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

Supporting information

Distinguishing ionic and radical mechanisms of hydroxylamine mediated electrocatalytic alcohol oxidation using NO–H bond dissociation energies

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The following theoretical treatments are used to calculate the barrier of hydrogen abstraction of TEMPO from benzyl alcohol: B3LYP/6-311+(d,p), B3LYP/6-311++G(df,pd)//B3LYP/6-311+(d,p), wB97XD/def2TZVP//B3LYP/6-311+(d,p), cam-B3LYP/def2TZVP//B3LYP/6-311+(d,p), BB1K/def2TZVP//B3LYP/6-311+(d,p), MPWB1K/def2TZVP//B3LYP/6-311+(d,p), wB97XD/def2TZVP//m062x/6-31g(d), m062x/6-31g(d), BB1K/def2TZVP//m062x/6-31g(d), and wB97XD/def2TZVP//m062x-D3/TZVP (Table S1). When using the same functional for single point energy, it can be seen that it does not make too much difference for methods of the geometry. When using the same geometry, most of the functionals for single point energy calculation give similar barrier values. In addition, calculation with or without dispersion correction give similar results. Other reactions are calculated at the selected level of calculation and it can also be seen that, the calculated reaction barriers do not vary with calculation level by a significant amount. With the ionic reaction, BB1K/def2TZVP//m062x/6-31g(d) barriers are 6 to 7 kcal/mol higher than the B3LYP/6-311+(d,p) barrier. But still in a reasonable amount that the ionic mechanism is feasible with TEMPO (TEMPO has the highest barrier among the catalysts). With the radical mechanism, a plot is sketched with the reaction barrier of four radicals with methanol calculated under BB1K/def2TZVP//m062x/6-31g(d) level against the BDEs (Figure S1). When the barrier is 25 kcal/mol, BDE is 84 to 85 kcal/mol, which is close to the value in the main text of 83 kcal/mol. Therefore, we conclude that, using different functionals will not significantly change the conclusions in our study.

Table S1. Reaction barriers of selected reactions calculated with different DFT methods with or without dispersion corrections.

Method	Reaction	Ea
B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	35.7
B3LYP/6-311+(d,p)	2+benzyl alcohol (radical)	30.8
B3LYP/6-311++G(df,pd)//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	35.6
wB97XD/def2TZVP//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	32.1
cam-B3LYP/def2TZVP//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	37.2
BB1K/def2TZVP//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	38.8
MPWB1K/def2TZVP//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	37.6
wB97X/def2TZVP//B3LYP/6-311+(d,p)	1+benzyl alcohol (radical)	36.8
wB97XD/def2TZVP//m062x/6-31g(d)	1+benzyl alcohol (radical)	31.1
wB97XD/def2TZVP//m062x/6-31g(d)	2+benzyl alcohol (radical)	29.6
m062x/6-31g(d)	1+benzyl alcohol (radical)	29.2

BB1K/def2TZVP//m062x/6-31g(d)	1+benzyl alcohol (radical)	38.3
wB97XD/def2TZVP//m062x-D3/TZVP	1+benzyl alcohol (radical)	31.0
B3LYP/6-311+(d,p)	2+methanol (radical)	36.2
B3LYP/6-311+(d,p)	7+methanol (radical)	33.7
B3LYP/6-311+(d,p)	13+methanol (radical)	27.6
B3LYP/6-311+(d,p)	14+methanol (radical)	29.1
B3LYP/6-311+(d,p)	15+methanol (radical)	29.6
B3LYP/6-311+(d,p)	18+methanol (radical)	18.9
BB1K/def2TZVP//m062x/6-31g(d)	2+methanol (radical)	40.3
BB1K/def2TZVP//m062x/6-31g(d)	7+methanol (radical)	39.4
BB1K/def2TZVP//m062x/6-31g(d)	13+methanol (radical)	31.0
BB1K/def2TZVP//m062x/6-31g(d)	14+methanol (radical)	35.2
BB1K/def2TZVP//m062x/6-31g(d)	15+methanol (radical)	34.0
BB1K/def2TZVP//m062x/6-31g(d)	18+methanol (radical)	20.4
B3LYP/6-311+(d,p)	1-cation+benzyl alcohol (ionic)	21.9
BB1K/def2TZVP//m062x/6-31g(d)	1-cation+benzyl alcohol (ionic)	27.7
B3LYP/6-311+(d,p)	1-cation+methanol (ionic)	16.5
BB1K/def2TZVP//m062x/6-31g(d)	1-cation+methanol (ionic)	23.2

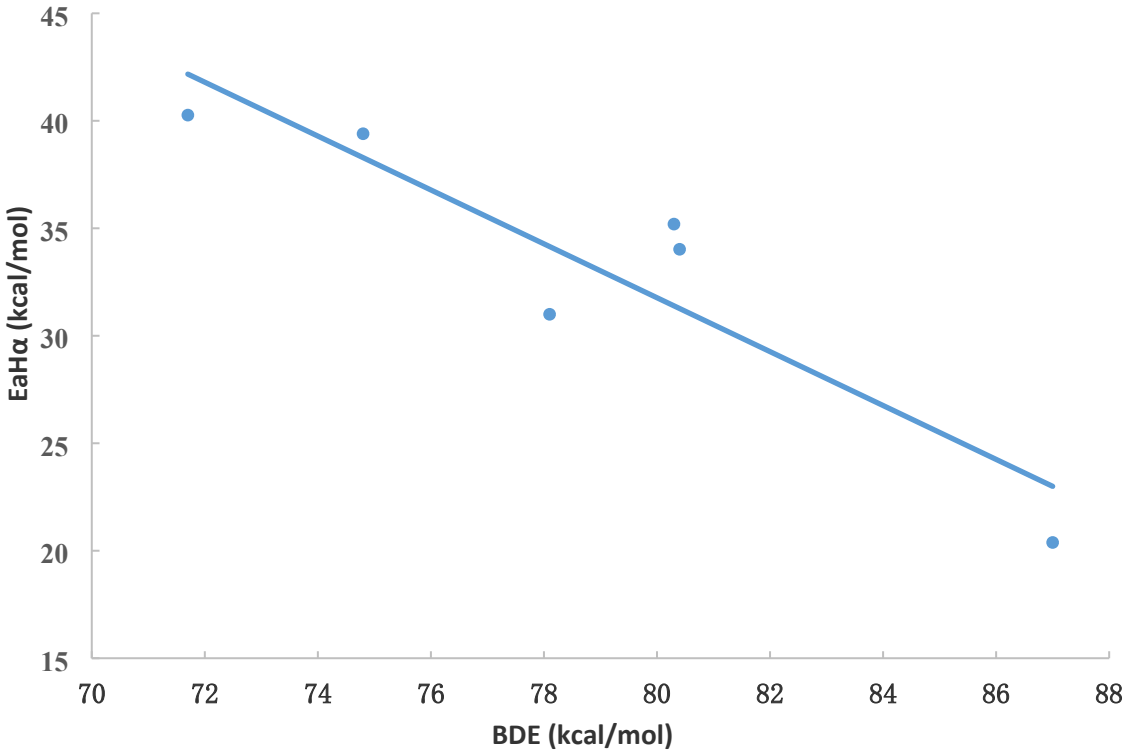

Figure S1. Plot of the reaction barrier of four radicals with methanol calculated under BB1K/def2TZVP//m062x/6-31g(d) level against the BDEs.

Cartesian coordinates for selected compounds and transition states.

Compound 1 (gas phase)

Charge 0 multiplicity 1

C	1.29585000	-0.04995600	-0.03365200
C	-1.29585000	-0.04995600	-0.03365200
C	-1.24997400	1.43213100	-0.46514600
C	0.00000000	2.16703500	0.01986300
C	1.24997400	1.43213200	-0.46514600
N	0.00000000	-0.66681700	-0.44677200
C	1.63224800	-0.18662200	1.46866800
C	2.40068000	-0.75799100	-0.83984900
C	-1.63224800	-0.18662200	1.46866800
C	-2.40068000	-0.75799100	-0.83984900
H	-1.28126300	1.47414500	-1.55988300
H	-2.15849400	1.92270400	-0.10133000
H	0.00000000	3.19298200	-0.36215600

H	0.00000000	2.24915600	1.11151300
H	1.28126300	1.47414500	-1.55988300
H	2.15849400	1.92270400	-0.10133000
H	1.47822800	-1.21504900	1.79823900
H	2.68349600	0.06836100	1.63091400
H	1.03529800	0.47022600	2.10063800
H	3.35605200	-0.24504800	-0.69767800
H	2.52387200	-1.79292300	-0.51504300
H	2.15902700	-0.75030500	-1.90572000
H	-2.68349600	0.06836100	1.63091400
H	-1.47822800	-1.21504900	1.79823900
H	-1.03529800	0.47022600	2.10063800
H	-2.52387200	-1.79292300	-0.51504300
H	-3.35605200	-0.24504800	-0.69767800
H	-2.15902700	-0.75030500	-1.90572000
O	0.00000000	-2.04368400	0.00244800
H	0.00000000	-2.54212400	-0.82124500

Compound 1 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	0.07316000	0.02183200	1.33295900
C	0.07316000	0.02183200	-1.33295900
C	-1.35909900	0.58372700	-1.24539000
C	-2.12100000	0.13361700	0.00000000
C	-1.35909900	0.58372700	1.24539000
O	2.02311200	-0.07189500	0.00000000
N	0.76258200	0.15123600	0.00000000
C	0.07316000	-1.46076800	1.76016800
C	0.88357300	0.84153400	2.34828600
C	0.07316000	-1.46076800	-1.76016800
C	0.88357300	0.84153400	-2.34828600
H	-1.30679800	1.67868100	-1.24544500
H	-1.89101100	0.29577400	-2.15755000
H	-3.12328200	0.57287100	0.00000000
H	-2.26317100	-0.95195200	0.00000000
H	-1.30679800	1.67868100	1.24544500
H	-1.89101100	0.29577400	2.15755000
H	1.08739100	-1.86046900	1.70740100
H	-0.28061000	-1.54832400	2.79119500
H	-0.57315700	-2.07451200	1.13020500
H	0.38562700	0.80762400	3.32122700
H	1.89274800	0.44499000	2.45263300
H	0.95579200	1.88522900	2.03285000
H	-0.28061000	-1.54832400	-2.79119500
H	1.08739100	-1.86046900	-1.70740100
H	-0.57315700	-2.07451200	-1.13020500
H	1.89274800	0.44499000	-2.45263300
H	0.38562700	0.80762400	-3.32122700
H	0.95579200	1.88522900	-2.03285000

Compound 1 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	0.07512100	0.01668600	1.33537900
C	0.07512100	0.01668600	-1.33537900
C	-1.35842100	0.57509700	-1.24511600
C	-2.11809200	0.12334400	0.00000000
C	-1.35842100	0.57509700	1.24511600
O	2.03646500	-0.02400600	0.00000000
N	0.76441800	0.14755100	0.00000000
C	0.07512100	-1.46418500	1.76449600
C	0.87405000	0.84043300	2.35524900
C	0.07512100	-1.46418500	-1.76449600
C	0.87405000	0.84043300	-2.35524900
H	-1.30781200	1.67015200	-1.24523300
H	-1.88684200	0.28160200	-2.15722500
H	-3.11884700	0.56651500	0.00000000
H	-2.25894200	-0.96221300	0.00000000
H	-1.30781200	1.67015200	1.24523300
H	-1.88684200	0.28160200	2.15722500
H	1.08760000	-1.87231800	1.71927700
H	-0.27992400	-1.54261600	2.79592600
H	-0.57412400	-2.07791700	1.13774600
H	0.34163700	0.83584900	3.31034800
H	1.87062300	0.42677700	2.51224500
H	0.97545600	1.87768800	2.02469600
H	-0.27992400	-1.54261600	-2.79592600
H	1.08760000	-1.87231800	-1.71927700
H	-0.57412400	-2.07791700	-1.13774600
H	1.87062300	0.42677700	-2.51224500
H	0.34163700	0.83584900	-3.31034800
H	0.97545600	1.87768800	-2.02469600

