Gas phase

1AB
SCF Energy = -1034.33411261 au

C	-5.76998500	-1.03924500	-0.03071100
C	-5.11746600	0.17330900	-0.00928100
C	-3.72386500	0.23285700	-0.01263500
C	-2.95523000	-0.94218600	-0.03752200
C	-3.64031700	-2.16364700	-0.05691100
C	-5.01874400	-2.21200000	-0.05396900
C	-3.08954500	1.56376100	0.00548100
C	-1.49540700	-0.86632400	-0.03312500
C	-0.85569000	0.40178700	0.01031800
C	-1.61233100	1.59851000	-0.00988800
C	-0.98797800	2.82561600	-0.06905100
H	-1.61188100	3.71124000	-0.08987600
C	0.40115600	2.90950900	-0.14154600
C	1.15734700	1.76397600	-0.09442900
C	0.56394800	0.49445300	0.02787500
H	-6.85259100	-1.08215600	-0.02858700
H	-5.65864100	1.11152200	0.00969600
H	-3.09106800	-3.09583700	-0.06948000
H	-5.51744500	-3.17467000	-0.06823100
H	0.88322300	3.87389800	-0.24964900
H	2.23283600	1.82905100	-0.19447900
C	1.35322100	-0.70083800	0.09262400
C	-0.69018500	-1.98301500	-0.09400600
C	0.70238900	-1.91194000	-0.02983500
H	-1.13440200	-2.96765800	-0.16337600
H	1.26725900	-2.83401700	-0.03100700
O	-3.74952600	2.58851700	0.02812700
C	3.53013000	-1.76735400	-0.14206000
C	3.31837800	0.10773100	1.33095200
C	5.02244300	-1.40982100	0.00400100
H	3.31387000	-2.64220400	0.49398600
C	4.62715400	0.76387300	0.87744100
H	2.61729500	0.84623300	1.71388500
H	5.60660300	-1.98635100	-0.71697200
H	5.28734500	0.87770500	1.74619800
N	2.73009300	-0.61660200	0.21682600
N	5.29955500	-0.00404100	-0.16083200
C	5.07088700	0.47903700	-1.50532900
H	5.41397400	1.51321700	-1.58189700
H	5.66513800	-0.11575400	-2.20395600
H	4.01931600	0.44184700	-1.82755900
H	5.37419800	-1.70500800	0.99757400
H	3.28699700	-2.04485000	-1.17123200
H	3.51157900	-0.59562900	2.15654500
H	4.43319900	1.76750100	0.49108000

2AB
SCF Energy = -995.075298425 au
C   5.57092200 -1.03649200 -0.25994500
C   4.91130300   0.17210300 -0.23224400
C   3.52472200   0.22508200 -0.08950400
C   2.76982700 -0.95383500   0.02853200
C   3.46232300 -2.17106400 -0.00158500
C   4.83371400 -2.21250600 -0.14289900
C   2.88436300   1.55368300 -0.06601000
C   1.31692400 -0.88566700   0.17566400
C   0.67502600   0.37948100   0.20572600
C   1.41655300   1.58103700   0.09505300
C   0.78257800   2.80409800   0.13601500
H   1.39505600   3.69376700   0.04837600
C   -0.60084400   2.88562500   0.29609700
C   -1.34412900   1.73587800   0.39996400
C   -0.73866900   0.46723100   0.34617400
H   6.64812800 -1.07371400 -0.37041600
H   5.44146900   1.11282300 -0.31888400
H   2.92401800 -3.10543100   0.08769500
H   5.33789600 -3.17228500 -0.16198100
H   -1.08526200   3.85369700   0.34547500
H   -2.41645500   1.79131600   0.54170400
C   -1.51979500 -0.72678000   0.43466300
C   0.52367900 -2.01042200   0.29280100
C   -0.86239600 -1.93946400   0.42420600
H   0.97520200 -2.99419600   0.27799400
H   -1.44677100 -2.84712400   0.51489800
O   3.53374800   2.58019300 -0.17462700
N   -2.88612200 -0.67513700   0.60968900
C   -3.70534400 -0.38471600 -0.33322700
N   -5.02146900 -0.21304700 -0.02398400
C   -3.30493700 -0.21158200 -1.77035200
H   -3.60472700   0.76748800 -2.14975400
H   -2.22555000 -0.30371200 -1.86462500
H   -3.77147400 -0.97250000 -2.39996500
C   -5.43819100 -0.45580300   1.33690100
H   -5.53457300 -1.52743100   1.55133400
H   -4.70001800 -0.04713000   2.02367800
H   -6.40329600   0.02543200   1.50119000
C   -6.05895800 -0.27757800 -1.02207700
H   -5.72792400   0.15420000 -1.96358800
H   -6.39403900 -1.30683800 -1.21141800
H   -6.92054700   0.29752500 -0.67834600

