Exploring Solvent Effects upon the Menshutkin Reaction using a Polarizable Force Field

Orlando Acevedo[†,*] **and William L. Jorgensen**[‡]

Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama 36849 and the Department of Chemistry, Yale University, 225 Prospect Street, New Haven, Connecticut 06520-8107. [†] *Auburn University.* [‡] *Yale University.*

Supporting Material

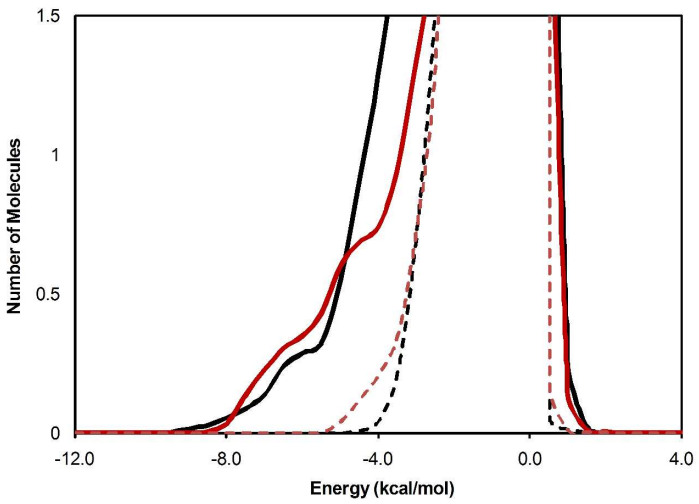

Figure S1. Solute-solvent energy pair distributions at 25 °C for the Menshutkin rearrangement of triethylamine and ethyl iodide in THF. OPLS-AA in black and OPLS-AAP in red with transition structures represented by solid lines and reactants by dashed lines.

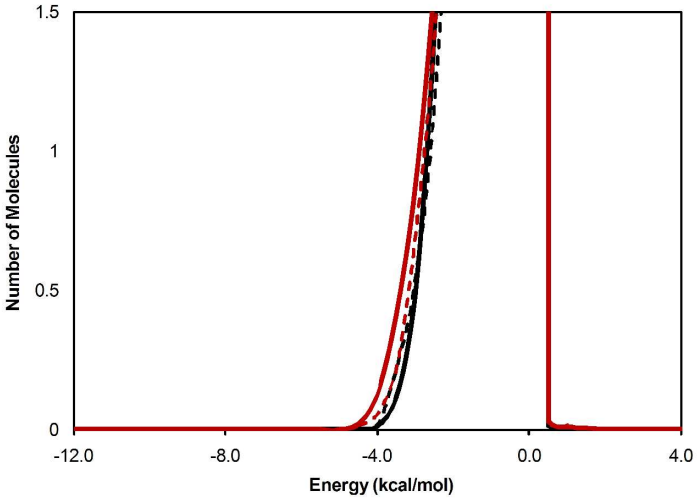

Figure S2. Solute-solvent energy pair distributions at 25 °C for the Menshutkin rearrangement of triethylamine and ethyl iodide in cyclohexane. OPLS-AA in black and OPLS-AAP in red with transition structures represented by solid lines and reactants by dashed lines.