Compound 1 oxoammonium ion (gas phase)

Charge 1 multiplicity 1

Compound 1 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	1.36137200	-0.07581900	0.02276100
C	-1.36139300	-0.07586400	0.02273900
C	-1.25067000	1.31681400	-0.63640000
C	-0.00008300	2.09889300	-0.25055200
C	1.25066600	1.31695200	-0.63615200

O	0.00003100	-1.94765500	-0.35884900
N	0.00002200	-0.78393500	-0.11913400
C	1.66441700	0.00570200	1.53792400
C	2.40749200	-0.94200000	-0.67319600
C	-1.66443400	0.00597600	1.53787800
C	-2.40743900	-0.94221200	-0.67307300
H	-1.27715700	1.18065000	-1.72171800
H	-2.15923700	1.85401300	-0.35328900
H	-0.00004900	3.05060200	-0.78856000
H	-0.00018900	2.34395300	0.81431600
H	1.27744100	1.18093000	-1.72148200
H	2.15910200	1.85421200	-0.35273700
H	1.57395500	-0.97319000	2.01231500
H	2.70322200	0.33249400	1.61751500
H	1.03690000	0.72369300	2.06017800
H	3.34362300	-0.38061100	-0.65861800
H	2.56992200	-1.88961900	-0.15898900
H	2.14053200	-1.13602100	-1.71426700
H	-2.70342600	0.33219200	1.61739600
H	-1.57341300	-0.97266900	2.01267600
H	-1.03732600	0.72453900	2.05982200
H	-2.56975300	-1.88979000	-0.15874900
H	-3.34362300	-0.38091200	-0.65852300
H	-2.14049000	-1.13632800	-1.71412900

Compound 2 (gas phase)

Charge 0 multiplicity 1

C	0.60271800	0.00026000	1.83841400
C	0.79167100	1.27518600	0.99455200
C	0.11554900	1.21357500	-0.39212900
N	0.48819100	-0.00016800	-1.15016800
C	0.11552500	-1.21368900	-0.39178700
C	0.79163100	-1.27491500	0.99492900
C	-1.42614600	-1.27118100	-0.39639200
C	-1.42612300	1.27109100	-0.39673000
C	-2.09593400	0.00003400	0.15315500
H	1.32486900	0.00037000	2.66138400
H	-0.38299200	0.00035100	2.30894300
H	1.86041300	1.43317400	0.82448500
H	0.42537700	2.15295600	1.53768000
H	0.47713100	2.06151700	-0.98112000
H	0.47710500	-2.06180400	-0.98053000
H	0.42529900	-2.15251500	1.53830600
H	1.86036800	-1.43299600	0.82491800
H	-1.75456300	-2.15202200	0.16470700
H	-1.74018300	-1.41855900	-1.43502600
H	-1.75451100	2.15208700	0.16414400
H	-1.74017100	1.41821200	-1.43539800
H	-2.06681300	0.00017500	1.24449100

H	-3.15654800	0.00000700	-0.11831100
O	1.93453900	-0.00019900	-1.30382400
H	2.03822400	-0.00036200	-2.26097200

Compound 2 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	-0.78943900	-1.78064100	0.02456700
C	-0.91955100	-0.95169700	-1.26948300
C	-0.12956200	0.37748000	-1.24111400
N	-0.51399300	1.10663900	-0.01518400
C	-0.12932900	0.41165500	1.23038000
C	-0.91892600	-0.91651800	1.29552600
O	-1.58182400	1.81523600	-0.02495500
C	1.40680200	0.30392800	1.27197700
C	1.40651800	0.26844300	-1.28029000
C	2.02746400	-0.31029600	0.00404200
H	-1.56937300	-2.54838000	0.03559700
H	0.15876700	-2.32168600	0.03174900
H	-1.97098500	-0.68704800	-1.42163500
H	-0.61159300	-1.54503200	-2.13671200
H	-0.46382600	1.00245400	-2.07099400
H	-0.46341900	1.05928500	2.04274100
H	-0.60972300	-1.48563600	2.17836700
H	-1.97032800	-0.64828000	1.44144900
H	1.70481100	-0.26616000	2.15775400
H	1.79743600	1.31876000	1.40462400
H	1.70414000	-0.32631700	-2.14978700
H	1.79737100	1.27901900	-1.44126100
H	1.92082500	-1.39663600	0.01919400
H	3.10458600	-0.11683900	0.00121500

Compound 2 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	-0.77225000	1.79281300	0.00014800
C	-0.91401700	0.94895200	1.28200900
C	-0.13845800	-0.38864600	1.23831700
N	-0.52644500	-1.09467500	-0.00008400
C	-0.13847900	-0.38844400	-1.23837800
C	-0.91404500	0.94915700	-1.28184300
O	-1.56583700	-1.85265400	-0.00013800
C	1.39892900	-0.29309700	-1.27622200
C	1.39895100	-0.29331400	1.27615400
C	2.02350600	0.29802200	0.00001100
H	-1.54253100	2.57055600	0.00022300
H	0.18525500	2.31569400	0.00017900
H	-1.97010900	0.70092700	1.43510100

H	-0.59162000	1.52218200	2.15678800
H	-0.47496300	-1.01928700	2.06285400
H	-0.47499100	-1.01895600	-2.06301100
H	-0.59167300	1.52252800	-2.15653800
H	-1.97014100	0.70115200	-1.43494900
H	1.69538200	0.28947600	-2.15367400
H	1.78165800	-1.30891900	-1.42481300
H	1.69542000	0.28910800	2.15370100
H	1.78167700	-1.30916300	1.42456700
H	1.92540000	1.38513300	0.00010700
H	3.09823100	0.09087300	-0.00001700

Compound 2 oxoammonium ion (gas phase)

Charge 1 multiplicity 1

C	1.58452000	1.22240500	-0.00000500
C	1.32919100	0.40384700	-1.27198800
C	0.00014800	-0.40881400	-1.25518100
N	-0.00003700	-1.19351100	0.00000100
C	0.00015500	-0.40881100	1.25518200
C	1.32920000	0.40384600	1.27198000
O	-0.00046800	-2.38510100	0.00000200
C	-1.32875100	0.40411800	1.27220800
C	-1.32876000	0.40411300	-1.27220100
C	-1.58498300	1.22221100	0.00000300
H	2.62824200	1.54761200	-0.00000900
H	0.98963300	2.13458100	-0.00000200
H	2.14071400	-0.31350900	-1.42886300
H	1.29632500	1.04030200	-2.15938500
H	0.00011100	-1.14756700	-2.05663000
H	0.00012100	-1.14756400	2.05663200
H	1.29634300	1.04030000	2.15937800
H	2.14072300	-0.31351200	1.42884700
H	-1.29558400	1.04103700	2.15926500
H	-2.14026200	-0.31309900	1.42971700
H	-1.29560000	1.04102800	-2.15926200
H	-2.14027100	-0.31310600	-1.42970100
H	-0.99163500	2.13548100	-0.00000100
H	-2.62918100	1.54590300	0.00000600

Compound 2 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	-1.58071800	-1.22341600	0.00000000
C	-1.32647700	-0.40507100	-1.26911400
C	0.00002900	0.41066600	-1.25109600
N	0.00010400	1.19173700	0.00000000
C	0.00002900	0.41066600	1.25109600

C	-1.32647700	-0.40507200	1.26911400
O	0.00026300	2.38724900	0.00000000
C	1.32638900	-0.40530900	1.26911600
C	1.32638900	-0.40530900	-1.26911600
C	1.58049500	-1.22369400	0.00000000
H	-2.62695600	-1.54265300	0.00000000
H	-0.98379200	-2.13432900	0.00000000
H	-2.13451800	0.31639700	-1.41995400
H	-1.28125000	-1.03927700	-2.15692900
H	0.00009300	1.14320100	-2.05673400
H	0.00009300	1.14320100	2.05673400
H	-1.28125000	-1.03927700	2.15692900
H	-2.13451800	0.31639700	1.41995400
H	1.28105100	-1.03950600	2.15693100
H	2.13455400	0.31602100	1.41995600
H	1.28105100	-1.03950600	-2.15693200
H	2.13455400	0.31602100	-1.41995700
H	0.98342000	-2.13450900	0.00000000
H	2.62668000	-1.54310300	0.00000000

Compound 3 (gas phase)

Charge 0 multiplicity 1

C	0.63092600	1.50745600	-0.00000200
C	-0.20943200	1.16726100	1.24699900
C	-0.55163500	-0.33554200	1.22299800
N	-1.29525000	-0.72645200	0.00000200
C	-0.55163600	-0.33554500	-1.22299500
C	-0.20943400	1.16725700	-1.24700100
C	1.92692600	0.66880200	-0.00000100
C	0.73962200	-1.17232400	-1.24581200
C	0.73962200	-1.17232100	1.24581400
C	1.58100900	-0.83568000	0.00000000
O	-2.54641600	0.01361300	-0.00000500
H	0.88198100	2.57335600	-0.00000400
H	0.34235200	1.40035400	2.16481700
H	-1.13030600	1.75570700	1.26062800
H	-1.18871500	-0.59989000	2.07062100
H	-1.18871700	-0.59989700	-2.07061500
H	0.34235000	1.40034900	-2.16481900
H	-1.13030800	1.75570200	-1.26063200
H	2.53253000	0.91332800	-0.88071500
H	2.53252800	0.91333000	0.88071400
H	0.48967900	-2.23751900	-1.26248200
H	1.29609200	-0.94846900	-2.16218400
H	1.29609200	-0.94846500	2.16218500
H	0.48968000	-2.23751700	1.26248600
H	2.50059500	-1.43017200	0.00000200

H	-3.20357100	-0.69011900	0.00002700

Compound 3 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	-0.78564500	0.00052600	1.44675300
C	0.08431300	1.25592900	1.22280200
C	0.61671100	1.24516400	-0.22576600
N	1.39934600	-0.00015100	-0.41745700
C	0.61669300	-1.24531200	-0.22485600
C	0.08430700	-1.25505900	1.22372000
C	-1.96057800	0.00013900	0.44560200
C	-0.54918900	-1.25174100	-1.22628000
C	-0.54925100	1.25086800	-1.22715400
C	-1.42150900	-0.00037600	-1.00063600
O	2.64038700	-0.00003000	-0.10129500
H	-1.17173200	0.00091000	2.47089800
H	-0.50033500	2.16707200	1.39053300
H	0.92876200	1.27233300	1.91811900
H	1.31109600	2.06650200	-0.40495900
H	1.31106400	-2.06678500	-0.40348400
H	-0.50037200	-2.16607500	1.39205700
H	0.92877300	-1.27104100	1.91902600
H	-2.59219700	-0.88020900	0.61040100
H	-2.59217000	0.88063400	0.60972300
H	-0.16080400	-1.27003100	-2.24918700
H	-1.13913500	-2.16310900	-1.08300800
H	-1.13921200	2.16229100	-1.08431800
H	-0.16093100	1.26857700	-2.25009100
H	-2.25643700	-0.00061000	-1.70826800

Compound 3 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	0.83131000	-0.00262500	1.42866900
C	-0.04484000	-1.25677700	1.23024800
C	-0.62272100	-1.24678400	-0.20153100
N	-1.40655900	0.00066800	-0.36936000
C	-0.62274600	1.24750200	-0.19693700
C	-0.04484400	1.25224700	1.23486500
C	1.97538300	-0.00069300	0.39279600
C	0.51350100	1.25329000	-1.23292100
C	0.51358500	-1.24875200	-1.23748700
C	1.39176500	0.00192700	-1.03539800
O	-2.66112700	0.00014200	-0.08817600
H	1.24722200	-0.00448100	2.44076800
H	0.54436200	-2.16888300	1.36993400
H	-0.86288500	-1.27522300	1.95751700