3AB
SCF Energy = -955.790147098 au
C   5.42454800 -0.89827100   0.32940000

C	4.72203300	0.28446200	0.26642200
C	3.33502400	0.28310100	0.11787500
C	2.62343800	-0.92477200	0.02946400
C	3.35914500	-2.11501000	0.09678800
C	4.73048300	-2.10294000	0.24343600
C	2.64668900	1.58552400	0.05576300
C	1.16955600	-0.91373600	-0.12350300
C	0.47967100	0.32425700	-0.17977500
C	1.17951900	1.55444200	-0.11062500
C	0.50685200	2.75292000	-0.20606900
H	1.08917100	3.66517400	-0.15185200
C	-0.87543200	2.78047900	-0.38893500
C	-1.58013800	1.60366500	-0.44328000
C	-0.93893800	0.35601100	-0.31755900
H	6.50192300	-0.89361200	0.44432900
H	5.21743300	1.24580900	0.32893900
H	2.85523300	-3.07048800	0.03557600
H	5.26861600	-3.04302100	0.29219500
H	-1.39022400	3.72771000	-0.49819700
H	-2.64900100	1.62718100	-0.61230400
C	-1.67117500	-0.87229500	-0.36200900
C	0.42271500	-2.07163900	-0.22990300
C	-0.96375900	-2.05675100	-0.35425400
H	0.91376200	-3.03599800	-0.20829800
H	-1.51542300	-2.98626300	-0.42391900
O	3.25735800	2.63807000	0.13770500
N	-3.04948400	-0.91222100	-0.46965500
C	-3.77363500	-0.35342600	0.42182300
N	-5.11365700	-0.25516300	0.34188800
C	-5.82777000	-0.81086100	-0.77803600
H	-6.59887900	-0.11073800	-1.11016000
H	-5.12352200	-0.99509700	-1.58657400
H	-6.31100000	-1.75749300	-0.50971500
C	-5.89035800	0.19967000	1.46210100
H	-5.23288100	0.62669800	2.21964700
H	-6.60158100	0.96950300	1.14815100
H	-6.45682300	-0.62097500	1.91849300
H	-3.35450100	0.08976200	1.33167700

4AB
SCF Energy = -1073.6424857 au

C	-6.09458200	-1.11653200	-0.17093900
C	-5.44852400	0.09604200	-0.26433800
C	-4.06260800	0.17856000	-0.12879500
C	-3.29441700	-0.97425800	0.10542100
C	-3.97339200	-2.19612500	0.19718000
C	-5.34414500	-2.26674700	0.06190900
C	-3.43732100	1.50993900	-0.23840600
C	-1.84263100	-0.87560000	0.24364400

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C    -1.21494300   0.39319800   0.14611000
C    -1.96996800   1.56960300  -0.08211000
C    -1.34992900   2.79795600  -0.16205100
H    -1.97242400   3.66772600  -0.33618900
C     0.03232000   2.91045900  -0.01101400
C     0.78810200   1.78439400   0.20406700
C     0.19763600   0.50986600   0.27486000
H    -7.17128100  -1.17663100  -0.27620100
H    -5.98913000   1.01750000  -0.44381600
H    -3.42459500  -3.11090300   0.37829500
H    -5.83750600  -3.22926900   0.13881900
H     0.50570300   3.88423500  -0.05588000
H     1.85969500   1.86437800   0.34045500
C     0.99405900  -0.66026100   0.47974400
C    -1.03651100  -1.97390700   0.47258900
C     0.34872400  -1.87493700   0.59346400
H    -1.47714600  -2.95912000   0.55753900
H     0.94298100  -2.76293200   0.77227100
O    -4.09821200   2.51327400  -0.44824800
N     2.35828700  -0.57303900   0.64258300
C     3.17366300  -0.37840600  -0.33090300
N     4.49576100  -0.24839800  -0.05691200
C     4.94397200  -0.33321000   1.32050400
H     4.33544100  -1.08239900   1.82906600
H     5.97726200  -0.69020900   1.30920800
C     5.50741300  -0.03038100  -1.06717100
H     5.06775700   0.48410800  -1.92163000
H     6.24611700   0.66125800  -0.64993600
C     4.84755000   0.99343900   2.05205500
H     5.43304800   1.76744200   1.54910800
H     3.80746100   1.31840700   2.10261300
H     5.22375000   0.89582900   3.07290300
C     6.19665100  -1.30731700  -1.51996700
H     5.48516300  -1.99268700  -1.98548700
H     6.98210500  -1.08381000  -2.24565200
H     6.65544900  -1.82607800  -0.67554400
C     2.74849900  -0.29107800  -1.76977900
H     1.70736000  -0.59287200  -1.86086500
H     2.83590300   0.73357700  -2.13975600
H     3.35654800  -0.93186900  -2.40948100