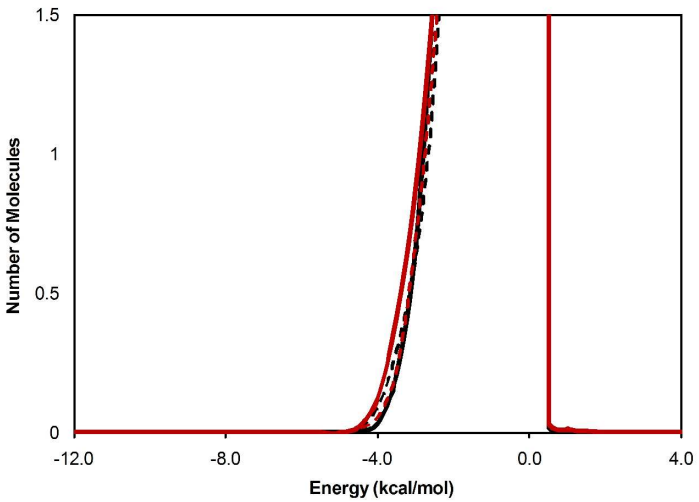

Figure S3. Solute-solvent energy pair distributions at 25 °C for the Menshutkin rearrangement of triethylamine and ethyl iodide in CCl_4. OPLS-AA in black and OPLS-AAP in red with transition structures represented by solid lines and reactants by dashed lines.

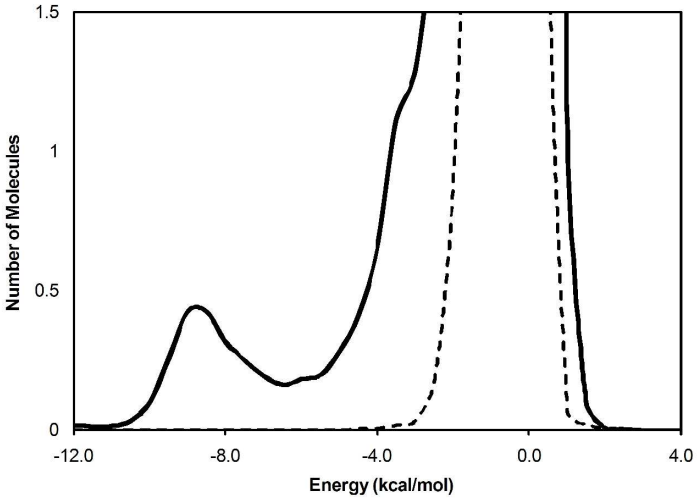

Figure S4. Solute-solvent energy pair distributions at 25 °C for the Menshutkin rearrangement of triethylamine and ethyl iodide in CH_3OH. The transition structure is represented by a solid line and reactants by a dashed line.

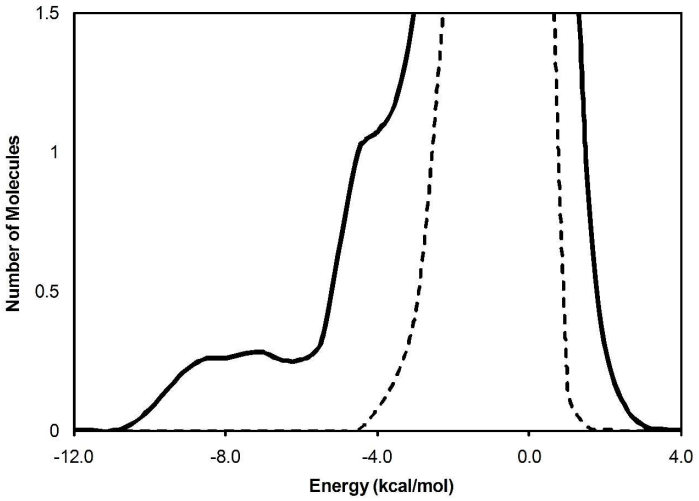

Figure S5. Solute-solvent energy pair distributions at 25 °C for the Menshutkin rearrangement of triethylamine and ethyl iodide in CH_3CN. The transition structure is represented by a solid line and reactants by a dashed line.