H	-1.31827700	-2.07103400	-0.36092400
H	-1.31832200	2.07231500	-0.35329800
H	0.54436700	2.16383000	1.37789500
H	-0.86288900	1.26803600	1.96219400
H	2.60875200	0.88140700	0.53901500
H	2.60875600	-0.88332200	0.53577200
H	0.09559700	1.27290700	-2.24436900
H	1.10368900	2.16537100	-1.10031100
H	1.10382700	-2.16126600	-1.10811900
H	0.09574600	-1.26475400	-2.24902400
H	2.20262400	0.00328700	-1.76995100

Compound 3 oxoammonium ion (gas phase)

Charge 1 multiplicity 1

C	1.12965700	1.26122700	-0.00000200
C	0.23106900	1.27912400	1.24571700
C	-0.65343100	0.00033700	1.26334200
N	-1.43407700	0.00041100	-0.00000100
C	-0.65342700	0.00033100	-1.26334200
C	0.23107400	1.27911800	-1.24572300
C	2.01636500	-0.00062700	0.00000100
C	0.23008400	-1.27912900	-1.24575200
C	0.23008200	-1.27912100	1.24576000
C	1.12877900	-1.26185200	0.00000500
O	-2.62600500	0.00031500	-0.00000300
H	1.75626800	2.15719600	-0.00000400
H	0.81494700	1.26597700	2.16954700
H	-0.40422900	2.16838000	1.27408300
H	-1.39103700	0.00061100	2.06506000
H	-1.39103200	0.00060000	-2.06506200
H	0.81495400	1.26596400	-2.16955100
H	-0.40422300	2.16837400	-1.27409600
H	2.66916000	-0.00083100	-0.87747300
H	2.66916000	-0.00082500	0.87747500
H	-0.40583800	-2.16794600	-1.27399200
H	0.81406700	-1.26654200	-2.16951600
H	0.81406300	-1.26652800	2.16952500
H	-0.40584100	-2.16793800	1.27400500
H	1.75464600	-2.15833400	0.00000700

Compound 3 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	1.12917800	1.26003300	-0.00000100
C	0.23124500	1.27730100	1.24314500
C	-0.65447400	-0.00008000	1.25965800
N	-1.43041700	-0.00015200	0.00000000

C	-0.65447400	-0.00008200	-1.25965800
C	0.23124500	1.27729900	-1.24314800
C	2.01677700	0.00017200	0.00000000
C	0.23151300	-1.27729600	-1.24315400
C	0.23151300	-1.27729400	1.24315600
C	1.12942400	-1.25986000	0.00000100
O	-2.62647800	-0.00007000	0.00000000
H	1.75396800	2.15765100	-0.00000200
H	0.81190300	1.25390800	2.16822900
H	-0.40967600	2.16181900	1.26222900
H	-1.38619700	-0.00015800	2.06529900
H	-1.38619700	-0.00016100	-2.06529900
H	0.81190300	1.25390400	-2.16823100
H	-0.40967600	2.16181700	-1.26223200
H	2.66341000	0.00023100	-0.88256300
H	2.66341000	0.00023200	0.88256200
H	-0.40925600	-2.16192600	-1.26224000
H	0.81217300	-1.25378600	-2.16823000
H	0.81217300	-1.25378300	2.16823200
H	-0.40925600	-2.16192300	1.26224300
H	1.75438600	-2.15736100	0.00000200

Compound 4 (gas phase)

Charge 0 multiplicity 1

C	-1.07190100	-1.28658500	-0.61600900
C	-1.81331300	0.00000000	-0.28572000
C	-1.07190100	1.28658600	-0.61600500
C	0.44943300	1.21846200	-0.37498900
C	0.84516800	1.26277200	1.11400400
C	0.40540000	-0.00000300	1.87076200
C	0.84516800	-1.26277500	1.11400000
C	0.44943300	-1.21846100	-0.37499200
N	0.93102200	0.00000200	-1.06514800
O	2.37809000	0.00000100	-0.99254400
O	-2.94324200	0.00000000	0.15322600
H	-1.52935300	-2.10918100	-0.06295500
H	-1.24370900	-1.46977200	-1.68384100
H	-1.24370900	1.46977600	-1.68383700
H	-1.52935300	2.10918100	-0.06294900
H	0.91348300	2.06385600	-0.88872100
H	0.42035600	2.16070700	1.57439000
H	1.93324400	1.35998700	1.16866500
H	0.83669000	-0.00000400	2.87620700
H	-0.68056100	-0.00000300	2.01387700
H	1.93324400	-1.35999000	1.16866100
H	0.42035700	-2.16071100	1.57438400
H	0.91348300	-2.06385400	-0.88872700
H	2.63496600	0.00000400	-1.92088100

Compound 4 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	-1.01864500	-0.62081300	1.29159600
C	-1.75750600	-0.29492400	-0.00004800
C	-1.01864100	-0.62039600	-1.29179700
C	0.49839500	-0.35338300	-1.23993700
C	0.87713400	1.14318500	-1.27105800
C	0.42961400	1.88437600	0.00029600
C	0.87712300	1.14278200	1.27142000
C	0.49838900	-0.35377500	1.23982700
N	1.03693000	-0.95066400	-0.00014800
O	2.23326700	-1.40706000	-0.00021800
O	-2.88844500	0.13863000	0.00002000
H	-1.49368600	-0.07979800	2.11226200
H	-1.17443400	-1.69180700	1.47200000
H	-1.17443700	-1.69133000	-1.47255200
H	-1.49367600	-0.07910900	-2.11228800
H	0.99225500	-0.87564400	-2.05972200
H	0.44811800	1.60986400	-2.16320900
H	1.96604400	1.20243400	-1.36766200
H	0.84862400	2.89465100	0.00045900
H	-0.65745800	2.01562200	0.00031300
H	1.96603200	1.20200300	1.36805400
H	0.44810000	1.60918000	2.16371500
H	0.99224800	-0.87629100	2.05944900

Compound 4 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	-1.02070100	-0.58579600	1.29118800
C	-1.75692900	-0.27879900	0.00000000
C	-1.02070100	-0.58579700	-1.29118800
C	0.50046000	-0.34378900	-1.24095600
C	0.90119300	1.14682000	-1.27053600
C	0.46475800	1.89261600	0.00000000
C	0.90119300	1.14682000	1.27053500
C	0.50046000	-0.34378800	1.24095600
N	1.02532000	-0.94795800	0.00000000
O	2.18416000	-1.50113900	0.00000000
O	-2.91038800	0.11338400	0.00000000
H	-1.47825900	-0.02733500	2.10995900
H	-1.19375500	-1.65262500	1.48260900
H	-1.19375500	-1.65262500	-1.48260900
H	-1.47825900	-0.02733600	-2.10995900
H	0.97720700	-0.87225000	-2.06599400
H	0.47300600	1.61255300	-2.16291700
H	1.99067000	1.19617500	-1.37011700
H	0.89751300	2.89723500	-0.00000100

H	-0.62107600	2.03775600	0.00000000
H	1.99067000	1.19617600	1.37011600
H	0.47300600	1.61255300	2.16291600
H	0.97720700	-0.87224900	2.06599400

Compound 4 oxoammonium ion (gas phase)

Charge 1 multiplicity 1

Compound 4 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	-1.01846500	-0.53486200	1.29119500
C	-1.75155100	-0.21750400	0.00000100
C	-1.01846500	-0.53486800	-1.29119300
C	0.51174800	-0.33744300	-1.25866700
C	0.97621800	1.15229100	-1.26009500
C	0.55072500	1.90361100	-0.00000400
C	0.97621900	1.15229700	1.26009000
C	0.51174900	-0.33743800	1.25866900
N	1.03428400	-0.91951400	0.00000200
O	1.89024700	-1.74887400	0.00000300
O	-2.90209000	0.16414900	0.00000000
H	-1.42420000	0.05774700	2.11186800
H	-1.22479400	-1.59031800	1.50599000
H	-1.22479200	-1.59032600	-1.50598100
H	-1.42420000	0.05773500	-2.11186800
H	0.99257500	-0.88720100	-2.06521400
H	0.55326600	1.59220500	-2.16581200
H	2.06444400	1.15615500	-1.36197400
H	1.02890000	2.88722500	-0.00000600
H	-0.52580500	2.09348400	-0.00000400
H	2.06444500	1.15616000	1.36196800
H	0.55326700	1.59221400	2.16580600
H	0.99257500	-0.88719300	2.06521800

Compound 6 (gas phase) 5,6-NO

Charge 0 multiplicity 1

N	-0.49673400	-1.12644900	0.00000100
C	0.10681600	-0.42572700	1.16241200
C	-0.38655000	1.02861100	1.27346300
C	-0.06150200	1.83232300	-0.00000600
C	-0.38651600	1.02860500	-1.27347900

C	0.10683600	-0.42573900	-1.16240600
C	1.59715800	-0.53297300	0.78086900
C	1.59717100	-0.53298900	-0.78084000
O	-1.93041800	-0.96021800	-0.00001300
H	-0.13159100	-0.97999900	2.07314500
H	0.06836000	1.50027300	2.15118000
H	-1.46669900	1.01161000	1.44158800
H	-0.61123000	2.77840800	-0.00001600
H	1.00102200	2.10109200	0.00000900
H	-1.46665900	1.01161100	-1.44163600
H	0.06842300	1.50025800	-2.15118500
H	-0.13156100	-0.98001700	-2.07313800
H	2.02094900	-1.46203100	1.16521000
H	2.17637800	0.29255400	1.19953800
H	2.02096800	-1.46205300	-1.16515900
H	2.17639800	0.29253100	-1.19951400
H	-2.24474900	-1.87001100	0.00000000

Compound 6 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

N	-0.86599600	-0.80626500	-0.00001400
C	-0.42322400	-0.02333900	-1.18017100
C	1.10740100	-0.19162200	-1.28220600
C	1.80766500	0.30363200	0.00003100
C	1.10735300	-0.19162100	1.28224400
C	-0.42326500	-0.02333900	1.18015700
C	-0.86178400	1.39809900	-0.78251400
C	-0.86183400	1.39808900	0.78248600
O	-0.87139100	-2.08028300	-0.00001800
H	-0.92466700	-0.40907900	-2.06804900
H	1.48388700	0.34902600	-2.15664100
H	1.31227100	-1.25475200	-1.44219200
H	2.85242700	-0.02002400	0.00005200
H	1.83169400	1.39906200	0.00003400
H	1.31222000	-1.25475100	1.44223900
H	1.48380300	0.34903100	2.15669100
H	-0.92473400	-0.40907900	2.06802000
H	-1.86282300	1.60462300	-1.16456900
H	-0.19090300	2.15404600	-1.19503700
H	-1.86291300	1.60455300	1.16447000
H	-0.19102400	2.15406900	1.19506900

Compound 6 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

N	-1.10108800	-0.41368400	-0.00000600
C	-0.39523000	0.13747200	-1.18237000

C	0.95600500	-0.60248700	-1.28218100
C	1.79170700	-0.41345000	0.00000900
C	0.95598800	-0.60249300	1.28218900
C	-0.39524100	0.13746800	1.18236700
C	-0.25552500	1.61758000	-0.78163100
C	-0.25554100	1.61757700	0.78163300
O	-1.64637800	-1.57079800	-0.00001200
H	-1.00423400	-0.02476300	-2.07180400
H	1.50568400	-0.23770500	-2.15519200
H	0.74792200	-1.66470200	-1.44911000
H	2.63257700	-1.11316000	0.00001400
H	2.22922900	0.59001800	0.00001600
H	0.74790000	-1.66470900	1.44910800
H	1.50565800	-0.23771800	2.15520800
H	-1.00425100	-0.02477000	2.07179600
H	-1.10240400	2.19025800	-1.16364300
H	0.65503100	2.05458500	-1.19437600
H	-1.10244500	2.19023200	1.16362500
H	0.65499300	2.05460300	1.19440400