Ethanol phase

1AB
SCF Energy =  -1034.36354764 au
C     5.75504100  -1.07316000   0.02606700
C     5.11593300   0.14503000   0.00904600
C     3.71895700   0.22341200   0.01520100
C     2.93737900  -0.94830800   0.04029100
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C	3.61265000	-2.17927700	0.05381200
C	4.98948800	-2.24026000	0.04707900
C	3.09398400	1.54969200	-0.00066100
C	1.48499200	-0.86034600	0.03897300
C	0.85752300	0.40942700	-0.01666900
C	1.62654300	1.60162400	0.00761700
C	1.00639800	2.83592100	0.07155400
H	1.62200400	3.72727400	0.09895700
C	-0.37847900	2.92910800	0.14607000
C	-1.14373100	1.78624400	0.08703500
C	-0.56341900	0.51484100	-0.04852400
H	6.83760800	-1.12759600	0.02110400
H	5.68282900	1.06824100	-0.00936900
H	3.05461700	-3.10679600	0.06232800
H	5.47927200	-3.20802700	0.05555300
H	-0.85575600	3.89505200	0.26206800
H	-2.21722900	1.87209600	0.18762000
C	-1.36625800	-0.67895700	-0.12059400
C	0.66608000	-1.97378400	0.12195100
C	-0.71956700	-1.89694700	0.05249800
H	1.10190200	-2.96096800	0.21240400
H	-1.28876300	-2.81631000	0.06858300
O	3.77106500	2.57915000	-0.01729400
C	-3.53358000	-1.77496600	0.01901800
C	-3.34446800	0.22098500	-1.30816500
C	-5.01859900	-1.40395400	-0.10841400
H	-3.31857200	-2.62114500	-0.65048700
C	-4.61809700	0.85509900	-0.75237900
H	-2.65191300	0.97631700	-1.67069500
H	-5.60211800	-2.05455200	0.54682800
H	-5.28211800	1.08797800	-1.59307800
N	-2.72020500	-0.61464300	-0.29482000
N	-5.30194200	-0.01717700	0.20337800
C	-5.01975700	0.31496300	1.58687500
H	-5.35291000	1.33511100	1.79239800
H	-5.58349200	-0.35697100	2.23994900
H	-3.95727800	0.24721400	1.86355500
H	-5.36035200	-1.59486900	-1.12952100
H	-3.29776300	-2.09412600	1.03726900
H	-3.58837200	-0.41616800	-2.16992900
H	-4.38916900	1.79945800	-0.25315900

2AB
SCF Energy = -995.10394219 au

C	-5.58867300	-0.98492200	0.25561400
C	-4.91557000	0.21455200	0.20765200
C	-3.52377700	0.25182400	0.07536100
C	-2.78187800	-0.94197100	-0.01148700
C	-3.49013100	-2.15200600	0.04094000

C	-4.86261100	-2.17321900	0.17157000
C	-2.86294600	1.56188700	0.03374400
C	-1.33130400	-0.89610600	-0.15079800
C	-0.67303300	0.35780200	-0.19497200
C	-1.40161700	1.57228700	-0.11402900
C	-0.74553900	2.78728000	-0.17376200
H	-1.33038800	3.69742700	-0.11070600
C	0.63763400	2.84648300	-0.32545700
C	1.36520500	1.68215300	-0.40263900
C	0.74393200	0.42411400	-0.32663000
H	-6.66749600	-1.00748400	0.35801100
H	-5.45137600	1.15413500	0.27151100
H	-2.96358700	-3.09571200	-0.01968200
H	-5.37869300	-3.12647100	0.20944100
H	1.13683400	3.80621600	-0.38972200
H	2.43871100	1.72913100	-0.53822100
C	1.51440100	-0.78374400	-0.39158800
C	-0.55250200	-2.03747900	-0.25061600
C	0.83203700	-1.98820400	-0.37444800
H	-1.01720100	-3.01515600	-0.22734600
H	1.39900400	-2.90937800	-0.44585700
O	-3.50666500	2.60772400	0.12086500
N	2.87426000	-0.76503700	-0.56540000
C	3.71235900	-0.37697800	0.33987100
N	5.01039900	-0.22877100	-0.00190600
C	3.33112100	-0.10267500	1.76220600
H	3.59147200	0.91715700	2.05374800
H	2.26144800	-0.24364800	1.90159900
H	3.85702200	-0.78370300	2.43554600
C	5.41921800	-0.57846800	-1.34268800
H	5.41667500	-1.66379900	-1.50091500
H	4.74741800	-0.12957300	-2.07398400
H	6.42891800	-0.20390600	-1.50938200
C	6.06314200	-0.13607000	0.98454000
H	5.73095700	0.40455500	1.86757400
H	6.42169200	-1.12588800	1.29388700
H	6.90250000	0.41172400	0.55441700

