-1.67115600	1.58300200	-0.77021400
H	-1.63641400	2.54779200	-0.67773900
H	1.46183300	0.35431100	1.48971600
O	-2.70068900	0.46856900	1.48492700
H	-2.38818300	0.93160900	0.65627900
H	-3.63004800	0.26478300	1.30139900

Sum of electronic and zero-point Energies= -618.568347
Sum of electronic and thermal Energies= -618.554147
Sum of electronic and thermal Enthalpies= -618.553203
Sum of electronic and thermal Free Energies= -618.609753

Int1-2.H_2O

Charge 1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z

C	1.94780400	-0.02633500	-0.06621400
N	0.78621800	-0.01108900	-0.12619100
C	3.37034900	-0.04982500	0.00747700
C	4.08480100	1.16158700	0.08721400
C	4.04728900	-1.28522900	-0.00155500
C	5.47352400	1.12816400	0.15799900
H	3.55143700	2.10663000	0.09263100
C	5.43634400	-1.29922600	0.06969800
H	3.48512100	-2.21130400	-0.06443500
C	6.14712500	-0.09742400	0.14919300
H	6.03158000	2.05701200	0.21954900
H	5.96576400	-2.24667000	0.06277800
H	7.23145700	-0.11604300	0.20421300
Cu	-1.07786200	0.01796200	-0.25637300
C	-3.76095500	1.11408700	-0.18233700
C	-3.85444600	-0.25291000	-0.85783000
H	-4.56698000	1.77099300	-0.53855700
H	-3.88154300	0.99430900	0.89992900
H	-4.84705200	-0.69075300	-0.68205600
H	-3.73190000	-0.15350100	-1.94373300
N	-2.42286200	1.70456700	-0.42037300
N	-2.77697400	-1.13839900	-0.35319400
C	-2.70611400	-2.42022600	-1.08961000
H	-2.41245200	-2.23521900	-2.12654500
H	-1.95326500	-3.06045900	-0.62417000
H	-3.67147600	-2.94476400	-1.08785700
C	-2.16725800	2.90298200	0.40719000
H	-2.13546800	2.61226200	1.46072600
H	-1.19842400	3.32804200	0.13421500
H	-2.94325700	3.67007800	0.27902600
H	-2.37323900	1.98742100	-1.40059100
H	-2.99501700	-1.34469900	0.63007500
O	-3.53425000	-1.26899000	2.50679700
H	-4.34540700	-1.67781100	2.84690700
H	-2.89330200	-1.35391400	3.22930500

Sum of electronic and zero-point Energies= -866.990770
Sum of electronic and thermal Energies= -866.970053
Sum of electronic and thermal Enthalpies= -866.969109
Sum of electronic and thermal Free Energies= -867.044271

Int1TS1.H_2O

Charge 0
Spin multiplicity 1

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z

C	-1.40420300	-0.23473200	-0.02292900
N	-0.60445400	-0.93017500	-0.61428500
C	-2.87691900	-0.08302900	-0.00970800
C	-3.63594400	-1.09374200	-0.62565200
C	-3.54247900	1.01503800	0.55591600
C	-5.02514400	-1.01360400	-0.66241400
H	-3.10965700	-1.93219100	-1.07087200
C	-4.93561600	1.09534800	0.51152400
H	-2.95949400	1.80724200	1.01136800
C	-5.68146000	0.08206000	-0.09239800
H	-5.59893500	-1.80549900	-1.13728200
H	-5.43809300	1.95443700	0.94895800
H	-6.76619800	0.14513200	-0.12212600
Cu	1.10360900	0.18467600	0.60249000
C	3.87857100	-0.05964300	-0.12591900
C	3.25189300	0.43841800	-1.43305700
H	4.75068400	-0.69206300	-0.35787500
H	4.23911800	0.78296200	0.47710500
H	4.02721200	0.93617300	-2.03962700
H	2.88959300	-0.42853000	-1.99464600
N	2.88102700	-0.80096500	0.67282700
N	2.10595600	1.31878400	-1.16607000
C	2.44518200	2.73128600	-0.98385700
H	1.52685800	3.30316600	-0.82423600
H	3.06984100	2.85127000	-0.09271100
H	2.98955500	3.16048700	-1.84251700
C	3.42062000	-1.25326900	1.96519800
H	3.64910400	-0.38762400	2.59452400
H	2.66930000	-1.86088600	2.47563500
H	4.33966700	-1.84943000	1.84586000
H	-1.06846600	0.65157000	1.92640000
O	-0.75649300	0.87080100	1.03024000
H	1.41624200	1.22178900	-1.90588000
H	2.58790700	-1.62201300	0.11866400
O	1.59117700	-2.50370300	-1.26362500
H	1.29142700	-3.42295700	-1.20714800
H	0.76748300	-1.96371700	-1.11624100

Sum of electronic and zero-point Energies= -942.939016
Sum of electronic and thermal Energies= -942.918404
Sum of electronic and thermal Enthalpies= -942.917460
Sum of electronic and thermal Free Energies= -942.989869