B3LYP/LANL2DZ transition structure:

	1	2	3
	A	A	A
Frequencies --	-341.0867	37.2959	61.4458
Red. masses --	8.0257	3.5417	2.9992
Frc consts --	0.5501	0.0029	0.0067
IR Inten --	910.4264	0.8306	3.0632

Sum of electronic and zero-point Energies= -382.655184
Sum of electronic and thermal Energies= -382.640696
Sum of electronic and thermal Enthalpies= -382.639752
Sum of electronic and thermal Free Energies= -382.698148

1|1|UNPC-UNK|FTS|RB3LYP|LANL2DZ|C8H20I1N1|PCUSER|30-May-2005|1||# B3LY
P/LANL2DZ OPT=(MNDOFC,TS,NOEIGEN,Z-MATRIX)||ET3N + EtI Menshutkin||0,1
|N|C,1,B1|C,1,B2,2,A1|C,1,B3,3,A2,2,D1,0|H,2,B4,1,A3,4,D2,0|C,2,B5,1,A
4,4,D3,0|H,2,B6,1,A5,4,D4,0|H,3,B7,1,A6,4,D5,0|C,3,B8,1,A7,4,D6,0|H,3,
B9,1,A8,4,D7,0|H,4,B10,1,A9,3,D8,0|C,4,B11,1,A10,3,D9,0|H,4,B12,1,A11,
3,D10,0|H,6,B13,2,A12,1,D11,0|H,6,B14,2,A13,1,D12,0|H,6,B15,2,A14,1,D1
3,0|H,9,B16,3,A15,1,D14,0|H,9,B17,3,A16,1,D15,0|H,9,B18,3,A17,1,D16,0|
H,12,B19,4,A18,1,D17,0|H,12,B20,4,A19,1,D18,0|H,12,B21,4,A20,1,D19,0|C
,1,B22,4,A21,12,D20,0|H,23,B23,1,A22,4,D21,0|C,23,B24,1,A23,4,D22,0|H,
23,B25,1,A24,4,D23,0|H,25,B26,23,A25,1,D24,0|H,25,B27,23,A26,1,D25,0|H
,25,B28,23,A27,1,D26,0|I,23,B29,1,A28,4,D27,0||B1=1.50995801|B2=1.5155
996|B3=1.50652828|B4=1.09333124|B5=1.53714642|B6=1.10436929|B7=1.09349
11|B8=1.53910683|B9=1.10410582|B10=1.0928208|B11=1.53791135|B12=1.1049
686|B13=1.09540257|B14=1.09418442|B15=1.09705551|B16=1.09473152|B17=1.
09731569|B18=1.09523976|B19=1.09506472|B20=1.09707298|B21=1.09482549|B
23=1.07968823|B24=1.51881946|B25=1.07945955|B26=1.09342058|B27=1.09776
134|B28=1.09335705|A1=110.25602236|A2=110.21053477|A3=107.0844497|A4=1
15.55433502|A5=108.33419109|A6=107.02918998|A7=116.104339|A8=107.95181
026|A9=107.54491003|A10=115.09537002|A11=108.37206163|A12=113.0248421|
A13=111.61689614|A14=108.42576068|A15=112.47468461|A16=108.04179173|A1
7=112.90979465|A18=111.70020451|A19=108.70856242|A20=112.76975834|A21=
113.65530817|A22=90.62648988|A23=108.53539139|A24=89.85520571|A25=110.
5982288|A26=112.11011378|A27=110.30390625|A28=154.06631375|D1=-122.835
55427|D2=180.9029277|D3=-58.08068072|D4=65.4899165|D5=59.91040819|D6=-
178.75249224|D7=-55.40218282|D8=181.12578205|D9=-57.29941147|D10=65.82
602995|D11=67.32886721|D12=-55.55336101|D13=-173.94268017|D14=-56.6393
9837|D15=-174.75937541|D16=67.02902906|D17=-52.78191074|D18=188.545699
69|D19=69.74630107|D20=58.15494682|D21=-88.37746045|D22=33.25649429|D2
3=154.83383239|D24=117.57345741|D25=-3.21972973|D26=-123.67689963|D27=
-148.29044247|B22=2.08283943|B29=2.919808||Version=x86-Win32-G03RevB.0
5|State=1-A|HF=-382.9309414|RMSD=5.231e-009|RMSF=5.797e-005|Dipole=0.3
66989,-4.7505932,1.430699|PG=C01 [X(C8H20I1N1)]||@