3AB
SCF Energy = -955.819365387 au

C	5.43726600	-0.86177400	0.29435900
C	4.72515700	0.31422800	0.23340400
C	3.33238800	0.30397900	0.10546500
C	2.62969000	-0.91420700	0.03618900
C	3.37751900	-2.09966100	0.10245700
C	4.75014300	-2.07435400	0.22871600
C	2.62819700	1.58967100	0.04730300
C	1.17832600	-0.91865600	-0.09871000
C	0.47696700	0.31041100	-0.15837000

C	1.16870600	1.54899000	-0.10968500
C	0.47918500	2.74135600	-0.21963200
H	1.03681500	3.66989300	-0.18389700
C	-0.90095000	2.75316400	-0.39979700
C	-1.59488400	1.56639900	-0.43318400
C	-0.94440100	0.32786800	-0.28592900
H	6.51660600	-0.84787200	0.39282500
H	5.22983200	1.27175100	0.28267900
H	2.88164200	-3.06045700	0.05706400
H	5.29704100	-3.00976600	0.27773700
H	-1.42591700	3.69314500	-0.52296900
H	-2.66395900	1.58789300	-0.60061100
C	-1.67149200	-0.91017300	-0.30736800
C	0.44120500	-2.08909000	-0.19019500
C	-0.94308000	-2.08883100	-0.29992400
H	0.94088800	-3.04935900	-0.16666200
H	-1.47994800	-3.02901400	-0.35303800
O	3.23598100	2.65783300	0.12667000
N	-3.04106700	-0.97949200	-0.40098500
C	-3.78357400	-0.32234200	0.42567100
N	-5.10663400	-0.23095700	0.30588100
C	-5.79471500	-0.87541700	-0.78599600
H	-6.74732700	-0.37083700	-0.95157900
H	-5.19410200	-0.81507800	-1.69297100
H	-5.99073900	-1.93144300	-0.56743400
C	-5.91083500	0.29789600	1.38056100
H	-5.26821500	0.77094600	2.12291100
H	-6.61346300	1.04124600	0.99609200
H	-6.48271500	-0.49764000	1.87031000
H	-3.37529700	0.19032700	1.29988900

4AB
SCF Energy = -1073.67238171 au

C	-6.11458900	-1.04869100	-0.19115500
C	-5.45002500	0.15467100	-0.25535600
C	-4.05898600	0.21483300	-0.12180900
C	-3.30925700	-0.95978500	0.08295800
C	-4.00909800	-2.17467100	0.14244900
C	-5.38060000	-2.21831100	0.00863100
C	-3.40789600	1.52808900	-0.19884800
C	-1.85998100	-0.89053600	0.22116200
C	-1.21059100	0.36630800	0.14585100
C	-1.94717400	1.56243100	-0.05195700
C	-1.29991100	2.78276500	-0.10341100
H	-1.89125200	3.67859200	-0.25240300
C	0.08199800	2.86599200	0.04636900
C	0.81748500	1.71841100	0.23001800
C	0.20598200	0.45441300	0.26814300
H	-7.19276900	-1.08868500	-0.29505200

H	-5.99239600	1.07977700	-0.41062500
H	-3.47597000	-3.10428800	0.29484100
H	-5.88998500	-3.17454300	0.06003100
H	0.57422900	3.83119200	0.02439700
H	1.89026900	1.78424500	0.36280900
C	0.98750200	-0.73655200	0.44232300
C	-1.07281200	-2.01123400	0.43383500
C	0.31122100	-1.94129000	0.54867800
H	-1.53106900	-2.98960600	0.50708200
H	0.88439500	-2.84792100	0.70563000
O	-4.05906900	2.55745900	-0.37971900
N	2.34624500	-0.69114200	0.59757200
C	3.17470000	-0.37466200	-0.34633700
N	4.48167200	-0.24454500	-0.05105500
C	4.93886500	-0.42040700	1.31620600
H	4.35163100	-1.21551600	1.77840500
H	5.97629900	-0.75925000	1.27269400
C	5.49800000	0.06856500	-1.03983700
H	5.05477800	0.64460000	-1.85127500
H	6.22324900	0.73054200	-0.55841700
C	4.83697900	0.85175300	2.13504900
H	5.42065500	1.65757500	1.68179100
H	3.79871000	1.18115200	2.21542800
H	5.22025500	0.68429400	3.14502300
C	6.20096600	-1.16020900	-1.58517400
H	5.49961500	-1.81334200	-2.11055700
H	6.98454000	-0.86452000	-2.28782600
H	6.66803600	-1.73605400	-0.78213900
C	2.75874800	-0.17106000	-1.77248600
H	1.71752800	-0.45831600	-1.90473600
H	2.86611100	0.87570400	-2.06681900
H	3.37111800	-0.77042900	-2.44794900