Int1-3.H_2O

Charge 0
Spin multiplicity 1

Atomic	Coordinates (Angstroms)		

Type	X	Y	Z
C	1.61106700	1.27910900	-0.43425200
N	0.36692900	1.09280800	-0.52916200
C	2.69476200	0.32313900	-0.02668300
C	2.38096800	-0.93349900	0.50963600
C	4.04928000	0.66496000	-0.17446600
C	3.38348600	-1.82697000	0.88066100
H	1.33367600	-1.20000200	0.63151100
C	5.05479800	-0.23049800	0.19238900
H	4.30682300	1.63535700	-0.58144300
C	4.72770700	-1.47989000	0.72155300
H	3.11660500	-2.79487300	1.29862100
H	6.09715700	0.05126300	0.06544500
H	5.51136900	-2.17565200	1.01071200
Cu	-0.83294200	-0.27905200	-0.25123100
C	-3.57135100	-1.13365300	-0.34609700
C	-3.78265400	-0.26659100	0.89719300
H	-4.33863000	-1.92229000	-0.38440000
H	-3.67278600	-0.53067100	-1.25537500
H	-4.80560600	0.15314100	0.85748800
H	-3.75052000	-0.90857200	1.79051200
N	-2.20977200	-1.73200800	-0.36553800
N	-2.73445600	0.73112100	1.02221800
C	-2.71858000	1.43045600	2.30352400
H	-2.50332200	0.72189300	3.11280500
H	-1.92091300	2.17773100	2.28617900
H	-3.66883000	1.94026700	2.54210400
C	-2.03094300	-2.66478100	-1.50078000
H	-2.09091500	-2.10387000	-2.43665500
H	-1.04213700	-3.12368900	-1.43829600
H	-2.80066700	-3.45080200	-1.50801700
H	-2.09881200	-2.26746600	0.49817100
H	1.40804100	3.06488400	-0.98693500
O	2.17025100	2.51522900	-0.73270400
H	-2.76280100	1.41463200	0.25656300
O	-1.90577100	2.62042900	-1.08678700
H	-2.01670600	2.50574100	-2.04276700
H	-1.01168000	2.20610100	-0.90329300

Sum of electronic and zero-point Energies= -942.967955
Sum of electronic and thermal Energies= -942.947376
Sum of electronic and thermal Enthalpies= -942.946432
Sum of electronic and thermal Free Energies= -943.019837

Int1TS2.H_2O

Charge 0

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.45860100	0.30567600	-1.27170400
N	0.20100200	0.13320800	-1.50188700
C	2.39225400	-0.37702800	-0.34568300
C	1.98328300	-1.46663200	0.43762900
C	3.71995900	0.06937700	-0.24928400
C	2.87695800	-2.08853200	1.30689900
H	0.95993100	-1.82044800	0.34704800
C	4.61341800	-0.55207100	0.62403300
H	4.03601600	0.89919400	-0.87243600
C	4.19457800	-1.63059000	1.40567100
H	2.54896400	-2.93418800	1.90633800
H	5.63837000	-0.19640700	0.69069200
H	4.89089300	-2.11597700	2.08472400
Cu	-1.29464400	-0.44661700	-0.60881500
C	-3.93235000	-0.09169700	0.52745800
C	-3.21733800	0.88844800	1.45965900
H	-4.82389600	-0.50405100	1.02383800
H	-4.27170400	0.42448800	-0.37841900
H	-3.94541800	1.64170800	1.81091800
H	-2.87308900	0.35148800	2.35452900
N	-3.02311000	-1.18579200	0.09525300
N	-2.04408800	1.45422700	0.80680500
C	-1.11673500	2.16015800	1.69861500
H	-0.69380800	1.44226700	2.41088400
H	-0.29779100	2.57966700	1.10502800
H	-1.60078800	2.96813900	2.27343600
C	-3.69811000	-2.14140100	-0.81402600
H	-3.94304800	-1.63327800	-1.74975500
H	-3.01805100	-2.96552300	-1.03827600
H	-4.62342000	-2.53947500	-0.37226000
H	-2.74996500	-1.70190400	0.93423800
H	0.68768600	1.17223000	-2.31583700
O	1.92009400	1.30467000	-2.04517800
H	-2.33039900	2.08313200	0.05830000
O	1.62611900	3.30446400	-0.05557200
H	2.25548300	2.91407100	0.56927800
H	1.74528400	2.74793500	-0.85743500

Sum of electronic and zero-point Energies= -942.923023
Sum of electronic and thermal Energies= -942.902368
Sum of electronic and thermal Enthalpies= -942.901424
Sum of electronic and thermal Free Energies= -942.975559