B3LYP/SVP transition structure:

	1	2	3
	A	A	A
Frequencies --	-373.6424	39.7830	55.7270
Red. masses --	7.9292	2.9074	2.1835

```
 Frc consts  --     0.6522                 0.0027                 0.0040
 IR Inten    --   967.2118                 1.3771                 0.6010

 Sum of electronic and zero-point Energies=          -7290.931573
 Sum of electronic and thermal Energies=             -7290.917126
 Sum of electronic and thermal Enthalpies=           -7290.916182
 Sum of electronic and thermal Free Energies=        -7290.974441


1|1|UNPC-UNK|FTS|RB3LYP|SVP|C8H20I1N1|PCUSER|31-May-2005|1||# B3LYP/SV
 P OPT=(TS,NOEIGEN,Z-MATRIX)||ET3N + EtI Menshutkin||0,1|N|C,1,B1|C,1,B
 2,2,A1|C,1,B3,3,A2,2,D1,0|H,2,B4,1,A3,4,D2,0|C,2,B5,1,A4,4,D3,0|H,2,B6
 ,1,A5,4,D4,0|H,3,B7,1,A6,4,D5,0|C,3,B8,1,A7,4,D6,0|H,3,B9,1,A8,4,D7,0|
 H,4,B10,1,A9,3,D8,0|C,4,B11,1,A10,3,D9,0|H,4,B12,1,A11,3,D10,0|H,6,B13
 ,2,A12,1,D11,0|H,6,B14,2,A13,1,D12,0|H,6,B15,2,A14,1,D13,0|H,9,B16,3,A
 15,1,D14,0|H,9,B17,3,A16,1,D15,0|H,9,B18,3,A17,1,D16,0|H,12,B19,4,A18,
 1,D17,0|H,12,B20,4,A19,1,D18,0|H,12,B21,4,A20,1,D19,0|C,1,B22,4,A21,12
 ,D20,0|H,23,B23,1,A22,4,D21,0|C,23,B24,1,A23,4,D22,0|H,23,B25,1,A24,4,
 D23,0|H,25,B26,23,A25,1,D24,0|H,25,B27,23,A26,1,D25,0|H,25,B28,23,A27,
 1,D26,0|I,23,B29,1,A28,4,D27,0||B1=1.48873796|B2=1.49519384|B3=1.48550
 145|B4=1.09749721|B5=1.52497875|B6=1.10784306|B7=1.09755689|B8=1.52784
 874|B9=1.10739148|B10=1.09732302|B11=1.52618091|B12=1.10835764|B13=1.0
 9986919|B14=1.09859581|B15=1.10084642|B16=1.10077365|B17=1.10106398|B1
 8=1.09994963|B19=1.09943145|B20=1.10084384|B21=1.09921099|B23=1.084347
 08|B24=1.50754478|B25=1.08415373|B26=1.09804783|B27=1.10218749|B28=1.0
 9802672|A1=109.85870825|A2=110.10395069|A3=106.88255253|A4=116.9154815
 8|A5=107.7497653|A6=106.85320929|A7=117.26148959|A8=107.34246306|A9=10
 7.30666612|A10=116.23134838|A11=107.99043639|A12=113.40040142|A13=112.
 11688471|A14=108.13094344|A15=113.02906348|A16=107.62492396|A17=113.19
 762516|A18=112.2454146|A19=108.43581875|A20=113.08134622|A21=113.27074
 006|A22=92.84467715|A23=109.45183141|A24=92.20371517|A25=110.65738494|
 A26=112.55746521|A27=110.36751243|A28=153.3713145|D1=-122.27723243|D2=
 175.70730996|D3=-62.59888986|D4=61.50730414|D5=54.64847564|D6=-183.502
 93468|D7=-59.52846119|D8=177.11397059|D9=-60.70849033|D10=62.95043643|
 D11=63.0519745|D12=-60.32063973|D13=-178.51946764|D14=-60.06431521|D15
 =-178.25008721|D16=64.07329068|D17=-54.72882634|D18=186.7145944|D19=68
 .2493053|D20=54.75243215|D21=-84.91985258|D22=37.1989416|D23=159.47899
 542|D24=118.54760396|D25=-2.13223126|D26=-122.71830589|D27=-143.868901
 27|B22=2.00611522|B29=2.92865915||Version=x86-Win32-G03RevB.05|State=1
 -A|HF=-7291.2042473|RMSD=9.365e-009|RMSF=1.938e-005|Dipole=0.2481397,-
 4.5347038,1.5317102|PG=C01 [X(C8H20I1N1)]||@
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B3LYP/MIDI! transition structure:

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                     1                      2                      3
                     A                      A                      A
 Frequencies --  -361.8232               40.7863               63.6437
 Red. masses --     8.0159                2.9091                2.4160
 Frc consts  --     0.6183                0.0029                0.0058
 IR Inten    --  1005.9903                1.3362                1.2376

 Sum of electronic and zero-point Energies=          -7259.304214
 Sum of electronic and thermal Energies=             -7259.289935
 Sum of electronic and thermal Enthalpies=           -7259.288991
 Sum of electronic and thermal Free Energies=        -7259.346793
```