Gas phase excited state optimization

1AB
SCF Energy = -1034.32721888 au

C	5.71348900	-1.04595200	0.04913000
C	5.06203700	0.17502800	0.05254100
C	3.67455100	0.24488100	0.03885900
C	2.91328500	-0.94599600	0.03015900
C	3.59770100	-2.17497800	0.01966500
C	4.97517700	-2.22792400	0.02931000
C	3.03841800	1.57586700	0.03856100
C	1.47534000	-0.86816500	0.02873500
C	0.82809600	0.42129200	-0.03260200
C	1.59530600	1.60928800	0.00658700
C	0.94767500	2.86141900	0.02535200
H	1.56947700	3.74636900	0.05189100
C	-0.42973200	2.93093100	0.04911300
C	-1.20491800	1.78528300	-0.00208100
C	-0.58511600	0.50540800	-0.08377100
H	6.79697100	-1.08316600	0.05704500
H	5.60508600	1.11238000	0.06528500
H	3.04597300	-3.10514400	-0.01197700
H	5.47855800	-3.18732900	0.01820300
H	-0.91801100	3.89740300	0.11739600
H	-2.27599800	1.86164600	0.10341900
C	-1.33774300	-0.70107000	-0.14524800
C	0.67635100	-2.01876600	0.11132400
C	-0.68891200	-1.94164000	0.02954100
H	1.13253900	-2.99273100	0.21551600
H	-1.27069800	-2.85335400	0.02257800
O	3.72768200	2.60039600	0.05484800
C	-3.51815100	-1.80450900	0.06950000
C	-3.33249300	0.13942200	-1.35116000
C	-5.00333500	-1.38341600	0.03637700
H	-3.39045900	-2.68877200	-0.57404600
C	-4.59936800	0.80221800	-0.77509700
H	-2.62571400	0.87497300	-1.72638600
H	-5.55247900	-1.97803800	0.76989100
H	-5.31720900	0.93485200	-1.59240900
N	-2.69086300	-0.70105700	-0.36610300
N	-5.20098300	0.01941000	0.28942900
C	-4.80848900	0.42861200	1.62126000
H	-5.10078700	1.46798600	1.78150900
H	-5.33991100	-0.18279900	2.35466500
H	-3.72867600	0.34775400	1.81940600
H	-5.43151100	-1.61478200	-0.94339000
H	-3.21254200	-2.08435900	1.07935700
H	-3.61257000	-0.50351200	-2.19833500
H	-4.36560100	1.79557200	-0.38802600

2AB
SCF Energy = -995.066714072 au
C   5.56533600 -0.88660000 -0.29777500
C   4.85979700   0.30030700 -0.20387300
C   3.47806800   0.30231800 -0.06179400
C   2.77665200 -0.92718600 -0.00797900
C   3.51783600 -2.12129600 -0.11049000
C   4.88761200 -2.10483300 -0.25340100
C   2.78580700   1.60131000   0.02962700
C   1.34949400 -0.92262900   0.14314200
C   0.64516700   0.33909500   0.20489000
C   1.34922000   1.56357700   0.16132600
C   0.64297300   2.78186700   0.25916800
H   1.21969900   3.69679800   0.22781000
C   -0.72940600   2.78415100   0.40716300
C   -1.44549000   1.59981000   0.43225500
C   -0.76736000   0.35676500   0.31200800
H   6.64375600 -0.86970700 -0.40795600
H   5.35505800   1.26330800 -0.23692800
H   3.01303900 -3.07776700 -0.08888900
H   5.43353400 -3.03748600 -0.33144900
H   -1.25664400   3.72688100   0.50912600
H   -2.51553700   1.61546500   0.58706500
C   -1.46919600 -0.88279900   0.31453000
C   0.61222100 -2.12064400   0.25255000
C   -0.74817800 -2.10304800   0.35416100
H   1.12297000 -3.07280400   0.26001600
H   -1.31978600 -3.01968800   0.43032900
O   3.42461900   2.65795500 -0.00808900
N   -2.81509600 -0.97515700   0.36103300
C   -3.66464500 -0.36446800 -0.40056800
N   -4.94534200 -0.27619800   0.00813300
C   -3.29933400   0.18099800 -1.74826100
H   -3.51529400   1.24948600 -1.81364200
H   -2.23494200   0.04144000 -1.91853800
H   -3.85432700 -0.33385800 -2.53563400
C   -5.31039300 -0.83845900   1.28916800
H   -5.44728800 -1.92383300   1.22548900
H   -4.52704200 -0.63932800   2.01727900
H   -6.24374200 -0.38260900   1.62041500
C   -6.03078900   0.08095800 -0.87108600
H   -5.67920300   0.68662500 -1.70158300
H   -6.53322200 -0.80708800 -1.27469500
H   -6.76726500   0.66486400 -0.31622100