Compound 6 oxoammonium ion (gas phase)

Charge 1 multiplicity 1

N	0.96554600	0.58432300	-0.00001800
C	0.38701100	-0.07298200	-1.19899900
C	-1.05914700	0.53064300	-1.27205300
C	-1.85669400	0.21653200	0.00004000
C	-1.05909400	0.53063200	1.27210200
C	0.38706000	-0.07299200	1.19898200
C	0.42675000	-1.55442300	-0.78369600
C	0.42678000	-1.55443000	0.78366400
O	1.68842300	1.52332600	-0.00002800
H	0.98020000	0.20880100	-2.06737300
H	-1.52572900	0.10282400	-2.16264700
H	-0.97308400	1.60859100	-1.43698900
H	-2.77824700	0.80457300	0.00006100
H	-2.16867700	-0.83070600	0.00004200
H	-0.97302400	1.60857900	1.43704200
H	-1.52563900	0.10280800	2.16271200
H	0.98028600	0.20878200	2.06733400
H	1.32952600	-2.02723200	-1.16979100
H	-0.42871400	-2.08725900	-1.19661200
H	1.32957000	-2.02724500	1.16972000
H	-0.42866900	-2.08726800	1.19660800

Compound 6 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

N	-0.96721200	-0.57105100	0.00000000
C	-0.38793700	0.07700100	-1.19620700
C	1.05215100	-0.54167400	-1.26881400
C	1.85109200	-0.23169700	0.00000000
C	1.05215100	-0.54167300	1.26881400
C	-0.38793700	0.07700100	1.19620700
C	-0.40753700	1.55659000	-0.78204800
C	-0.40753700	1.55659000	0.78204700
O	-1.70233700	-1.50568700	0.00000000
H	-0.97968400	-0.19806000	-2.06631300
H	1.51443000	-0.11330700	-2.16063900
H	0.95110200	-1.61895500	-1.42595300
H	2.76549800	-0.83172600	0.00000000
H	2.16480600	0.81474600	0.00000000
H	0.95110200	-1.61895500	1.42595400
H	1.51443000	-0.11330600	2.16063900
H	-0.97968400	-0.19806000	2.06631300
H	-1.30874900	2.03216800	-1.16687600
H	0.45899700	2.07165900	-1.19365600
H	-1.30874900	2.03216800	1.16687600
H	0.45899700	2.07165900	1.19365600

Compound 13 (gas phase)

Charge 0 multiplicity 1

C	-2.54166100	0.11694500	0.00143500
C	-2.05785900	-1.21473700	-0.00137400
C	-0.70469300	-1.50554600	-0.00828900
C	0.15518900	-0.40131700	-0.00949700
C	-0.30536000	0.92851700	-0.00234700
C	-1.68208500	1.19981400	0.00042800
N	1.50715300	-0.23491800	-0.02856300
N	1.86177100	1.06860300	0.01214500
N	0.78111800	1.77896300	0.00190800
O	2.44403700	-1.22337700	0.11355800
H	-3.61243900	0.28268400	0.00626400
H	-2.77215200	-2.03000600	0.00324300
H	-0.33153000	-2.52131700	-0.00582400
H	-2.04244600	2.22107100	0.00371000
H	2.97478000	-1.19601600	-0.69642100

Compound 13 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	2.49100800	-0.21846000	0.00017700
C	2.08360500	1.12907700	0.00019800
C	0.73799900	1.48771100	-0.00014300
C	-0.16825400	0.43378100	-0.00058400

C	0.22099400	-0.90467600	-0.00036900
C	1.56588800	-1.26015000	-0.00006800
N	-1.56102200	0.38144900	-0.00004200
N	-1.96936700	-0.98860700	0.00030100
N	-0.92825000	-1.71130700	0.00007100
O	-2.38081000	1.31812200	0.00017200
H	3.55016900	-0.44646200	0.00048800
H	2.83811800	1.90680500	0.00056300
H	0.41164200	2.51974200	-0.00009500
H	1.86959300	-2.29949600	0.00009300

Compound 13 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	-2.49167600	0.21343900	-0.00001700
C	-2.08105300	-1.13243100	0.00000400
C	-0.73386300	-1.49163300	0.00003600
C	0.16922400	-0.43525700	0.00006100
C	-0.22512400	0.90448600	0.00002700
C	-1.57015000	1.25987900	-0.00000500
N	1.56013300	-0.37665600	-0.00006200
N	1.96443300	0.98278300	0.00012500
N	0.91882500	1.70913900	-0.00008100
O	2.39637900	-1.30209700	-0.00005200
H	-3.55135900	0.43917500	-0.00005900
H	-2.83367200	-1.91211000	-0.00002700
H	-0.41399400	-2.52575600	0.00003500
H	-1.87988200	2.29770600	-0.00004400

Compound 13 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

Decomposed

Compound 15 (gas phase)

Charge 0 multiplicity 1

C	0.19534700	1.41760700	-0.00082100
N	1.51660600	0.94581900	-0.00030000
C	1.96624100	-0.36257800	-0.00021100
N	0.94643100	-1.32365200	-0.00013800
C	-0.40645500	-1.08969500	-0.00020600
C	-0.82565400	0.32566100	-0.00026100
O	-0.03976400	2.59845200	0.00053200
O	-1.21441100	-2.01752700	0.00014300

O	3.13213800	-0.67118400	0.00051500
N	-2.06827900	0.71261900	0.00009500
O	-3.02954300	-0.20253300	0.00022100
H	2.24064400	1.65446400	0.00019700
H	1.25313100	-2.28975100	0.00012500
H	-2.62133400	-1.11184500	-0.00021100

Compound 15 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	-0.08226000	1.39589300	-0.00046500
N	-1.42401900	1.01433000	0.00016800
C	-1.95413400	-0.27083200	0.00024600
N	-1.00601000	-1.29394100	-0.00010400
C	0.37684300	-1.17180300	0.00020000
C	0.84549300	0.24031400	0.00001200
O	0.25133600	2.55689700	-0.00000400
O	1.11619500	-2.12876800	-0.00019400
O	-3.14061700	-0.49060300	-0.00000800
N	2.12100800	0.49332300	-0.00003500
O	3.08978700	-0.21094900	0.00020400
H	-2.10434900	1.76479500	0.00011500
H	-1.38176000	-2.23482400	-0.00025100

Compound 15 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	0.08994400	1.38943300	0.00025600
N	1.42249300	1.01775000	0.00006400
C	1.94167400	-0.26801900	0.00018500
N	1.00542200	-1.29454600	0.00023200
C	-0.36776000	-1.17246000	0.00056300
C	-0.84041000	0.23702200	0.00020600
O	-0.25977100	2.55216200	-0.00011100
O	-1.11671700	-2.12805000	-0.00024200
O	3.13438700	-0.48681200	-0.00045000
N	-2.11017400	0.49118400	-0.00011400
O	-3.09017400	-0.20567700	-0.00022300
H	2.10815500	1.76752700	-0.00020700
H	1.38517600	-2.23708200	-0.00011900

Compound 15 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	-0.10647400	1.37331100	-0.11347200
N	1.23112600	1.18858500	0.01613100
C	1.95855600	0.00001600	0.08997100
N	1.23116200	-1.18856000	0.01598200
C	-0.10646100	-1.37332400	-0.11338000

C	-0.87070300	-0.00003500	-0.02222100
O	-0.68704200	2.40329400	-0.25997700
O	-0.68698500	-2.40333200	-0.25992400
O	3.15526300	0.00002900	0.19532300
N	-2.08394200	0.00002600	0.14275200
O	-3.21773500	-0.00001500	0.28621500
H	1.79700300	2.03849800	0.01882500
H	1.79705800	-2.03845800	0.01862400

Compound 16 (gas phase)

Charge 0 multiplicity 1

C	1.68540500	-1.42201400	0.00400600
C	0.50376900	-0.69952100	0.00563300
C	0.50377100	0.69951700	0.00562700
C	1.68540700	1.42200900	0.00401500
C	2.88470500	0.69858300	-0.00263900
C	2.88470400	-0.69859000	-0.00264500
C	-0.90614800	1.17843600	0.00983300
C	-0.90615000	-1.17843600	0.00988600
O	-1.35503100	2.29938300	-0.03677700
O	-1.35504600	-2.29937500	-0.03679800
N	-1.67088600	0.00000400	0.08794300
H	1.68529100	-2.50551200	0.00519900
H	1.68529500	2.50550700	0.00520300
H	3.82855400	1.23127800	-0.00858300
H	3.82855100	-1.23128700	-0.00859000
O	-3.02827800	0.00001700	-0.12285000
H	-3.43742600	-0.00013000	0.76028500

Compound 16 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	1.63698300	-1.42082300	0.00003600
C	0.45112900	-0.70006800	0.00027200
C	0.45112900	0.70006800	0.00019300
C	1.63698400	1.42082300	0.00009500
C	2.83326700	0.70000900	-0.00005100
C	2.83326700	-0.70000900	-0.00010200
C	-0.94201400	1.20422500	0.00007300
C	-0.94201400	-1.20422500	0.00077600
O	-1.37706400	2.31912800	0.00002200
O	-1.37706400	-2.31912800	-0.00013200
N	-1.76444500	0.00000000	-0.00012700
O	-3.02209500	0.00000000	-0.00071500
H	1.62626700	-2.50391200	0.00008700
H	1.62626800	2.50391200	0.00004000
H	3.77798800	1.23102400	-0.00017700

H	3.77798800	-1.23102400	-0.00021700

Compound 16 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	-1.63781100	-1.42292700	0.00001900
C	-0.45162400	-0.70240100	-0.00000900
C	-0.45162300	0.70240000	0.00003300
C	-1.63780900	1.42292700	-0.00001800
C	-2.83343300	0.70012600	-0.00002600
C	-2.83343300	-0.70012500	0.00000300
C	0.93469000	1.20193600	0.00020300
C	0.93468900	-1.20193700	-0.00015700
O	1.39156200	2.31292900	-0.00006200
O	1.39156200	-2.31292900	0.00006400
N	1.75679000	0.00000000	-0.00000300
O	3.01579200	0.00000000	-0.00003100
H	-1.63741900	-2.50611200	-0.00000500
H	-1.63741700	2.50611200	0.00000300
H	-3.77794500	1.23120400	-0.00003500
H	-3.77794600	-1.23120200	-0.00000800

Compound 16 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

C	-1.62889800	1.42742600	-0.00003500
C	-0.43380200	0.71540700	0.00004300
C	-0.43380200	-0.71540700	0.00006500
C	-1.62889800	-1.42742600	0.00008000
C	-2.81816900	-0.70366700	-0.00000700
C	-2.81816900	0.70366700	-0.00008100
C	0.88922900	-1.29597700	-0.00004000
C	0.88922900	1.29597600	0.00016500
O	1.39494300	-2.36330700	-0.00009600
O	1.39494300	2.36330700	-0.00007400
N	1.79971000	0.00000000	0.00024500
O	2.97137900	0.00000000	-0.00015300
H	-1.63089600	2.50999900	-0.00008800
H	-1.63089600	-2.50999900	0.00009600
H	-3.76330900	-1.23232800	-0.00007200
H	-3.76330900	1.23232800	-0.00019900

Compound 17 (gas phase)