1|1|UNPC-UNK|FTS|RB3LYP|MIDIx|C8H20I1N1|PCUSER|31-May-2005|1||# B3LYP/
MIDIX OPT=(TS,NOEIGEN,Z-MATRIX)||ET3N + EtI Menshutkin||0,1|N|C,1,B1|C
,1,B2,2,A1|C,1,B3,3,A2,2,D1,0|H,2,B4,1,A3,4,D2,0|C,2,B5,1,A4,4,D3,0|H,
2,B6,1,A5,4,D4,0|H,3,B7,1,A6,4,D5,0|C,3,B8,1,A7,4,D6,0|H,3,B9,1,A8,4,D
7,0|H,4,B10,1,A9,3,D8,0|C,4,B11,1,A10,3,D9,0|H,4,B12,1,A11,3,D10,0|H,6
,B13,2,A12,1,D11,0|H,6,B14,2,A13,1,D12,0|H,6,B15,2,A14,1,D13,0|H,9,B16
,3,A15,1,D14,0|H,9,B17,3,A16,1,D15,0|H,9,B18,3,A17,1,D16,0|H,12,B19,4,
A18,1,D17,0|H,12,B20,4,A19,1,D18,0|H,12,B21,4,A20,1,D19,0|C,1,B22,4,A2
1,12,D20,0|H,23,B23,1,A22,4,D21,0|C,23,B24,1,A23,4,D22,0|H,23,B25,1,A2
4,4,D23,0|H,25,B26,23,A25,1,D24,0|H,25,B27,23,A26,1,D25,0|H,25,B28,23,
A27,1,D26,0|I,23,B29,1,A28,4,D27,0||B1=1.5017002|B2=1.50821726|B3=1.49
891088|B4=1.09451536|B5=1.53871153|B6=1.10465843|B7=1.09478821|B8=1.54
271401|B9=1.10440058|B10=1.0938806|B11=1.54022565|B12=1.10538061|B13=1
.09703077|B14=1.09610422|B15=1.0991168|B16=1.09836645|B17=1.09950051|B
18=1.09708658|B19=1.09689199|B20=1.09910217|B21=1.09647926|B23=1.07973
648|B24=1.51897173|B25=1.07991521|B26=1.09591086|B27=1.10016891|B28=1.
09584305|A1=109.29655323|A2=109.46253385|A3=106.58663228|A4=115.474849
59|A5=108.15270071|A6=106.56023425|A7=116.22240537|A8=107.68065652|A9=
107.06196664|A10=114.90927346|A11=108.26713768|A12=112.90481778|A13=11
1.28841045|A14=108.19457935|A15=112.49084226|A16=107.55314764|A17=112.
78612264|A18=111.42704263|A19=108.46129498|A20=112.61640974|A21=114.55
866982|A22=92.46121719|A23=108.89895045|A24=91.78247696|A25=110.387627
69|A26=112.381503|A27=110.22292111|A28=154.28200345|D1=-120.79599037|D
2=175.48472761|D3=-63.90248628|D4=59.99299115|D5=56.13483441|D6=-182.9
4665871|D7=-59.2376197|D8=176.57126153|D9=-62.20585243|D10=61.07864024
|D11=65.1489345|D12=-57.72684147|D13=-176.10671903|D14=-58.87302071|D1
5=-177.05082579|D16=64.99164694|D17=-52.20045218|D18=189.18494705|D19=
70.45347605|D20=53.75849811|D21=-85.69671761|D22=36.00184155|D23=157.8
1508091|D24=119.71571667|D25=-1.09248111|D26=-121.95317766|D27=-145.00
041856|B22=1.9958077|B29=2.89202073||Version=x86-Win32-G03RevB.05|Stat
e=1-A|HF=-7259.5799437|RMSD=3.635e-009|RMSF=3.130e-005|Dipole=0.354001
9,-4.6073681,1.5550361|PG=C01 [X(C8H20I1N1)]||@