Int1TS2-1.H_2O
Charge -2
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.16261400	-0.00969500	-0.25476000
N	1.33475600	-0.81356000	0.30647300
C	3.65011300	-0.20036100	0.03741600
C	4.08229000	-1.22125800	0.90166900
C	4.63127700	0.62174300	-0.54453400
C	5.43483500	-1.41479800	1.17664000
H	3.30050300	-1.84102800	1.33399000
C	5.98974800	0.43044300	-0.27303800
H	4.28952100	1.40777500	-1.20969500
C	6.40388100	-0.58853800	0.58938200
H	5.74321700	-2.21418700	1.85252300
H	6.73220900	1.08207700	-0.73700000
H	7.46288600	-0.73854000	0.80215100
Cu	-0.48609300	-0.49178000	0.03222700
C	-3.56703100	-0.15386100	0.09038400
C	-3.44594600	0.04732600	1.61371500
H	-4.55580300	-0.59401700	-0.16754000
H	-3.48637000	0.81131600	-0.42978500
H	-4.37811700	-0.26322100	2.12167300
H	-2.65048600	-0.63029100	1.99389300
N	-2.48458100	-1.00227100	-0.45869900
N	-3.17503500	1.44413500	1.91906200
C	-2.72123100	1.62832700	3.28112500
H	-1.85371700	0.99471700	3.56243500
H	-2.42869600	2.67512300	3.43155800
H	-3.53081000	1.40333400	3.99875400
C	-2.58711700	-1.10462300	-1.92637200
H	-2.51424600	-0.09101000	-2.33478500
H	-1.76326200	-1.71539400	-2.30474200
H	-3.55520500	-1.54835300	-2.25027300
H	-2.54397100	-1.93503800	-0.05102500
H	0.87994900	1.27700600	-1.41399400
O	1.98471000	1.01364500	-1.09562200
H	-2.42888400	1.73969900	1.24965500
C	-1.24867200	1.82203300	-1.23189400
O	-1.09174800	1.68163300	0.06349800
O	-0.19701100	1.62402000	-2.00083000
O	-2.38224600	2.07855900	-1.75045700
O	-4.80523800	-3.43570800	-0.49448200
H	-4.89093500	-2.58248600	-0.04018000

H	-4.23336600	-3.21160900	-1.24529000

Sum of electronic and zero-point Energies= -1206.717939
Sum of electronic and thermal Energies= -1206.692553
Sum of electronic and thermal Enthalpies= -1206.691608
Sum of electronic and thermal Free Energies= -1206.776537

Int1-3-1.H_2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.12771600	-0.33117200	-0.00052900
N	0.62719500	-1.36951000	-0.59526600
C	2.64457800	-0.17349800	-0.00258600
C	3.46970200	-1.11167500	-0.64354600
C	3.25433300	0.91516400	0.63912600
C	4.85652400	-0.96792400	-0.64277500
H	2.97698300	-1.94582300	-1.13431800
C	4.64401200	1.06282300	0.64264400
H	2.60450800	1.63272000	1.12919100
C	5.45409400	0.12215600	0.00186500
H	5.47886200	-1.70716500	-1.14649900
H	5.09749600	1.91563600	1.14732700
H	6.53735900	0.23542100	0.00289800
Cu	-1.20394200	-1.19847600	-0.42651900
C	-3.65811700	0.51914600	-0.41948600
C	-2.91762700	1.82939500	-0.12770300
H	-4.68606900	0.62363600	-0.02673900
H	-3.72639000	0.37097100	-1.50316700
H	-3.58563200	2.63394000	-0.47397000
H	-2.83679500	1.95278600	0.97259300
N	-3.03985900	-0.68474700	0.18539000
N	-1.64812000	1.97420900	-0.81706400
C	-1.13338800	3.33311600	-0.72725100
H	-1.07801800	3.72983000	0.30654900
H	-0.12126200	3.35398500	-1.14187500
H	-1.76108900	4.02306200	-1.31227300
C	-3.99397800	-1.79967400	0.27409500
H	-4.26875700	-2.13320800	-0.73217500
H	-3.52530500	-2.63840700	0.79580900
H	-4.91696500	-1.51329400	0.80736500
H	-2.69539300	-0.44152300	1.13336300
O	0.50370000	0.66119800	0.62959000
H	-0.93200500	1.36342000	-0.38501900
O	-1.27432400	-0.12536900	2.40759000

H	-0.96585200	-1.03939900	2.51819200
H	-0.57798200	0.22579500	1.73982700

Sum of electronic and zero-point Energies= -942.413003
Sum of electronic and thermal Energies= -942.393260
Sum of electronic and thermal Enthalpies= -942.392316
Sum of electronic and thermal Free Energies= -942.462483

Int1TS2-2.H_2O

Charge -2
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.94752000	1.61284700	0.01678000
N	-0.74060700	1.27862200	0.43210300
C	-2.94981300	0.49432300	-0.42067500
C	-2.59383500	-0.82071200	-0.75845700
C	-4.31264200	0.83219200	-0.50127000
C	-3.55329600	-1.76145300	-1.14802900
H	-1.53605800	-1.07695800	-0.70528200
C	-5.27950100	-0.10322900	-0.87249600
H	-4.56107600	1.86347500	-0.26773300
C	-4.90588300	-1.41149700	-1.20161000
H	-3.24361200	-2.77291800	-1.41574800
H	-6.33111000	0.18558000	-0.91235700
H	-5.65616400	-2.14397800	-1.50057400
Cu	0.52772400	-0.10783000	0.39209600
C	2.66007000	-2.40310000	0.18141000
C	3.03199500	-1.85280400	-1.20917700
H	2.80382700	-3.50088200	0.22321800
H	3.34033700	-1.95683400	0.91283300
H	3.56712400	-2.63269800	-1.78150000
H	2.08956600	-1.65743100	-1.77020800
N	1.28338200	-2.06870200	0.60126700