Charge 0 multiplicity 1

C	-0.07527100	2.13670700	1.05967300
C	0.29392800	2.76873600	-0.11874200
C	1.28100500	2.21644500	-0.92993200

C	1.86137700	1.03859400	-0.48739800
C	1.46369200	0.44954400	0.69581100
C	2.90262300	0.17283900	-1.12468000
N	3.10073100	-0.86628700	-0.18932000
C	2.23888600	-0.82569900	0.91643900
O	2.18907000	-1.61049300	1.82063600
O	3.47501300	0.31433000	-2.16642500
O	3.77820500	-2.01082600	-0.51212800
C	-0.00744000	0.29186700	2.67829600
N	0.51715700	0.99385900	1.47618700
H	-0.86498900	2.51382500	1.69031000
H	-0.22914800	3.67170300	-0.40228700
H	1.57371700	2.66865400	-1.86946600
H	4.68814400	-1.88913900	-0.20258300
H	-0.46924200	1.03458700	3.32383700
H	0.81085900	-0.21117000	3.18392100
H	-0.75209600	-0.43069600	2.33798100
F	-0.77223300	-0.35166600	-0.65802500
F	-4.01216100	-0.54910300	-0.09262800
F	-2.47671800	-1.78872100	-1.33859200
F	-2.30266100	0.88338800	0.58430100
P	-2.42885300	-0.47343300	-0.40381700
F	-2.66891700	0.51174600	-1.67642200
F	-2.09406100	-1.39315000	0.92736700

Compound 17 *N*-oxyl (gas phase)

Charge 0 multiplicity 2

C	0.42102900	2.75703500	-0.06748900
C	0.80636900	2.65281900	-1.39343600
C	1.48888800	1.52108000	-1.83412900
C	1.77111800	0.55273400	-0.88431500
C	1.37696500	0.70934100	0.43414000
C	2.43941700	-0.76737700	-1.04393800
N	2.43195400	-1.34250100	0.29168800
C	1.80966700	-0.46650800	1.25652700
O	1.74867800	-0.65982900	2.43145100
O	2.91528700	-1.27559800	-2.01019700
O	2.93311900	-2.45344300	0.58553000
C	0.16936200	1.90834200	2.22658600
N	0.71677500	1.80265400	0.84655100
H	-0.15117600	3.59672400	0.29975900
H	0.53183400	3.44611400	-2.07519600
H	1.77559100	1.38880000	-2.87008700
H	-0.74678300	1.31463800	2.25675800
H	0.89650200	1.51786900	2.93194600
H	-0.03836000	2.95694300	2.42484500
F	-3.67238600	0.01792500	-0.35576600
F	-0.56814100	-1.03220700	0.03809200
F	-2.67819800	-1.99048600	0.30122600

F	-1.55785000	0.96454600	-0.61273000
P	-2.16700200	-0.53757100	-0.17169100
F	-2.14021700	-0.00998300	1.39965700
F	-2.08068200	-1.00228900	-1.72362200

Compound 17 *N*-oxyl (solvent=acetonitrile)

Charge 0 multiplicity 2

C	1.71829100	2.69346900	-0.22258500
C	2.12486300	2.35727800	-1.50856000
C	2.33104800	1.02749900	-1.85492500
C	2.11858100	0.08368000	-0.85630300
C	1.72110900	0.46653600	0.41401400
C	2.23738800	-1.39403100	-0.90812900
N	1.88970200	-1.83480600	0.43309800
C	1.57069200	-0.72278100	1.30098100
O	1.28102000	-0.82648500	2.45523200
O	2.53956700	-2.13052300	-1.79848700
O	1.87460300	-3.03433200	0.80393900
C	1.08361700	2.16551500	2.09173500
N	1.51543600	1.75720300	0.73056600
H	1.54511300	3.71830600	0.07417800
H	2.26827300	3.15384000	-2.22600800
H	2.64012700	0.74122100	-2.85233300
H	0.20388800	1.59177500	2.37126300
H	1.90004000	1.97877000	2.78790600
H	0.84724000	3.22489100	2.06106900
F	-3.67996000	0.92136400	-0.56486100
F	-1.19527000	-1.09509900	0.19462700
F	-3.41366000	-1.38479200	-0.43609500
F	-1.46063100	1.21008200	0.06568000
P	-2.44108100	-0.08681400	-0.18572500
F	-2.89102700	-0.05065200	1.39256400
F	-1.98383900	-0.12264000	-1.76288100

Compound 17 oxoammonium ion (solvent=acetonitrile)

Charge 1 multiplicity 1

Decomposed

Transition state (compound 2 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	-3.57563400	-1.34550000	-1.09754400
C	-3.18543100	-1.66877800	0.35736400
C	-2.40135400	-0.54025000	1.05965900
N	-1.23321600	-0.13607800	0.23332200

C	-1.66434700	0.39368200	-1.08766600
C	-2.41529300	-0.69820500	-1.87741800
O	-0.33733600	-1.17345000	0.08897200
C	-2.43031400	1.70568800	-0.83249800
C	-3.19329400	0.73690800	1.39747100
C	-3.59317600	1.56986400	0.16699300
H	-3.87518900	-2.26964800	-1.60184200
H	-4.45448700	-0.69770500	-1.11899400
H	-2.54291400	-2.55407000	0.36641300
H	-4.07439900	-1.91447500	0.94753300
H	-1.98574100	-0.94004400	1.98821400
H	-0.74395600	0.63389900	-1.62513000
H	-2.77470700	-0.27989200	-2.82322200
H	-1.67999000	-1.46811900	-2.12851300
H	-2.79139300	2.09958300	-1.78761200
H	-1.70996700	2.43538500	-0.44634900
H	-4.07936400	0.46465100	1.97934100
H	-2.56488300	1.34904700	2.05417700
H	-4.46173300	1.12576900	-0.32239100
H	-3.90937700	2.56598100	0.49164600
C	3.18157100	1.05194300	-0.36177700
C	4.38220400	1.02220200	-1.06333600
C	5.27492300	-0.03725200	-0.89354000
C	4.95936400	-1.06911900	-0.00695500
C	3.76343400	-1.04071600	0.69981500
C	2.85411200	0.01938800	0.53248900
C	1.57553300	0.00212800	1.25735200
O	0.87862900	1.19748000	1.30522700
H	2.49077000	1.87701700	-0.48187000
H	4.62642800	1.83035200	-1.74432600
H	6.20947000	-0.05733100	-1.44268000
H	5.65018600	-1.89285200	0.13527400
H	3.52516800	-1.84299000	1.39138200
H	0.71312700	-0.77348700	0.58612400
H	1.60565400	-0.53189200	2.21569000
H	-0.06432700	0.98922600	1.07784500

Transition state (compound 3 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	3.46042800	0.46965000	0.88788500
C	2.21883300	0.25612200	1.77843900
C	1.10570500	-0.39787200	0.93387800
N	0.76979000	0.45778100	-0.22972500
C	1.94402500	0.72434300	-1.09571300
C	3.07045900	1.39580900	-0.28209700
C	3.94263300	-0.88913800	0.33584100
C	2.42748000	-0.62170700	-1.65960700
C	1.57779600	-1.75762600	0.39457000
C	2.81968400	-1.54798000	-0.49311600

O	0.16500800	1.62382700	0.15956400
H	4.25990700	0.93410500	1.47450600
H	2.45956400	-0.38718300	2.63246600
H	1.86181900	1.21064800	2.17536400
H	0.18709300	-0.50897300	1.51289200
H	1.59671000	1.38102500	-1.89620000
H	3.93237300	1.58413900	-0.93213900
H	2.72054300	2.36206500	0.09140900
H	4.83388300	-0.74631000	-0.28663100
H	4.23459900	-1.54816400	1.16197400
H	1.63559200	-1.07925500	-2.26060700
H	3.28447000	-0.44845200	-2.31919500
H	1.81333000	-2.41594200	1.23761800
H	0.77176500	-2.22779900	-0.17642600
H	3.16245700	-2.51147900	-0.88436500
C	-3.68095000	0.22901300	0.76937200
C	-4.16229200	-1.04056000	1.07392000
C	-3.81969100	-2.13553400	0.28077900
C	-2.99301800	-1.94661500	-0.82909100
C	-2.50920000	-0.68154500	-1.13599900
C	-2.84389600	0.43351000	-0.34181300
C	-2.25786900	1.74005200	-0.66423500
O	-2.73655000	2.88165700	-0.02865700
H	-3.98633100	1.06937700	1.38304000
H	-4.81609400	-1.17426400	1.92882600
H	-4.19871900	-3.12269800	0.51896100
H	-2.72905400	-2.78993400	-1.45786100
H	-1.86524700	-0.54357200	-1.99765900
H	-0.93049200	1.62813700	-0.26349200
H	-2.13901600	1.95053800	-1.72611600
H	-2.70612200	2.75614600	0.92637500

Transition state (compound 5 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	3.27921700	-1.04630700	0.16572600
C	2.80965400	-0.84797600	-1.27514900
C	1.91309500	0.40861200	-1.31821200
N	0.74806900	0.24046500	-0.40410100
C	1.17803600	-0.01203000	1.00021400
C	2.06503000	-1.27330800	1.06668300
C	1.95866400	1.21817400	1.48724500
C	2.70419700	1.64327900	-0.85789400
C	3.19207800	1.42209600	0.58641500
C	4.08691200	0.16287200	0.64238100
F	4.10862800	-2.19251500	0.22045300
O	-0.08932800	-0.75833300	-0.84953400
H	3.67064000	-0.71739800	-1.93734600
H	2.24851800	-1.72249000	-1.61079600
H	1.50257400	0.55229400	-2.31892000

H	0.26495300	-0.15442900	1.57959800
H	2.38816900	-1.45245600	2.09627700
H	1.50330600	-2.14585100	0.72701100
H	1.31542200	2.10297000	1.46444600
H	2.25998300	1.06091500	2.52752000
H	3.55156800	1.79501400	-1.53371800
H	2.07547000	2.53672600	-0.91796700
H	3.76230100	2.29190000	0.92462400
H	4.44087500	-0.01577400	1.66250300
H	4.96782200	0.28536400	0.00452100
C	-3.62403900	0.60110900	0.91181700
C	-4.75818200	0.10390700	1.54489200
C	-5.62536700	-0.75623300	0.86927900
C	-5.35284700	-1.11192500	-0.45334100
C	-4.22353400	-0.61358300	-1.09119900
C	-3.34023600	0.24952000	-0.41815500
C	-2.12703700	0.72456600	-1.09957500
O	-1.48230400	1.80546000	-0.52071100
H	-2.95459200	1.27796200	1.42754400
H	-4.97059700	0.39001400	2.56928700
H	-6.50795500	-1.14234200	1.36648400
H	-6.02524500	-1.77461000	-0.98672100
H	-4.01833800	-0.88939600	-2.12092300
H	-1.19346300	-0.22155100	-1.00472500
H	-2.21768200	0.79621400	-2.19086000
H	-0.51866700	1.58266100	-0.48801000

Transition state (compound 15 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	2.73108100	1.21015000	-0.14253600
N	4.09591400	1.03063100	0.06597600
C	4.77946800	-0.16238700	0.27170000
N	3.97652900	-1.29516500	0.26097000
C	2.59386800	-1.37291000	0.06920900
C	1.94228500	-0.05472600	-0.13968600
O	2.26365900	2.31639600	-0.30639000
O	2.02249700	-2.43937400	0.07854600
O	5.97516000	-0.20807300	0.44525400
N	0.66956000	0.12287700	-0.33218800
O	-0.15368900	-0.86342000	-0.34780700
H	4.66654100	1.86700400	0.07310900
H	4.45952100	-2.17328500	0.40678000
H	-1.27957100	-0.26496000	-0.53357100
C	-5.15359000	0.22940800	1.43316700
C	-3.91702700	0.67940900	0.98797600
C	-5.92268600	-0.62428400	0.63898800
H	-5.52231200	0.54343000	2.40301200
C	-3.43627500	0.28596200	-0.27285600
H	-3.31747200	1.34312000	1.59768700

C	-5.44975500	-1.02557200	-0.61204900
H	-6.88566700	-0.97430400	0.99271300
C	-4.21701700	-0.57520000	-1.06561400
C	-2.12309800	0.71601100	-0.76094200
H	-6.04503300	-1.68563000	-1.23227700
H	-3.85211300	-0.88486100	-2.03969500
H	-2.01790900	0.74913900	-1.85368900
O	-1.57392000	1.79082200	-0.10435500
H	-0.63318500	1.86597000	-0.34351700