B3LYP/6-311G(d,p) transition structure:

	1	2	3
	A	A	A
Frequencies --	-365.6897	41.1876	62.7579
Red. masses --	8.0357	3.5203	3.2866
Frc consts --	0.6331	0.0035	0.0076
IR Inten --	999.4154	1.1262	4.3120

Sum of electronic and zero-point Energies=	-7290.966553
Sum of electronic and thermal Energies=	-7290.952088
Sum of electronic and thermal Enthalpies=	-7290.951144
Sum of electronic and thermal Free Energies=	-7291.009339

1|1|UNPC-UNK|FTS|RB3LYP|Gen|C8H20I1N1|PCUSER|18-Aug-2005|1||# B3LYP/6-
311G** EXTRABASIS OPT=(CALCFC,TS,NOEIGEN,Z-MATRIX)||ET3N + EtI Menshut
kin + 6-311G** for I||0,1|N|C,1,B1|C,1,B2,2,A1|C,1,B3,3,A2,2,D1,0|H,2,
B4,1,A3,4,D2,0|C,2,B5,1,A4,4,D3,0|H,2,B6,1,A5,4,D4,0|H,3,B7,1,A6,4,D5,
0|C,3,B8,1,A7,4,D6,0|H,3,B9,1,A8,4,D7,0|H,4,B10,1,A9,3,D8,0|C,4,B11,1,
A10,3,D9,0|H,4,B12,1,A11,3,D10,0|H,6,B13,2,A12,1,D11,0|H,6,B14,2,A13,1
,D12,0|H,6,B15,2,A14,1,D13,0|H,9,B16,3,A15,1,D14,0|H,9,B17,3,A16,1,D15
,0|H,9,B18,3,A17,1,D16,0|H,12,B19,4,A18,1,D17,0|H,12,B20,4,A19,1,D18,0