N	3.87213500	-0.67782700	-1.08277600
C	4.02563400	0.06109600	-2.32309100
H	3.07402300	0.19490100	-2.87873100
H	4.39574000	1.05951100	-2.07162200
H	4.73637300	-0.43612200	-3.00878000
C	1.01640300	-2.48611300	1.98731200
H	1.68303100	-1.92311900	2.64733700
H	-0.01189900	-2.22569400	2.25418700
H	1.19945700	-3.56803600	2.14482900
H	0.63205800	-2.55582800	-0.01193000
O	-2.46413600	2.76614200	-0.04299600
H	3.41640900	-0.02945300	-0.39741500
H	0.27397700	2.19612700	0.50684200
C	2.38057500	2.17018800	0.32440100
O	2.34923100	0.87295400	0.62003100
O	1.25189400	2.85320100	0.45291000
O	3.43566900	2.72361600	-0.05697400
O	-1.79563000	-0.57258100	2.59789100
H	-2.43853800	-0.85206800	1.92649500
H	-1.29118600	0.09775200	2.06372700

Sum of electronic and zero-point Energies= -1206.731594

Sum of electronic and thermal Energies= -1206.706661

Sum of electronic and thermal Enthalpies= -1206.705717

Sum of electronic and thermal Free Energies= -1206.789709

Int1-4.H_2O

Charge 0

Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.57766700	-1.76225500	-0.51223300

N	0.21971400	-1.70417000	-0.30357100
C	2.39657400	-0.58938100	-0.01250000
C	2.01372800	0.21582700	1.07173300
C	3.62114800	-0.33621000	-0.64518700
C	2.83202100	1.26726000	1.49349600
H	1.09450600	-0.00104400	1.60753200
C	4.42805700	0.72515700	-0.23674400
H	3.92240200	-0.99231500	-1.45562000
C	4.03446500	1.53291800	0.83374100
H	2.53508800	1.87194900	2.34758800
H	5.36918400	0.91730400	-0.74615000
H	4.66726400	2.35451400	1.16046800
Cu	-0.81341500	-0.16477300	-0.66010600
C	-2.52552100	1.92938700	0.23354700
C	-3.63347600	0.87516400	0.27347200
H	-2.97163300	2.93047000	0.12999600
H	-1.95183800	1.91728800	1.16684800
H	-4.32692100	1.13014900	1.09589900
H	-4.22173500	0.93660800	-0.65410200
N	-1.56894800	1.67060600	-0.87520200
N	-3.08258400	-0.46971400	0.36579200
C	-4.06741800	-1.52964400	0.16265100
H	-4.45264600	-1.48967700	-0.86312500
H	-3.57910000	-2.49781900	0.30433100
H	-4.92863100	-1.47171000	0.85136600
C	-0.53938600	2.73109900	-0.98328300
H	0.11079500	2.69163100	-0.10645100
H	0.07224600	2.54694500	-1.86881400
H	-0.99338800	3.73052700	-1.05282400
H	-2.10246400	1.66326900	-1.74708100
H	-0.16873600	-2.56892100	-0.68446300
O	2.15390400	-2.70677400	-1.05842800
H	-2.60545600	-0.61814100	1.25925700
O	-0.97591100	-1.26240900	2.25957900
H	-0.47708700	-1.52585900	1.44016600
H	-0.63118900	-1.82628000	2.96776200

Sum of electronic and zero-point Energies= -942.996741
Sum of electronic and thermal Energies= -942.976077
Sum of electronic and thermal Enthalpies= -942.975133
Sum of electronic and thermal Free Energies= -943.048461

Int2-1.H_2O

Charge -1
Spin multiplicity 1
Atomic Coordinates (Angstroms)

Type	X	Y	Z
Cu	-1.14887600	-0.75014800	0.08065100
C	1.94178700	0.54935000	-0.40436900
C	0.69751100	1.12055500	-1.09291200
H	2.82263300	0.80630900	-1.03606500
H	2.06768100	1.06485100	0.55672200
H	0.92825400	2.19326700	-1.27972800
H	0.62039400	0.66779300	-2.11127100
N	1.85976800	-0.88268500	-0.15468800
N	-0.52466800	1.00616700	-0.32346300
C	-1.53905200	1.86227000	-0.91271000
H	-1.80492100	1.60337100	-1.96160000
H	-2.46313900	1.81644800	-0.32506700
H	-1.21488900	2.92868500	-0.93861000
C	3.11931900	-1.49132000	0.21379900
H	3.45546000	-1.08464500	1.17702700
H	2.98561800	-2.57210900	0.33891900
H	3.94649700	-1.32568800	-0.51271600
H	1.43928800	-1.36053200	-0.94780100
O	-1.74333300	-2.42559400	0.48216400
H	-2.63236200	-2.46533700	0.09277400
O	0.28329300	2.56397900	1.84574700
H	0.23422000	3.38213900	1.32867200
H	-0.05009300	1.88315400	1.18078900