3AB
SCF Energy = -955.78244505 au
C   5.39693800 -0.86719200   0.33589700

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C     4.68643600   0.31666700   0.24340900
C     3.30490200   0.31260100   0.09647600
C     2.60954600  -0.92000200   0.03498800
C     3.35593300  -2.11101200   0.13712900
C     4.72499900  -2.08864400   0.28549600
C     2.60591000   1.60612800   0.00749600
C     1.18324800  -0.92241200  -0.12237600
C     0.46971700   0.33473600  -0.17409100
C     1.16857300   1.56116700  -0.12633900
C     0.46103800   2.77901400  -0.22259000
H     1.03615800   3.69470800  -0.18644800
C    -0.90937600   2.77693600  -0.38086700
C    -1.62207500   1.59063400  -0.40702700
C    -0.94614400   0.34516800  -0.28043500
H     6.47483700  -0.84562200   0.45031000
H     5.17730900   1.28171400   0.28159300
H     2.85537100  -3.06961000   0.11281900
H     5.27489700  -3.01892100   0.36360500
H    -1.43938200   3.71712300  -0.49128400
H    -2.68756400   1.61127300  -0.58807100
C    -1.63538900  -0.90031900  -0.28675300
C     0.45589300  -2.12419800  -0.25103500
C    -0.90435800  -2.11270300  -0.34893400
H     0.97338600  -3.07231400  -0.27599600
H    -1.47149700  -3.03140800  -0.43251900
O     3.23634000   2.66780500   0.04948900
N    -2.98826600  -1.03366800  -0.28348800
C    -3.75378100  -0.29338000   0.44113700
N    -5.08599800  -0.30904000   0.34498800
C    -5.75757100  -1.09473600  -0.65966500
H    -6.20151900  -0.44752500  -1.42292700
H    -5.03222000  -1.75557200  -1.12931600
H    -6.55389000  -1.68329600  -0.19689100
C    -5.90319900   0.50436300   1.20560300
H    -5.27416100   1.04706300   1.91030600
H    -6.47913100   1.22937400   0.62153300
H    -6.60656100  -0.11768300   1.76778800
H    -3.36433600   0.36032600   1.22397100

4AB
SCF Energy =  -1073.63401076 au
C    -6.07919800  -0.95616600  -0.27123800
C    -5.38671800   0.24164900  -0.24592700
C    -4.00487900   0.26685900  -0.10472600
C    -3.29049600  -0.94917500   0.02041300
C    -4.01777800  -2.15479000  -0.01377900
C    -5.38797600  -2.16189900  -0.15746500
C    -3.32665300   1.57649400  -0.08942600
C    -1.86241400  -0.92006000   0.17254200
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C    -1.17129200   0.35008800   0.15321700
C    -1.88949800   1.56235400   0.04075900
C    -1.19700600   2.79189900   0.06773300
H    -1.78389000   3.69718200  -0.01413500
C     0.17530400   2.81789700   0.21450300
C     0.90473700   1.64489300   0.30365900
C     0.24081600   0.38891500   0.25389500
H    -7.15768100  -0.95752300  -0.38224700
H    -5.89235000   1.19573100  -0.33430200
H    -3.50206300  -3.10279900   0.06097800
H    -5.92318300  -3.10368500  -0.18248300
H     0.69175000   3.77082600   0.26441200
H     1.97412400   1.68117700   0.45948900
C     0.95645600  -0.84080800   0.33236900
C    -1.11365200  -2.09940300   0.36268900
C     0.24734400  -2.06139300   0.46130600
H    -1.61495200  -3.05377600   0.43699000
H     0.82755900  -2.96574700   0.59694200
O    -3.97707200   2.62224700  -0.18749500
N     2.30247100  -0.91574100   0.37216300
C     3.13950800  -0.34122900  -0.43300800
N     4.42716400  -0.24418600  -0.05854000
C     4.81938300  -0.68319200   1.27038300
H     4.23136100  -1.56920100   1.51583100
H     5.87079600  -0.97582800   1.22005000
C     5.46869600   0.28919500  -0.91310100
H     5.03424300   1.00205500  -1.61307600
H     6.14911500   0.86260000  -0.27716300
C     4.60930000   0.39014100   2.32234600
H     5.17815700   1.29319800   2.08791800
H     3.55253200   0.65317300   2.39029300
H     4.93502500   0.03044500   3.30048100
C     6.23682600  -0.78819700  -1.66005700
H     5.58001600  -1.34376100  -2.33242200
H     7.03645100  -0.34111300  -2.25446800
H     6.68924000  -1.50136300  -0.96799200
C     2.74811600   0.14491200  -1.79606600
H     1.72146200  -0.14821400  -2.00242100
H     2.79687300   1.23510900  -1.84912900
H     3.40097900  -0.27086500  -2.56505500