Transition state (compound 16 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	4.05886900	0.88591700	-1.08935600
C	4.08662600	1.27469000	0.25315500
C	3.13203500	0.80262200	1.16059300
C	2.16359700	-0.06315700	0.67962900
C	2.13582000	-0.45171100	-0.66194000
C	3.07574900	0.01265000	-1.56733900
C	1.03399500	-0.71761000	1.39857600
N	0.37912900	-1.48731800	0.40265200
C	0.98724100	-1.37791100	-0.87657500
O	0.61616400	-1.93255800	-1.87779500
O	0.70232300	-0.64062900	2.55390100
O	-0.63022600	-2.30438000	0.66344700
H	4.81190600	1.26764500	-1.76915800
H	4.86096000	1.95199200	0.59459500
H	3.14504900	1.09762100	2.20288500
H	3.04545600	-0.29469600	-2.60569700
C	-2.30666900	2.13082800	-1.45153700
C	-2.60830400	0.79537500	-1.21177400
C	-1.99189100	2.98527500	-0.39287500
H	-2.31489200	2.50848000	-2.46783500
C	-2.61032300	0.29713100	0.10285400
H	-2.84999900	0.12809700	-2.02906500
C	-1.98272100	2.49626700	0.91513300
H	-1.75510300	4.02549800	-0.58565900
C	-2.28773100	1.16387700	1.16308400
C	-2.88900100	-1.11614500	0.38582500
H	-1.73939400	3.15530200	1.74069600
H	-2.27197400	0.78462300	2.17943100
H	-1.72022600	-1.68224800	0.52232900
H	-3.29764200	-1.31259500	1.38423800
O	-3.55569500	-1.77407800	-0.63884100
H	-3.61233100	-2.71393200	-0.43573800

Transition state (compound 17 *N*-oxyl + benzyl alcohol, gas phase)

Charge 0 multiplicity 2

C	1.35010000	2.16904000	-0.91762800
C	1.24899300	2.83325400	0.29368100
C	0.48992000	2.29090400	1.32922400
C	-0.14851400	1.09096900	1.06934300
C	-0.01887300	0.46533800	-0.15636300
C	-1.00369100	0.23749500	1.94941800
N	-1.30033100	-0.90458500	1.15014100
C	-0.80139500	-0.81607500	-0.15126700
O	-1.03655600	-1.58024300	-1.05860500
O	-1.37870500	0.43617100	3.06716200
O	-1.98468800	-1.94486600	1.58442500
C	0.95985700	0.26612900	-2.41825400
N	0.70521200	1.00025400	-1.15072900
H	1.96219400	2.53702300	-1.72608600
H	1.79924300	3.75535700	0.42124500
H	0.41080800	2.77100600	2.29672700
H	1.78932700	-0.42135800	-2.24018100
H	0.06402500	-0.27771900	-2.70042700
H	1.23125700	0.99466500	-3.17820600
F	5.51395200	-0.43758400	-0.63170000
F	2.45575200	-0.36036800	0.59446800
F	4.31805600	-1.73046000	0.89934400
F	3.64773900	0.92624400	-0.93208800
P	4.02724600	-0.42079300	0.00146000
F	3.45884500	-1.35730300	-1.23572500
F	4.48970800	0.57622800	1.20176900
C	-4.19672800	-0.12933000	-1.51517200
C	-4.44301300	1.20300100	-1.83321300
C	-4.86430000	2.09667700	-0.84757000
C	-5.04754000	1.64887300	0.46293600
C	-4.80729900	0.31897900	0.78457600
C	-4.38108000	-0.58950800	-0.20190900
C	-4.13608400	-2.00395600	0.17912500
O	-3.73516100	-2.89806500	-0.78683100
H	-3.90070700	-0.82506400	-2.29079500
H	-4.32288500	1.54202100	-2.85610900
H	-5.06079500	3.13229700	-1.10030600
H	-5.38202700	2.33661300	1.23100100
H	-4.94827300	-0.02494400	1.80426200
H	-3.16479400	-1.94518200	1.00028700
H	-4.92589700	-2.44917800	0.78768300
H	-2.87203300	-2.62884900	-1.14226100

Transition state (compound 2 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	2.25471400	-1.20689600	-0.12920900
C	1.35115500	-1.04555300	-1.36673500
C	0.26258900	0.03462600	-1.20808800
N	-0.52279900	-0.19569900	0.03335000
C	0.34635900	-0.12092300	1.23673200
C	1.44491700	-1.20408300	1.18122100
O	-1.17735800	-1.42174600	-0.02402400
C	0.82954500	1.33670500	1.36204800
C	0.74774600	1.49655300	-1.17977500
C	1.51821200	1.87762600	0.09668600
H	2.80674900	-2.14889900	-0.20741600
H	3.01234000	-0.42063000	-0.10789900
H	0.83533200	-1.99093700	-1.55798600
H	1.95276600	-0.82628100	-2.25486200
H	-0.44813400	-0.07022200	-2.03136400
H	-0.30281400	-0.33869900	2.08891600
H	2.11044000	-1.08987200	2.04322800
H	0.94353200	-2.16981600	1.29292200
H	1.49631400	1.41973400	2.22598100
H	-0.04752800	1.95525300	1.58412800
H	1.36011000	1.68672500	-2.06672100
H	-0.13683300	2.13684500	-1.26905600
H	2.54471600	1.51136200	0.04151100
H	1.59305600	2.96749000	0.16299000
C	-3.47411300	-0.37835600	0.15027300
O	-3.00347300	0.86443700	-0.19846200
H	-4.24969500	-0.73522600	-0.52644700
H	-2.31512100	-1.15648200	0.01542100
H	-3.69537600	-0.51866800	1.21493400
H	-2.04035800	0.87848100	0.03924300

Transition state (compound 3 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	-2.01284400	-1.05361100	0.14397200
C	-1.09780300	-1.04560000	1.38583000
C	-0.03621000	0.05702600	1.22011100
N	0.77315600	-0.17946700	-0.01103200
C	-0.08146200	-0.23434600	-1.23228600
C	-1.14366500	-1.34063000	-1.09786100
C	-2.69479700	0.32291700	-0.00801700
C	-0.75513600	1.13790400	-1.39543200
C	-0.71054100	1.43148800	1.08171400
C	-1.62608200	1.42607900	-0.15726600
O	1.50621900	-1.35463700	0.11677900
H	-2.77360300	-1.83354500	0.25050700

H	-1.67862200	-0.85541500	2.29506100
H	-0.60350400	-2.01299200	1.50661900
H	0.66992400	0.05142800	2.05239600
H	0.59110600	-0.44040300	-2.06778800
H	-1.75801900	-1.36617700	-2.00460400
H	-0.64954300	-2.31126300	-1.00625400
H	-3.35490100	0.32070200	-0.88323900
H	-3.32505900	0.52927900	0.86479700
H	0.00326600	1.91757900	-1.52151200
H	-1.36544100	1.12840300	-2.30443400
H	-1.28853700	1.63615300	1.98872400
H	0.04810000	2.21612400	0.99677100
H	-2.10985600	2.40209200	-0.26474000
C	3.72768300	-0.17622300	-0.13863000
O	3.17521400	1.05069300	0.13762800
H	4.52893700	-0.43884200	0.55131200
H	2.62559500	-1.01936600	0.05362100
H	3.95223200	-0.36724600	-1.19478500
H	2.20950800	0.98129500	-0.08330600

Transition state (compound 5 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	-1.88549200	-0.61819200	0.06264600
C	-1.00445100	-0.84345000	1.29091600
C	0.21104600	0.10291800	1.18847800
N	0.97810600	-0.16737700	-0.05958000
C	0.12499000	-0.01611900	-1.27112000
C	-1.09313300	-0.96331900	-1.19736300
C	-0.34332900	1.44633100	-1.34125400
C	-0.25639800	1.56640800	1.15013300
C	-1.16166100	1.77565400	-0.07851800
C	-2.38063000	0.82871600	0.00982000
F	-3.00941800	-1.47626500	0.14321600
O	1.52866900	-1.44286500	-0.01574200
H	-1.56969300	-0.63265900	2.20346700
H	-0.67082900	-1.88239800	1.32695800
H	0.90127100	-0.06702300	2.01579500
H	0.75331300	-0.26957600	-2.12666500
H	-1.72120100	-0.83749900	-2.08427500
H	-0.76029300	-2.00240300	-1.15802600
H	0.51985800	2.11411200	-1.42239400
H	-0.94850100	1.58471900	-2.24266200
H	-0.79796200	1.79208100	2.07392000
H	0.60844500	2.23534600	1.10889900
H	-1.50585900	2.81309500	-0.11674300
H	-3.03535300	0.95798200	-0.85777700
H	-2.97321500	1.04322000	0.90466700
C	3.90751300	-0.60085800	-0.12436100
O	3.55293600	0.66599000	0.27307100

H	4.64039000	-1.05247700	0.54254800
H	2.69209600	-1.27286300	-0.03072100
H	4.12583600	-0.71792300	-1.19229200
H	2.61614600	0.79876300	-0.01148700

Transition state (compound 13 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	3.31508800	0.16726100	0.42363200
C	2.88551800	-1.17316200	0.25596300
C	1.57884200	-1.48993600	-0.07183500
C	0.70749600	-0.40518200	-0.21889400
C	1.11421400	0.93164300	-0.05384000
C	2.44628200	1.23190000	0.27161800
N	-0.61479800	-0.28697500	-0.54217200
N	-0.99393400	1.02064400	-0.54814500
N	0.03009500	1.75724700	-0.25157400
O	-1.49168500	-1.25672900	-0.78303600
H	4.35215100	0.35451100	0.67575500
H	3.60586000	-1.97240500	0.38683000
H	1.24513300	-2.51023900	-0.20826600
H	2.76692000	2.25899300	0.39428600
C	-3.22675600	-0.56380000	0.94114900
O	-3.75082400	0.49399300	0.26250200
H	-3.99468200	-1.28710700	1.20496400
H	-2.36610100	-1.13884700	0.07903800
H	-2.52311000	-0.31589800	1.74459600
H	-3.01975300	1.08412400	-0.00645300

Transition state (compound 15 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	-0.53326600	-1.24626400	0.09515400
N	-1.92165900	-1.31250700	0.04031600
C	-2.82586000	-0.25880700	-0.04202600
N	-2.24202200	1.00105900	-0.06775300
C	-0.88372600	1.32623500	-0.02117700
C	0.01418000	0.14324700	0.06419300
O	0.14025000	-2.25118300	0.16055100
O	-0.51617300	2.47777200	-0.04861600
O	-4.02143900	-0.42795000	-0.08690800
N	1.30809600	0.18828500	0.11487000
O	1.93668500	1.32026200	0.08700300
H	-2.33202400	-2.23810700	0.05687800
H	-2.88784800	1.77909900	-0.12669700
H	3.08672900	0.95667300	0.12094200
C	4.15161800	0.08193900	0.19984600
O	3.76443300	-0.99925700	-0.52934700
H	5.02007800	0.56539200	-0.24020200
H	4.17734800	-0.05244500	1.28591600

H	2.95708900	-1.38373200	-0.14627500

Transition state (compound 17 *N*-oxyl + methanol, gas phase)