Sum of electronic and zero-point Energies= -618.001435
Sum of electronic and thermal Energies= -617.986681
Sum of electronic and thermal Enthalpies= -617.985736
Sum of electronic and thermal Free Energies= -618.044445

Int2-2.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.85735500	-0.21079700	-0.14290500
N	-0.69771900	-0.28842200	-0.20896200
C	-3.27832200	-0.12837700	-0.06238700
C	-3.97423800	0.81168800	-0.84651200
C	-3.98138600	-0.98905200	0.80259000
C	-5.36135400	0.88384400	-0.76079700
H	-3.42392700	1.47041000	-1.51058000
C	-5.36841000	-0.90342600	0.87667400
H	-3.43612500	-1.70992200	1.40313800

C	-6.05931500	0.02970400	0.09806000
H	-5.89909600	1.60810900	-1.36535800
H	-5.91151500	-1.56643000	1.54348300
H	-7.14193200	0.09127400	0.16054400
Cu	1.13927700	-0.37872000	-0.29261500
C	3.34414500	1.45034000	-0.59519900
C	3.92935500	0.02984500	-0.67110800
H	4.15539600	2.18002100	-0.41826500
H	2.87949200	1.71215500	-1.55635000
H	4.41692100	-0.07620300	-1.65879100
H	4.75049900	-0.05582900	0.07299400
N	2.29618800	1.52802100	0.43011100
N	2.91643400	-0.98664400	-0.44833200
C	3.35913200	-2.29173200	-0.89914400
H	4.28517000	-2.61994600	-0.38471200
H	2.59128000	-3.04471000	-0.69302200
H	3.57970200	-2.32759500	-1.98421500
C	1.76543500	2.87217800	0.62741700
H	1.27192800	3.21273400	-0.29097500
H	1.02032000	2.85653500	1.42931000
H	2.53986800	3.61575500	0.88649900
H	2.65213500	1.14154700	1.31010400
O	3.11146300	-0.60625000	2.32885700
H	3.00422400	-0.91828300	1.38047800
H	4.02449300	-0.83270800	2.56084500

Sum of electronic and zero-point Energies= -866.545921
Sum of electronic and thermal Energies= -866.526399
Sum of electronic and thermal Enthalpies= -866.525455
Sum of electronic and thermal Free Energies= -866.596865

Int2TS1.H2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.33609000	-0.59536900	0.13118400
N	-0.72262600	-1.33737900	0.88252800
C	-2.78196300	-0.26200100	0.00173800
C	-3.66616800	-0.84737800	0.92632400
C	-3.31132000	0.59275200	-0.97796300
C	-5.03215500	-0.58345000	0.87697100
H	-3.23891200	-1.50908200	1.67399200
C	-4.68297300	0.85559600	-1.02760800
H	-2.63218700	1.03848000	-1.69494900

C	-5.55003900	0.27191400	-0.10235700
H	-5.69836800	-1.04525900	1.60349300
H	-5.07498100	1.52042400	-1.79538900
H	-6.61772300	0.47864100	-0.14260100
Cu	1.21228500	-0.80745900	-0.69550700
C	2.84187400	1.72139000	-0.46619600
C	3.73386400	0.48014800	-0.28046700
H	3.50017200	2.60364900	-0.35065000
H	2.46990900	1.73936000	-1.50230400
H	4.46060100	0.51442100	-1.12513400
H	4.35196000	0.63781100	0.63339200
N	1.69318600	1.81812400	0.45016800
N	3.03733200	-0.78538900	-0.20872100
C	3.96123700	-1.88778900	-0.32818600
H	4.75246900	-1.86057000	0.45318100
H	3.43103700	-2.84086100	-0.21771100
H	4.50100300	-1.92034600	-1.30221500
C	1.41643800	3.16987600	0.90558600
H	1.09461900	3.79980000	0.06395300
H	0.59958700	3.14852800	1.63584300
H	2.28362900	3.67634100	1.37637300
H	1.79204500	1.17707100	1.24626600
H	-0.10969000	0.95610800	-0.53249700
O	-0.53915100	0.20711000	-1.01177000
O	1.80152400	-0.51642700	2.35188300
H	2.34493700	-0.74536300	1.54896800
H	0.92315700	-0.83993400	2.05481300

Sum of electronic and zero-point Energies= -942.370552
Sum of electronic and thermal Energies= -942.350697
Sum of electronic and thermal Enthalpies= -942.349753
Sum of electronic and thermal Free Energies= -942.420797