|H,12,B21,4,A20,1,D19,0|C,1,B22,4,A21,12,D20,0|H,23,B23,1,A22,4,D21,0|
C,23,B24,1,A23,4,D22,0|H,23,B25,1,A24,4,D23,0|H,25,B26,23,A25,1,D24,0|
H,25,B27,23,A26,1,D25,0|H,25,B28,23,A27,1,D26,0|I,23,B29,1,A28,4,D27,0
||B1=1.49213776|B2=1.49810212|B3=1.48885538|B4=1.0890969|B5=1.52647002
|B6=1.09956024|B7=1.0892976|B8=1.52851715|B9=1.09922071|B10=1.08878159
|B11=1.52751634|B12=1.10010483|B13=1.09115509|B14=1.09031216|B15=1.092
5981|B16=1.09144573|B17=1.09282722|B18=1.09105064|B19=1.09110881|B20=1
.09255746|B21=1.09050925|B23=1.07470364|B24=1.50596231|B25=1.07454491|
B26=1.08931153|B27=1.09371821|B28=1.08928098|A1=109.83732686|A2=109.80
443126|A3=106.88893229|A4=116.27870241|A5=107.91380075|A6=106.80279825
|A7=116.68843958|A8=107.55727978|A9=107.38935375|A10=115.66800911|A11=
108.02177033|A12=113.24467088|A13=111.93093638|A14=108.08264195|A15=11
2.76153773|A16=107.66039745|A17=113.03785043|A18=112.01982305|A19=108.
43900883|A20=112.874561|A21=113.64886693|A22=91.88245802|A23=108.79450
497|A24=91.30217865|A25=110.58009741|A26=112.20448298|A27=110.41497173
|A28=154.10193046|D1=-121.84422077|D2=177.79253295|D3=-60.9317438|D4=6
3.00383022|D5=58.34412206|D6=-180.11053454|D7=-56.35211085|D8=178.8175
242|D9=-59.26072255|D10=64.16556444|D11=64.99137429|D12=-58.33054126|D
13=-176.51905006|D14=-57.42325559|D15=-175.4590639|D16=66.65676421|D17
=-53.05808568|D18=188.35799096|D19=69.76972114|D20=56.57476393|D21=-86
.97783659|D22=34.96921625|D23=156.9306463|D24=119.13477804|D25=-1.3683
4476|D26=-121.80799074|D27=-146.05413099|B22=2.03846975|B29=2.92510329
||Version=x86-Win32-G03RevB.05|State=1-A|HF=-7291.2397287|RMSD=2.175e-
009|RMSF=2.134e-005|Dipole=0.3350088,-4.7199304,1.5303196|PG=C01 [X(C8
H20I1N1)]||@

MP2/LANL2DZ transition structure:

	1	2	3
	A	A	A
Frequencies --	-488.8166	47.3891	52.6367
Red. masses --	8.0680	3.5211	2.1292
Frc consts --	1.1358	0.0047	0.0035
IR Inten --	2005.5705	0.6256	0.9259

Sum of electronic and zero-point Energies=	-380.582365
Sum of electronic and thermal Energies=	-380.568317
Sum of electronic and thermal Enthalpies=	-380.567372
Sum of electronic and thermal Free Energies=	-380.624413

1|1|UNPC-UNK|FTS|RMP2-FC|LANL2DZ|C8H20I1N1|PCUSER|01-Jun-2005|1||# MP2
/LANL2DZ OPT=(TS,NOEIGEN,Z-MATRIX)||ET3N + EtI Menshutkin||0,1|N|C,1,B
1|C,1,B2,2,A1|C,1,B3,3,A2,2,D1,0|H,2,B4,1,A3,4,D2,0|C,2,B5,1,A4,4,D3,0
|H,2,B6,1,A5,4,D4,0|H,3,B7,1,A6,4,D5,0|C,3,B8,1,A7,4,D6,0|H,3,B9,1,A8,
4,D7,0|H,4,B10,1,A9,3,D8,0|C,4,B11,1,A10,3,D9,0|H,4,B12,1,A11,3,D10,0|
H,6,B13,2,A12,1,D11,0|H,6,B14,2,A13,1,D12,0|H,6,B15,2,A14,1,D13,0|H,9,
B16,3,A15,1,D14,0|H,9,B17,3,A16,1,D15,0|H,9,B18,3,A17,1,D16,0|H,12,B19
,4,A18,1,D17,0|H,12,B20,4,A19,1,D18,0|H,12,B21,4,A20,1,D19,0|C,1,B22,4
,A21,12,D20,0|H,23,B23,1,A22,4,D21,0|C,23,B24,1,A23,4,D22,0|H,23,B25,1
,A24,4,D23,0|H,25,B26,23,A25,1,D24,0|H,25,B27,23,A26,1,D25,0|H,25,B28,
23,A27,1,D26,0|I,23,B29,1,A28,4,D27,0||B1=1.52624762|B2=1.53291188|B3=
1.52374463|B4=1.10082677|B5=1.55445372|B6=1.11254105|B7=1.10131007|B8=
1.5563176|B9=1.11234512|B10=1.09890727|B11=1.55567892|B12=1.11316297|B
13=1.10239953|B14=1.10128298|B15=1.10515918|B16=1.10184342|B17=1.10537
518|B18=1.1021664|B19=1.10215315|B20=1.10511773|B21=1.1019805|B23=1.08