Charge 0 multiplicity 2

C	-1.00720300	1.89432500	1.77843100
C	-1.02389200	2.88255100	0.81021900
C	-0.13927000	2.82375600	-0.26667800
C	0.73691400	1.75396100	-0.29233700
C	0.72315400	0.79592100	0.70370600
C	1.77388000	1.36961700	-1.30010300
N	2.29778300	0.13811800	-0.81132700
C	1.77279900	-0.24073400	0.41968100
O	2.16410400	-1.14629700	1.12271400
O	2.12003900	1.94420000	-2.28891500
O	3.19424400	-0.58540500	-1.47370900
C	-0.21242500	-0.22103900	2.74827300
N	-0.12170900	0.86806300	1.74222200
H	-1.70872700	1.87919000	2.59869700
H	-1.76105200	3.66964400	0.88962600
H	-0.14758500	3.56199200	-1.05873700
H	-0.76718600	-1.03910300	2.29157700
H	0.78921900	-0.54268200	3.01693900
H	-0.74459400	0.16442900	3.61389800
F	-3.04158100	-2.26779000	0.15589100
F	-2.03195700	0.62555900	-1.01266200
F	-2.36099800	-1.48610600	-1.93195100
F	-2.71529500	-0.15298100	1.05752000
P	-2.57789200	-0.84525300	-0.46548100
F	-0.98357700	-1.20853400	-0.06965700
F	-4.10202700	-0.42068500	-0.79726900
C	5.17425000	-0.88990100	0.10072000
O	4.85969300	-2.11493900	0.60423500
H	6.14017400	-0.90509600	-0.39907400
H	4.26437500	-0.63567500	-0.81137000
H	5.02330300	-0.04043300	0.77796100
H	3.97296400	-2.07313900	1.00350300

Transition state (compound 1 oxoammonium ion + 2,6-lutidine + benzyl alcohol)

Charge 1 multiplicity 1

C	2.47198600	-1.12526600	-1.28516100
C	2.99847800	-1.00028600	1.38783600
C	2.14739100	-2.27281000	1.51130600
C	2.16547000	-3.16228500	0.26660000
C	1.66223400	-2.38701100	-0.95307400
O	3.13644900	0.84172300	-0.11089600
C	1.73581800	-0.25310700	-2.30318600

C	3.88047200	-1.43417300	-1.82737400
C	2.71964100	-0.02877100	2.53551600
C	4.51204000	-1.29885700	1.37437900
N	2.65114200	-0.28068500	0.03409000
H	1.11361000	-1.98933600	1.73493000
H	2.51326800	-2.82204900	2.38394600
H	3.16672400	-3.56629900	0.09206600
H	1.51945700	-4.02790300	0.43528100
H	0.61965300	-2.09658300	-0.79172200
H	1.68045600	-3.02168200	-1.84441900
H	0.70651600	-0.06732200	-2.00439300
H	1.71667300	-0.79253500	-3.25288700
H	2.25091900	0.69396700	-2.46112900
H	3.76269600	-1.83482300	-2.83647500
H	4.42313500	-2.17367000	-1.24399600
H	4.47875700	-0.52448500	-1.89515100
H	3.02475600	-0.50909000	3.46727600
H	1.66178800	0.21338100	2.62311700
H	3.29339400	0.89100600	2.42413800
H	4.78991100	-2.10976600	0.70647400
H	4.80058800	-1.59320800	2.38563800
H	5.07963000	-0.40660600	1.10695800
C	-0.28023400	2.43803600	-1.19995300
C	-0.02360900	3.74501900	-1.58929700
C	0.78192700	4.57125700	-0.79667700
C	1.31972600	4.08367000	0.39006000
C	1.06073200	2.77175800	0.78416000
C	0.25197900	1.93552900	-0.00219500
C	-0.04992000	0.52852600	0.43596900
O	-0.94784400	-0.17107500	-0.22760100
H	-0.90617300	1.79258000	-1.80395600
H	-0.45053300	4.12972200	-2.50859500
H	0.98244700	5.59043600	-1.10614400
H	1.94117600	4.72038100	1.00865800
H	1.47010300	2.40763100	1.71780400
H	-0.11426200	0.46327000	1.53933900
H	-2.37745900	-0.36084700	0.06104600
H	1.06003800	-0.00968200	0.30005900
C	-3.96572900	-1.61311100	-0.50783900
C	-5.33771300	-1.83490400	-0.46187800
C	-6.15086900	-0.95004900	0.23765100
C	-5.59012600	0.14903200	0.88290000
C	-4.21761600	0.35125000	0.82073400
N	-3.46053000	-0.53486500	0.13279200
H	-7.22167600	-1.11274900	0.27677100
H	-5.75519900	-2.69101800	-0.97533500
H	-6.20743200	0.85164300	1.42671100
C	-3.51825000	1.50150500	1.48054000
H	-4.24217100	2.21870600	1.86492800
H	-2.90881700	1.15064100	2.31874400
H	-2.85407700	2.01207000	0.77963500

C	-3.00504000	-2.51765200	-1.21857900
H	-2.18210600	-1.95051000	-1.65407100
H	-2.57419100	-3.23438500	-0.51188900
H	-3.51744800	-3.08104200	-1.99818000

Transition state (compound 2 oxoammonium ion + 2,6-lutidine + benzyl alcohol)

Charge 1 multiplicity 1

C	-0.23051000	2.22681700	-1.18001700
C	-0.03218700	3.50712800	-1.68987600
C	0.52958200	4.49873200	-0.88780100
C	0.89392100	4.21081800	0.43248000
C	0.69733100	2.93506400	0.94152300
C	0.12037200	1.92970200	0.14463400
C	-0.09142300	0.55448500	0.71391000
O	-0.82596900	-0.31802100	0.01782100
H	-0.66717800	1.44417000	-1.78746800
H	-0.31061400	3.73127300	-2.71310800
H	0.68348400	5.49559800	-1.28463300
H	1.32244800	4.98604000	1.05711600
H	0.96732500	2.71649500	1.97105200
H	1.01434500	0.15026700	0.75711700
H	-0.32123300	0.61175500	1.79710700
H	-2.17912400	-0.47848800	0.13715100
C	4.61992800	-1.88931800	-0.77738500
C	4.77552900	-0.47977600	-0.17757800
C	3.54353300	0.00752900	0.64237800
N	2.39204700	-0.17995400	-0.30059300
C	2.05505600	-1.61340000	-0.57494800
C	3.24763800	-2.11250900	-1.43879500
O	2.21971200	0.65221400	-1.18662300
C	1.78745600	-2.36919400	0.73541500
C	3.27458900	-0.70351700	1.97456700
C	2.84869000	-2.17366000	1.83205300
H	5.39900800	-2.03282300	-1.53138400
H	4.80146500	-2.64902500	-0.01698800
H	4.92482200	0.24932800	-0.97891100
H	5.65241300	-0.42717600	0.47274600
H	3.62138000	1.08545100	0.78913900
H	1.14314000	-1.57631500	-1.17289200
H	3.08787300	-3.17160100	-1.65627100
H	3.19949000	-1.57702800	-2.39113800
H	1.69012100	-3.43019000	0.48881100
H	0.80812600	-2.04722100	1.09700400
H	4.17716300	-0.62180800	2.58610000
H	2.49615200	-0.14348000	2.50240000
H	3.72003700	-2.79986500	1.63944700
H	2.44040600	-2.51855100	2.78532500
C	-3.72247500	-1.76018700	-0.60880000
C	-5.08483500	-2.02595600	-0.70528500

C	-5.99145700	-1.18676800	-0.06784000
C	-5.52956400	-0.09132100	0.65577400
C	-4.16316500	0.15047800	0.73158000
N	-3.30961700	-0.68818000	0.10246200
H	-7.05520400	-1.38244800	-0.13710800
H	-5.42166500	-2.88038200	-1.27754200
H	-6.21793900	0.57727200	1.15556500
C	-3.57796000	1.30838800	1.48499400
H	-2.97046600	0.95666100	2.32355800
H	-2.93521700	1.91155800	0.83920400
H	-4.36789100	1.94533400	1.88078200
C	-2.67352400	-2.62119300	-1.24744400
H	-3.10984000	-3.23316900	-2.03643100
H	-1.86726200	-2.01238700	-1.65769100
H	-2.23167000	-3.28991200	-0.50195500

Transition state (compound 3 oxoammonium ion + 2,6-lutidine + benzyl alcohol)

Charge 1 multiplicity 1

C	4.48234400	-1.61767300	-0.58343900
C	4.63116600	-0.12829600	-0.21983600
C	3.37355600	0.33688000	0.56219700
N	2.23682200	0.09823600	-0.39843500
C	1.97862000	-1.34932500	-0.71705200
C	3.24769200	-1.79759700	-1.48908000
C	4.31551200	-2.45020300	0.70565800
C	1.81531200	-2.16104900	0.57293100
C	3.18762900	-0.49540100	1.83464300
C	3.05693300	-1.98556000	1.46625100
O	2.01582300	0.94306600	-1.26034000
H	5.37415700	-1.94474700	-1.12518600
H	5.50190200	0.03595400	0.42108600
H	4.75342000	0.49224200	-1.11127300
H	3.38307900	1.41192700	0.74121600
H	1.07981700	-1.35091400	-1.33316200
H	3.11557200	-2.84585800	-1.77093000
H	3.33996900	-1.21612200	-2.41007600
H	4.23234600	-3.51309800	0.45787900
H	5.20163500	-2.34051800	1.33875800
H	0.89990600	-1.86417200	1.08808700
H	1.69395900	-3.21024500	0.28769700
H	4.05903200	-0.32738200	2.47390600
H	2.31241500	-0.15161100	2.39297200
H	2.93440500	-2.57417800	2.37896000
H	0.85809700	0.30940200	0.66738700
C	-0.53537400	2.37942400	-1.16609100
C	-0.42011200	3.68775300	-1.62821200
C	0.09244400	4.68022200	-0.79489000
C	0.49256800	4.36481400	0.50850000
C	0.37919200	3.06112500	0.96999500

C	-0.14929500	2.05444200	0.14189400
C	-0.27144400	0.64914700	0.66105000
O	-0.96650800	-0.23848400	-0.05465100
H	-0.93343300	1.59562500	-1.79809700
H	-0.72594600	3.93362400	-2.63851800
H	0.18029100	5.69902200	-1.15433500
H	0.88297400	5.14003400	1.15767000
H	0.67700700	2.81999200	1.98677900
H	-0.48162300	0.65285500	1.74973600
H	-2.28970300	-0.52319900	0.11075000
C	-4.28559100	-0.13338300	0.85562500
C	-5.62881400	-0.48792500	0.82116500
C	-6.03607300	-1.54654200	0.01442600
C	-5.09895200	-2.23568600	-0.74673100
C	-3.76066200	-1.85917300	-0.68892700
N	-3.40068700	-0.82832200	0.10658700
H	-7.08160900	-1.82950000	-0.02352700
H	-6.34216200	0.06590700	1.41708500
H	-5.39405100	-3.05761300	-1.38578800
C	-2.67985100	-2.55603300	-1.46099700
H	-3.10470100	-3.11489500	-2.29452600
H	-1.94542100	-1.84121100	-1.83342900
H	-2.15078200	-3.26142900	-0.81236200
C	-3.75735600	0.99544300	1.69100200
H	-3.08769800	0.61927100	2.46963700
H	-3.19237800	1.70322100	1.07958900
H	-4.57460600	1.52913600	2.17438000

Transition state (compound 6 oxoammonium ion+ 2,6-lutidine + benzyl alcohol)

Charge 1 multiplicity 1

N	1.94927700	-0.91791800	-0.03471100
C	2.39552000	-1.51002600	1.29577900
C	3.46111500	-2.55970700	0.91246200
C	2.87942100	-3.65263200	-0.00431100
C	2.02973300	-3.07077100	-1.14973700
C	1.05564100	-1.99227600	-0.63450400
C	1.09105600	-2.10534100	1.83738400
C	0.21915300	-2.42567800	0.57742100
O	2.75230900	-0.28441200	-0.74230300
H	2.82466600	-0.70866200	1.89606900
H	3.85518700	-2.99656300	1.83387300
H	4.28582900	-2.03665000	0.42171000
H	3.69395200	-4.25022500	-0.41977800
H	2.27260000	-4.34397600	0.58828700
H	2.66336700	-2.61607500	-1.91547900
H	1.44552200	-3.85638800	-1.63608700
H	0.48483400	-1.53755400	-1.44309100
H	0.58290000	-1.39725500	2.49395200
H	1.29353000	-2.99772100	2.42951100