Int2-3.H_2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.55591900	1.23286800	-0.09223100
N	-0.34047800	0.89956900	-0.09834200
C	-2.76252600	0.34616800	0.02920900
C	-2.61128800	-1.04129100	0.17653100
C	-4.06541000	0.87310900	0.00260600
C	-3.72167900	-1.87516700	0.29203900
H	-1.60274800	-1.44680100	0.19766900

C	-5.17845000	0.03803600	0.11763100
H	-4.19134100	1.94375500	-0.10840700
C	-5.01386100	-1.34096400	0.26308600
H	-3.57823800	-2.94797900	0.40573500
H	-6.17861900	0.46759800	0.09409900
H	-5.88097100	-1.99245700	0.35348300
Cu	0.82028300	-0.52753100	-0.10091400
C	3.89566500	-0.06390000	-0.38204200
C	3.53643200	-1.55170000	-0.31459300
H	4.95805300	0.02689200	-0.70338400
H	3.28773200	0.41231000	-1.16308400
H	3.96350800	-2.01765300	-1.23746700
H	4.14472000	-2.00034200	0.51483300
N	3.64746200	0.63922500	0.87058400
N	2.14048600	-1.83303900	-0.17210900
C	1.90340500	-3.24861100	-0.18226400
H	2.40867000	-3.78787100	0.65534400
H	0.83179300	-3.46382700	-0.09774600
H	2.26505900	-3.75431100	-1.11131400
C	3.99393400	2.05000200	0.83292600
H	3.27636700	2.58640900	0.20110200
H	3.91343300	2.47254400	1.84148100
H	5.01827200	2.26074900	0.45386600
H	4.15328100	0.16723000	1.61740300
H	-1.13230500	3.08222900	-0.29124500
O	-1.96550500	2.56515400	-0.20318000
O	0.77343700	3.33561400	-0.50180700
H	0.87055000	3.26276300	-1.46515700
H	0.56701500	2.36942800	-0.24913200

Sum of electronic and zero-point Energies= -942.412469
Sum of electronic and thermal Energies= -942.391839
Sum of electronic and thermal Enthalpies= -942.390895
Sum of electronic and thermal Free Energies= -942.465311

Int2TS2.H_2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.02768400	-1.72267900	-0.13627600
N	-0.78466000	-2.07940600	-0.17171200
C	-2.65224900	-0.38371700	0.03433000
C	-1.88604600	0.78411000	0.17479100
C	-4.05304100	-0.28443400	0.05782000
C	-2.51331400	2.01976000	0.33624800

H	-0.80025500	0.72906900	0.15625300
C	-4.67694700	0.95298100	0.21937600
H	-4.63132800	-1.19560300	-0.05221100
C	-3.90819300	2.11102700	0.35957100
H	-1.90435300	2.91393800	0.44534000
H	-5.76363500	1.01339700	0.23634700
H	-4.39212700	3.07765300	0.48677500
Cu	0.90141400	-1.33599300	-0.06605800
C	2.19749300	1.33288700	-1.37465300
C	3.18128500	0.25591000	-0.90082500
H	2.76557100	2.00246300	-2.05548600
H	1.40872800	0.86485500	-1.98409100
H	3.54401500	-0.26563600	-1.81363200
H	4.07762300	0.77964300	-0.49425800
N	1.58057500	2.08341100	-0.28640200
N	2.66581600	-0.66520900	0.09396900
C	3.68770500	-1.65257800	0.40230200
H	4.61611400	-1.17830000	0.79288300
H	3.32949300	-2.34478500	1.17281600
H	4.00252500	-2.26113100	-0.47173300
C	1.20669800	3.43505500	-0.63669900
H	0.40608000	3.42561700	-1.39025300
H	0.81910000	3.95252100	0.24914900
H	2.03336300	4.05093400	-1.05603300
H	2.14905400	2.04629700	0.56047600
H	-1.62523600	-3.20714200	-0.32648500
O	-2.82135500	-2.78594600	-0.28199800
O	3.01274400	1.08661300	2.18029900
H	3.97850000	1.10222400	2.09817000
H	2.74829100	0.37093800	1.50835000

Sum of electronic and zero-point Energies= -942.379620
Sum of electronic and thermal Energies= -942.359371
Sum of electronic and thermal Enthalpies= -942.358427
Sum of electronic and thermal Free Energies= -942.431329

Int2-4.H_2O

Charge -1
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.54110000	1.30623600	0.13748900
N	-0.27151500	0.91058800	0.11591900
C	-2.63946300	0.26722400	0.02824200
C	-2.40298900	-1.11058600	-0.07729400
C	-3.96760900	0.71866200	0.03456400