Ethanol phase excited state optimization

1AB
SCF Energy =  -1034.35884038 au
C     5.71137800  -1.04520900   0.07719200
C     5.06345700   0.17454300   0.07195000
C     3.66822600   0.25326300   0.04435800
C     2.90554700  -0.94119600   0.03002600
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C     3.58778800  -2.16756600   0.02813300
C     4.96760700  -2.22453700   0.05206100
C     3.02865600   1.56343100   0.03608000
C     1.46323000  -0.86811400   0.01000700
C     0.81743000   0.41059900  -0.05641000
C     1.58639200   1.60315100  -0.00772100
C     0.93641400   2.85141400   0.01405900
H     1.54022700   3.74877500   0.05152000
C    -0.44352300   2.92005800   0.02880500
C    -1.21360900   1.77243300  -0.03435100
C    -0.60006700   0.49803400  -0.12436000
H     6.79504400  -1.08429100   0.09685000
H     5.63048700   1.09756100   0.08872600
H     3.03563300  -3.09799900  -0.00323700
H     5.46724900  -3.18648000   0.04830300
H    -0.93540000   3.88483900   0.09884800
H    -2.28635500   1.85511500   0.04303300
C    -1.36013800  -0.70972500  -0.19676100
C     0.66174900  -2.01823600   0.07982200
C    -0.70391100  -1.94337400  -0.01866500
H     1.11316800  -2.99512800   0.18145500
H    -1.28144000  -2.85831900  -0.03434400
O     3.71180300   2.61715200   0.05671400
C    -3.53323400  -1.81415700   0.03627500
C    -3.38458400   0.14276000  -1.36085800
C    -5.01049100  -1.36069600   0.10012100
H    -3.47387300  -2.67813400  -0.64012800
C    -4.61544300   0.82316300  -0.71317100
H    -2.69660200   0.86935600  -1.78368200
H    -5.51361700  -1.95718400   0.86345300
H    -5.36943100   0.94169800  -1.49713200
N    -2.70472300  -0.72333500  -0.43149600
N    -5.15614000   0.04609100   0.38653400
C    -4.61289300   0.42162300   1.67565200
H    -4.85709200   1.46520700   1.88463600
H    -5.06469600  -0.19836800   2.45370000
H    -3.51980500   0.31370500   1.74454100
H    -5.50042100  -1.56582500  -0.85450500
H    -3.17412100  -2.12633700   1.01707800
H    -3.73680600  -0.49403900  -2.18300100
H    -4.36043200   1.81937800  -0.34855200

2AB
SCF Energy =  -995.096959935 au
C    -5.60055700  -0.81654300   0.23434800
C    -4.87721500   0.35697300   0.13738700
C    -3.48489600   0.34222100   0.03060200
C    -2.80171700  -0.90164900   0.01465900
C    -3.56072900  -2.07926400   0.11888600
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C    -4.93643700  -2.04297100   0.22793500
C    -2.76612500   1.60724900  -0.06212300
C    -1.36719700  -0.92624800  -0.10229600
C    -0.63874000   0.31209800  -0.15548300
C    -1.32626400   1.55144100  -0.15459200
C    -0.59723300   2.75354700  -0.25593300
H    -1.14088400   3.68937800  -0.25654000
C     0.77973500   2.73080800  -0.36866900
C     1.47275500   1.53243800  -0.35363700
C     0.78001200   0.30682600  -0.22564700
H    -6.68128600  -0.78248700   0.31765000
H    -5.38161800   1.31582300   0.14313000
H    -3.07028000  -3.04365800   0.12401300
H    -5.49481200  -2.96840500   0.30948500
H     1.32763700   3.66176400  -0.47199700
H     2.54761000   1.53795000  -0.47090000
C     1.47190800  -0.94900100  -0.21590200
C    -0.64914700  -2.13838300  -0.19350700
C     0.71301100  -2.14747700  -0.27207400
H    -1.17383700  -3.08347000  -0.20472000
H     1.25663500  -3.08289700  -0.33557600
O    -3.38052300   2.70157200  -0.05854000
N     2.80328600  -1.08039700  -0.24519400
C     3.69808200  -0.41358300   0.44197800
N     4.93970900  -0.36021900  -0.03394200
C     3.39590300   0.17189100   1.78493300
H     3.57984000   1.24823500   1.79988200
H     2.35498900  -0.01039800   2.04215100
H     4.02934500  -0.29131500   2.54509500
C     5.22564000  -0.88760100  -1.35159900
H     4.76332100  -1.86829400  -1.47316100
H     4.83971600  -0.22534400  -2.13197800
H     6.30482500  -0.97798100  -1.46410100
C     6.03486300   0.29629800   0.64131400
H     5.73042900   0.68805600   1.60609000
H     6.85320200  -0.41316400   0.79153200
H     6.40446900   1.12352200   0.02874700