H	-0.72535600	-1.88131300	0.61068100
H	-0.02412100	-3.48632800	0.51402500
C	1.68448700	2.38918200	-1.35527500
C	2.73272000	3.26847700	-1.59284300
C	3.48045100	3.76838400	-0.52689600
C	3.18359900	3.39153100	0.78833200
C	2.14083000	2.51436900	1.03342900
C	1.36599100	2.01801500	-0.03559500
C	0.26532600	1.09406000	0.25052500
O	-0.61859300	0.84935100	-0.72516900
H	1.08824000	2.00294100	-2.17142100
H	2.97008300	3.56411000	-2.60748700
H	4.29673600	4.45577700	-0.71647300
H	3.76384400	3.79114800	1.61114300
H	1.89830400	2.23180200	2.05328800
H	0.97482600	0.02034600	0.37135900
H	-0.14539600	1.15789100	1.26484800
H	-1.57281400	0.60537700	-0.39142000
C	-3.79780900	0.90210000	0.89174300
C	-5.17273700	0.72276200	1.03182300
C	-5.84393400	-0.09919600	0.13392100
C	-5.12776700	-0.71766300	-0.88319600
C	-3.75284700	-0.50370100	-0.97554600
N	-3.10958100	0.28868200	-0.09298500
H	-6.91368000	-0.24980800	0.22210900
H	-5.70420800	1.22673500	1.82895500
H	-5.62308700	-1.35524100	-1.60442300
C	-2.93197400	-1.15001100	-2.05993700
H	-2.28527900	-0.41998400	-2.55109100
H	-2.29280300	-1.93506500	-1.64346100
H	-3.57252800	-1.60840500	-2.81327600
C	-3.02606900	1.79199200	1.82940000
H	-2.30732900	1.21033400	2.41561400
H	-2.47515300	2.55683300	1.27540600
H	-3.69169500	2.29583200	2.53001500

Transition state (compound 1 oxoammonium ion+ 2,6-lutidine + methanol)

Charge 1 multiplicity 1

C	2.76161400	-1.19477300	-0.17153600
C	2.10894300	1.26651100	0.76447100
C	3.33151900	1.78063200	-0.01266100
C	4.45188600	0.75088700	-0.17713500
C	3.93616900	-0.50640600	-0.88235500
O	0.57406800	-0.54693200	0.53354200
N	1.67540900	-0.10936100	0.15160800
C	3.17799500	-1.87574900	1.14507700
C	2.12004000	-2.25372100	-1.07298800
C	2.39922600	1.06437100	2.26295900
C	0.93026200	2.23468400	0.63542600

H	3.00595200	2.11831800	-1.00326100
H	3.70026100	2.66980500	0.50694100
H	5.25923200	1.18979600	-0.76868300
H	4.89334300	0.49960800	0.79140900
H	3.63076100	-0.24683300	-1.90228000
H	4.73604100	-1.24550200	-0.98343800
H	2.30033400	-2.17774200	1.71859500
H	3.74062600	-2.77732800	0.89374800
H	3.81589700	-1.26018700	1.77415600
H	2.86597800	-3.02712800	-1.26706100
H	1.26152200	-2.71930500	-0.59109000
H	1.80618300	-1.85041500	-2.03396000
H	2.47159100	2.04949600	2.72883100
H	1.58376900	0.52297700	2.74513100
H	3.33246000	0.54299300	2.45805300
H	0.05093800	1.85313500	1.15429100
H	1.21695100	3.18184500	1.09645300
H	0.67692000	2.43800100	-0.40418100
C	0.41807400	0.38183100	-2.08068200
O	-0.56158000	-0.20931600	-1.47994200
H	0.33973600	1.46669600	-2.26393400
H	1.36654300	0.34306900	-1.24599200
H	0.88060100	-0.15192800	-2.92591800
H	-1.96622800	-0.01863600	-0.75817600
C	-3.28965700	-1.23758200	0.26813800
C	-4.53884700	-1.30919200	0.87518900
C	-5.36990700	-0.19474100	0.87163900
C	-4.95282100	0.98730100	0.26326400
C	-3.70205600	1.04224800	-0.33366100
N	-2.92289500	-0.06569700	-0.30248900
H	-6.34504000	-0.24517800	1.34201100
H	-4.84834600	-2.23533700	1.34074200
H	-5.58831300	1.86256700	0.24923300
C	-3.15386400	2.25631900	-1.01954200
H	-3.86610300	3.07839000	-0.96856700
H	-2.21905700	2.57666900	-0.55254800
H	-2.94346800	2.04395400	-2.07122600
C	-2.33511300	-2.38671900	0.18475900
H	-2.59758000	-3.15124500	0.91525600
H	-2.38137400	-2.83531100	-0.81284800
H	-1.30841300	-2.05526600	0.34350300

Transition state (compound 2 oxoammonium ion + 2,6-lutidine + methanol)

Charge 1 multiplicity 1

C	3.65173800	1.42230500	1.49479600
C	2.68561900	0.38095200	2.08903400
C	2.20619000	-0.68898800	1.07848300
N	1.64268000	0.08323600	-0.08786000
C	2.69856900	0.85036400	-0.84397700

C	3.18478600	1.95226400	0.12640600
O	0.52082400	0.60887600	0.03911200
C	3.76023200	-0.12217400	-1.37889700
C	3.25688200	-1.69007600	0.57530700
C	4.34484300	-1.07744700	-0.32400800
H	3.73075100	2.26320300	2.18899100
H	4.65716700	1.00794700	1.41843100
H	1.79086500	0.88545400	2.46618800
H	3.14442600	-0.13035100	2.93957000
H	1.35549700	-1.22344600	1.50421500
H	2.16722700	1.31516400	-1.67576100
H	3.98408400	2.51444400	-0.36353700
H	2.34937300	2.64471900	0.26683600
H	4.55590200	0.46705900	-1.84242000
H	3.30610100	-0.70533300	-2.18628500
H	3.70866400	-2.17406100	1.44541000
H	2.73347900	-2.48019800	0.02663700
H	5.09116000	-0.56410300	0.28215400
H	4.87983200	-1.88349300	-0.83221900
C	0.32563500	-1.48223300	-1.71399200
O	-0.63222600	-0.63619700	-1.44611100
H	1.29323200	-1.08166400	-1.10722500
H	0.22060200	-2.50885400	-1.31877700
H	0.70376600	-1.46683000	-2.74966400
H	-1.97714100	-0.42472000	-0.66304200
C	-3.63385700	-1.07797200	0.41122600
C	-4.85560500	-0.71297400	0.95695000
C	-5.30406300	0.59860000	0.81432700
C	-4.53239400	1.52942300	0.12804300
C	-3.31148300	1.14389900	-0.41554600
N	-2.91300000	-0.13838800	-0.24542600
H	-6.25692400	0.89290800	1.23868500
H	-5.44437700	-1.45029000	1.48592300
H	-4.86679300	2.55104400	0.00622000
C	-2.42342900	2.05670500	-1.20198600
H	-2.67515900	3.09727600	-0.99936300
H	-1.37248400	1.87578400	-0.97469800
H	-2.55969100	1.87410200	-2.27287500
C	-3.05658500	-2.45825600	0.49638300
H	-3.70744800	-3.11041300	1.07678700
H	-2.93640300	-2.88838800	-0.50174000
H	-2.07145800	-2.43848700	0.96944900

Phenol (gas phase)

Charge 0 multiplicity 1

C	0.26277100	1.19765600	-0.00001000
C	-1.13148000	1.21719200	-0.00000200
C	-1.85509200	0.02724900	0.00000500
C	-1.16963600	-1.18910800	-0.00000100

C	0.22071200	-1.22148100	0.00000600
C	0.93793300	-0.02383700	0.00000600
O	2.30551300	-0.11040100	-0.00003800
H	0.82256300	2.12870500	-0.00003100
H	-1.64898300	2.16995800	-0.00000800
H	-2.93831500	0.04554400	0.00001600
H	-1.72209000	-2.12209100	-0.00000100
H	0.76458900	-2.15846600	0.00002000
H	2.68689200	0.77352800	0.00027900

Phenol radical (gas phase)

Charge 0 multiplicity 2

C	0.28952500	1.23846700	-0.00000100
C	-1.08557200	1.22369900	-0.00000400
C	-1.78244200	0.00000000	0.00000200
C	-1.08557100	-1.22369900	0.00000000
C	0.28952500	-1.23846700	-0.00000400
C	1.04749400	0.00000000	0.00002300
O	2.30030800	0.00000000	-0.00000800
H	0.85478600	2.16308200	-0.00000600
H	-1.64171100	2.15438800	-0.00001300
H	-2.86636000	0.00000000	-0.00000500
H	-1.64171300	-2.15438700	0.00000300
H	0.85478500	-2.16308200	-0.00002200

Methanol (gas phase)

Charge 0 multiplicity 1

C	-0.66723800	-0.02025800	0.00000100
O	0.74957800	0.12205600	0.00000100
H	-1.02903000	-0.54469000	0.89303200
H	-1.08412500	0.98697500	-0.00015800
H	-1.02900800	-0.54495400	-0.89288400
H	1.14896900	-0.75223100	0.00000000

Benzyl alcohol (gas phase)

Charge 0 multiplicity 1

C	0.07198700	-1.09557500	0.20816200
C	1.43720200	-1.30989800	0.04290500
C	2.30185300	-0.22788600	-0.13187000
C	1.79125800	1.06754700	-0.14474100
C	0.42126600	1.27916100	0.01518000
C	-0.45138300	0.20345400	0.19680200
C	-1.93480800	0.43291600	0.39041800
O	-2.75162100	-0.38507600	-0.44980700

H	-0.60037000	-1.93615600	0.34037200
H	1.82955400	-2.32083600	0.05404300
H	3.36539000	-0.39582800	-0.25921900
H	2.45548500	1.91312700	-0.28492800
H	0.02764900	2.29086700	-0.00235900
H	-2.23308800	0.17070200	1.40903300
H	-2.16644900	1.49575900	0.24501100
H	-2.48945500	-0.23534100	-1.36462900

Lutidine (gas phase)

Charge 0 multiplicity 1

C	1.15732600	-0.26590700	-0.00000600
C	1.19838200	1.13215400	-0.00000200
C	0.00000000	1.83724200	-0.00000300
C	-1.19838200	1.13215400	-0.00000500
C	-1.15732700	-0.26590600	-0.00001000
N	0.00000000	-0.94127800	-0.00000900
H	0.00000100	2.92191800	-0.00000100
H	2.14985300	1.65089800	-0.00000500
H	-2.14985400	1.65089800	-0.00000200
C	-2.41591600	-1.09458400	-0.00000300
H	-3.31190200	-0.47094200	-0.00016900
H	-2.44049100	-1.74420100	-0.87902900
H	-2.44065500	-1.74394600	0.87921000
C	2.41591600	-1.09458400	0.00002100
H	2.44062400	-1.74396900	0.87921800
H	2.44052400	-1.74417800	-0.87902100
H	3.31190100	-0.47094100	-0.00009800

Lutidine (solvent=acetonitrile)

Charge 0 multiplicity 1

C	1.16157300	-0.26792500	-0.00003400
C	1.19973700	1.12998500	-0.00004400
C	-0.00000200	1.83458500	0.00000200
C	-1.19974300	1.12998500	0.00004600
C	-1.16157200	-0.26792100	-0.00000300
N	0.00000400	-0.94373000	-0.00001200
H	0.00001100	2.91941000	0.00001000
H	2.15132600	1.64826200	-0.00010000
H	-2.15134600	1.64823600	0.00011900
C	-2.42231400	-1.09065500	-0.00001900
H	-3.31206600	-0.45873900	-0.00018200
H	-2.45562700	-1.73930400	-0.88092600
H	-2.45581600	-1.73906800	0.88106000
C	2.42231800	-1.09065000	0.00003200
H	2.45573300	-1.73904600	0.88112700

H	2.45570000	-1.73933000	-0.88084900
H	3.31207400	-0.45873700	-0.00006500