C	-3.46568500	-2.01062100	-0.17476600
H	-1.37725800	-1.47103200	-0.08050500
C	-5.03120100	-0.17814500	-0.06309700
H	-4.13107700	1.78776100	0.11873400
C	-4.78456000	-1.54963600	-0.16874000
H	-3.26084700	-3.07629700	-0.25577000
H	-6.05484000	0.19232900	-0.05688900
H	-5.61209300	-2.25257500	-0.24540000
Cu	0.89176200	-0.57458300	-0.00792400
C	3.98342000	-0.22044200	-0.34240100
C	3.53402900	-1.58198500	0.19937200
H	5.06398300	-0.08401800	-0.12023700
H	3.87385400	-0.22286400	-1.43547600
H	4.25315000	-2.33119000	-0.20300200
H	3.72987600	-1.58353800	1.30627900
N	3.17091000	0.87495300	0.17573500
N	2.18388400	-1.92808600	-0.14861800
C	1.90136400	-3.28822000	0.23511600
H	1.96758100	-3.48486800	1.33339100
H	0.89021000	-3.57525400	-0.07810600
H	2.60544300	-4.01227500	-0.23552400
C	3.55993100	2.19801600	-0.28355300
H	3.48168700	2.23019800	-1.37787700
H	2.86808700	2.94550900	0.12038800
H	4.59900200	2.48887500	-0.02196900
H	3.15872900	0.84162400	1.19337800
H	0.31445100	1.74146400	0.20996400
O	-1.91401700	2.51469200	0.24364900
O	0.33570300	4.07445700	0.07316300
H	0.46219100	3.90527800	-0.87278800
H	-0.52650500	3.60538500	0.24588000

Sum of electronic and zero-point Energies= -942.446960
Sum of electronic and thermal Energies= -942.426357
Sum of electronic and thermal Enthalpies= -942.425413
Sum of electronic and thermal Free Energies= -942.499509

Int1TS3.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.05868700	1.90411500	-0.02525800
N	0.83418900	1.63241800	-0.54240200
C	3.19305300	1.00765700	-0.49060200
C	3.10141800	0.21143900	-1.64359600

C	4.39440200	1.01271000	0.23385800
C	4.18243800	-0.57367100	-2.05151000
H	2.18082300	0.23332300	-2.21765300
C	5.47121000	0.22101600	-0.16662700
H	4.46102700	1.66358200	1.10012000
C	5.36789700	-0.57548300	-1.31080900
H	4.10466900	-1.17555100	-2.95402900
H	6.39539300	0.23237500	0.40616400
H	6.20952100	-1.18560700	-1.62939300
Cu	-0.17228200	0.00099900	0.09155200
C	1.17213300	-1.60325000	2.23734600
C	0.92111100	-0.24296400	2.88208800
H	2.05315300	-2.07891900	2.69802200
H	0.31433300	-2.26372300	2.41559200
H	0.89012900	-0.35752800	3.97849900
H	1.75026500	0.43738000	2.65323600
N	1.33740300	-1.45883200	0.78032400
N	-0.30996700	0.36195800	2.35319100
C	-0.44618600	1.77188400	2.75518600
H	0.37677900	2.35037200	2.32431100
H	-1.38909500	2.16598900	2.36682900
H	-0.43683800	1.89759900	3.85036700
C	1.49346800	-2.74740400	0.09428700
H	0.55239100	-3.30473900	0.14005000
H	1.73956400	-2.56579900	-0.95439800
H	2.28643500	-3.36458200	0.54351600
H	2.17483600	-0.90339700	0.59833000
H	0.23066400	2.40204600	-0.24210900
O	2.32795200	2.82142700	0.77580000
H	-1.10984300	-0.17324000	2.69757500
C	-2.58473500	2.71908100	-1.89543300
C	-1.95879200	1.47417400	-1.84562800
C	-2.13363900	0.67781400	-0.70624800
C	-2.99146100	1.06807600	0.33027700
C	-3.60900600	2.32030300	0.25803100
C	-3.40895500	3.14694500	-0.84897100
H	-2.42521100	3.35547900	-2.76165400
H	-1.31316700	1.14990700	-2.65295800
H	-3.16071000	0.41863500	1.18247100
H	-4.25807900	2.63854700	1.06995400
H	-3.90088800	4.11362600	-0.90370100
I	-1.94782000	-1.61765600	-1.01232400
O	-2.55846800	-1.67097700	2.67873000
H	-3.48659500	-1.77088700	2.93995500
H	-2.53442900	-1.91515800	1.73668700

Sum of electronic and zero-point Energies= -1185.904389

Sum of electronic and thermal Energies= -1185.876116
Sum of electronic and thermal Enthalpies= -1185.875172
Sum of electronic and thermal Free Energies= -1185.966266