3AB
SCF Energy =  -955.813399581 au
C     5.42595700  -0.85424300   0.25059400
C     4.71429100   0.32718300   0.16925200
C     3.32141000   0.32738500   0.06530900
C     2.62554100  -0.90972100   0.03713700
C     3.37403200  -2.09640300   0.12534200
C     4.74970900  -2.07456100   0.23110400
C     2.61478700   1.59816600  -0.01331100
C     1.19199700  -0.92000400  -0.07642000
C     0.47323500   0.32428800  -0.11805500
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C     1.17318400   1.55594400  -0.10712600
C     0.45978100   2.76803300  -0.19977800
H     1.01526400   3.69675800  -0.19107500
C    -0.91552800   2.76126200  -0.31908200
C    -1.62237900   1.57012900  -0.31273100
C    -0.94919400   0.33318400  -0.18771900
H     6.50716200  -0.83184200   0.33152700
H     5.22834700   1.28076900   0.18483900
H     2.87473200  -3.05618600   0.11998300
H     5.29952200  -3.00611000   0.29981000
H    -1.45379700   3.69788300  -0.42093700
H    -2.69533500   1.59633500  -0.44117700
C    -1.64753800  -0.91868900  -0.18190000
C     0.46424600  -2.12665400  -0.17689500
C    -0.89694600  -2.12152500  -0.24935800
H     0.98079500  -3.07579900  -0.19980100
H    -1.45020600  -3.05094600  -0.31755300
O     3.23652900   2.68807100   0.00192800
N    -2.98563400  -1.07019600  -0.17769800
C    -3.80645500  -0.29299000   0.47221400
N    -5.11247200  -0.31151000   0.27566000
C    -5.71742300  -1.09389900  -0.77593800
H    -5.94545700  -0.45989400  -1.63847600
H    -5.03390200  -1.88180700  -1.08559300
H    -6.64662400  -1.52957700  -0.40575500
C    -5.99096100   0.53645600   1.04530900
H    -5.42158600   1.07595000   1.80062200
H    -6.48723800   1.25646100   0.38822900
H    -6.75665800  -0.07121900   1.53426500
H    -3.47099800   0.36654400   1.27225300

4AB
SCF Energy =  -1073.66628532 au
C    -6.10959900  -0.90421700  -0.21554800
C    -5.40555900   0.28450400  -0.18336500
C    -4.01293400   0.29815300  -0.07926200
C    -3.30927700  -0.93180600  -0.00183800
C    -4.04888100  -2.12552700  -0.04002500
C    -5.42544000  -2.11751900  -0.14515400
C    -3.31510500   1.57791900  -0.05104900
C    -1.87397100  -0.92660900   0.11154400
C    -1.16641600   0.32490200   0.10383200
C    -1.87462900   1.55093800   0.04485000
C    -1.16608300   2.76861700   0.08908200
H    -1.72553100   3.69397800   0.04458900
C     0.21095000   2.77446400   0.20602000
C     0.92405300   1.58873600   0.24756800
C     0.25218500   0.34689100   0.17300800
H    -7.19092000  -0.89236400  -0.29727900
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H	-5.92601000	1.23311600	-0.23873500
H	-3.54281100	-3.08082500	0.00566900
H	-5.96892200	-3.05489200	-0.17369600
H	0.74287500	3.71831600	0.26738200
H	1.99814200	1.61673700	0.36897900
C	0.96548000	-0.89600200	0.21577500
C	-1.13551000	-2.12014500	0.26111300
C	0.22699600	-2.10274200	0.33404400
H	-1.64433000	-3.07194300	0.32200400
H	0.78656700	-3.02473800	0.44070800
O	-3.94741900	2.66039200	-0.10879100
N	2.29854400	-1.00531000	0.23955800
C	3.17509700	-0.34228200	-0.47622100
N	4.41927200	-0.23339300	-0.01770100
C	4.75526300	-0.72116600	1.31204500
H	4.20368900	-1.64755500	1.48268700
H	5.82017000	-0.95840200	1.30636600
C	5.49945600	0.36744700	-0.78481200
H	5.08727500	1.09493400	-1.48196600
H	6.11909200	0.92523000	-0.07856800
C	4.44052900	0.28827900	2.39792400
H	4.97502000	1.22674300	2.23021500
H	3.36960100	0.49955600	2.43614600
H	4.74564900	-0.10662300	3.36988800
C	6.33413300	-0.66493400	-1.51781300
H	5.73283700	-1.20566400	-2.25238700
H	7.15468300	-0.17001600	-2.04287700
H	6.76418600	-1.39048900	-0.82330300
C	2.85020200	0.18641100	-1.83735700
H	1.83279100	-0.08723800	-2.10799100
H	2.93922700	1.27474900	-1.86897000
H	3.53572200	-0.23068800	-2.57770000