Int1-5.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.33867500	0.50174000	1.62215600
N	1.01011200	0.15609600	1.60811500
C	3.25878800	0.00624900	0.53337800
C	2.83410300	-0.49659500	-0.70462000
C	4.63649000	0.08291200	0.78885600
C	3.76051400	-0.91823900	-1.66124800
H	1.77650500	-0.54479200	-0.94605500
C	5.56260500	-0.34782500	-0.15841700
H	4.95355000	0.48977000	1.74290800
C	5.12770700	-0.85025900	-1.38798000
H	3.41106300	-1.29275500	-2.61983300
H	6.62566900	-0.28709400	0.05931500
H	5.84933900	-1.18039100	-2.13057800
Cu	-0.31167600	-0.20684500	0.26002100
C	-1.40465000	-2.78328300	1.32258100
C	-1.83251100	-1.91610500	2.50114600
H	-1.26991600	-3.82079100	1.66490300
H	-2.17365200	-2.79203900	0.54221300
H	-2.72401200	-2.36554400	2.97115700
H	-1.03817100	-1.92850000	3.25988900
N	-0.15250600	-2.27798900	0.71713800
N	-2.04809000	-0.52410900	2.09818700
C	-2.17518900	0.36232700	3.26043600
H	-1.23828600	0.36524500	3.82927600
H	-2.36733300	1.38479100	2.92542100
H	-2.98417300	0.06208400	3.94687600
C	0.39909700	-3.21896100	-0.27728700
H	-0.26763300	-3.26078300	-1.14143100
H	1.37944900	-2.86750200	-0.60446800
H	0.50412800	-4.22711500	0.14766600
H	0.53654200	-2.13179500	1.45795100
H	0.56225300	0.68190300	2.35783400
O	2.81201400	1.13164300	2.57449600
H	-2.91243900	-0.45932400	1.54983400
C	0.57571900	3.77969000	-0.87504500
C	0.68274800	2.39704400	-0.68342100

C	-0.37444400	1.71249200	-0.09225000
C	-1.53391000	2.37774600	0.30119000
C	-1.62472500	3.76269100	0.10957900
C	-0.57154400	4.46577500	-0.47475700
H	1.40441700	4.31500000	-1.33152800
H	1.58766300	1.88530700	-0.99097200
H	-2.37901600	1.83579300	0.70985100
H	-2.53176300	4.28197200	0.41032400
H	-0.64561200	5.53974100	-0.62124000
I	-1.60926800	-0.58570000	-1.94303600
O	-4.40809700	-0.14211600	0.28585000
H	-3.84230600	-0.30014000	-0.49577800
H	-4.74124900	0.75894600	0.15414500

Sum of electronic and zero-point Energies= -1185.917436
Sum of electronic and thermal Energies= -1185.889169
Sum of electronic and thermal Enthalpies= -1185.888225
Sum of electronic and thermal Free Energies= -1185.978832

Int1TS4.H_2O

Charge 0
Spin multiplicity 1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.00068900	0.37472400	1.81129100
N	0.68260900	0.61741100	1.51594500
C	3.03997600	0.40686100	0.72472300
C	3.09521100	1.40770000	-0.25297800
C	4.05171200	-0.56544100	0.76320500
C	4.11984300	1.41021000	-1.20441300
H	2.35809800	2.20168500	-0.24512800
C	5.06147800	-0.57515600	-0.19800400
H	4.03838400	-1.29968500	1.56275500
C	5.09493800	0.41063900	-1.18921900
H	4.16348800	2.20228700	-1.94762200
H	5.83107900	-1.34176000	-0.16631400
H	5.88780900	0.41062000	-1.93236500
Cu	-0.37661100	-0.23352200	0.14157100
C	0.76464500	-2.32590200	-1.78761000
C	1.04803300	-2.83047600	-0.37593200
H	1.50500100	-2.74491300	-2.48830200
H	-0.22222500	-2.67803600	-2.11080900
H	1.09880400	-3.93095700	-0.37985000
H	2.02105800	-2.46313700	-0.02907000
N	0.73747200	-0.85327700	-1.83141500
N	0.02002400	-2.33649200	0.55365100

C	0.27425600	-2.69845100	1.96131800
H	1.17956500	-2.19747900	2.31181400
H	-0.56135600	-2.34835000	2.57102600
H	0.39569500	-3.78484000	2.08619300
C	0.24610900	-0.36588300	-3.13046700
H	-0.81275300	-0.62139300	-3.22704800
H	0.33380300	0.72180200	-3.17526400
H	0.79881600	-0.79891300	-3.97899000
H	1.68564700	-0.50543800	-1.68368300
H	0.11948400	0.60298800	2.36663600
O	2.34121600	0.10752000	2.96687200
H	-0.88497500	-2.71905400	0.27429000
C	-0.62209300	3.71985400	-1.10488100
C	-0.09792000	2.44876900	-0.83570900
C	-0.57791300	1.74430100	0.26587900
C	-1.50557000	2.30668200	1.14473100
C	-2.01323100	3.57433500	0.86029900
C	-1.57548600	4.28657800	-0.26119000
H	-0.27229200	4.25991400	-1.98124000
H	0.64175500	2.02134200	-1.49924600
H	-1.85262200	1.75348300	2.01122900
H	-2.75528600	4.00642500	1.52671900
H	-1.96988100	5.27703100	-0.46849400
I	-2.88806400	-0.83300500	-0.59529500
O	-2.08127200	-0.42593600	2.97345900
H	-2.81415000	-0.33703800	3.60197100
H	-2.51216800	-0.58738200	2.10967900

Sum of electronic and zero-point Energies= -1185.907325
Sum of electronic and thermal Energies= -1185.879196
Sum of electronic and thermal Enthalpies= -1185.878252
Sum of electronic and thermal Free Energies= -1185.968843

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2. Full citation for reference 15

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