519514|B24=1.54083738|B25=1.08531149|B26=1.10093846|B27=1.10302693|B28
=1.10089194|A1=109.9984028|A2=108.99896444|A3=106.76525766|A4=114.8958
4178|A5=108.2135148|A6=106.62347103|A7=115.49364096|A8=107.82676342|A9
=107.62399015|A10=113.91887873|A11=108.06174966|A12=112.88876253|A13=1
11.3093729|A14=108.03316905|A15=112.12561032|A16=107.72913311|A17=112.
63144523|A18=111.26713423|A19=108.59576712|A20=112.39275167|A21=115.29
882864|A22=88.86208891|A23=105.06506541|A24=88.06275381|A25=110.149608
12|A26=112.15966489|A27=110.15815414|A28=158.87322522|D1=-121.50485589
|D2=178.91564364|D3=-60.92361539|D4=62.51837739|D5=63.06876234|D6=-176
.29990643|D7=-53.20763691|D8=178.2429138|D9=-60.50833565|D10=61.993181
89|D11=65.75094835|D12=-57.28035435|D13=-175.49506119|D14=-55.26043843
|D15=-173.31669599|D16=68.47696923|D17=-50.39791214|D18=190.93640055|D
19=72.02765002|D20=55.30881596|D21=-87.93553424|D22=32.94658392|D23=15
3.59291489|D24=120.0092518|D25=-0.71412604|D26=-121.66551226|D27=-148.
31638353|B22=2.07457348|B29=2.78634286||Version=x86-Win32-G03RevB.05|S
tate=1-A|HF=-380.0027025|MP2=-380.859439|RMSD=1.896e-009|RMSF=1.531e-0
05|Dipole=0.6523323,-4.4328332,1.3770578|PG=C01 [X(C8H20I1N1)]||@

MP2/LANL2DZd transition structure:

	1	2	3
	A	A	A
Frequencies --	-488.6499	46.9138	52.6899
Red. masses --	8.1106	3.5349	2.1300
Frc consts --	1.1410	0.0046	0.0035
IR Inten --	1931.1510	0.7587	0.7911

Sum of electronic and zero-point Energies=	-380.675682
Sum of electronic and thermal Energies=	-380.661588
Sum of electronic and thermal Enthalpies=	-380.660644
Sum of electronic and thermal Free Energies=	-380.717788

1 1\1\ ASN_ALTIX-ALTIX7\Freq\RMP2-FC\Gen\C8H20I1N1\AUBOXA\04-Oct-2007\1\
\# MP2/LANL2DZ ExtraBasis freq\\ET3N + EtI Menshutkin extra d orbital
on I\\0,1\N\C,1,B1\C,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,2,B4,1,A3,4,D2,0\C
,2,B5,1,A4,4,D3,0\H,2,B6,1,A5,4,D4,0\H,3,B7,1,A6,4,D5,0\C,3,B8,1,A7,4,
D6,0\H,3,B9,1,A8,4,D7,0\H,4,B10,1,A9,3,D8,0\C,4,B11,1,A10,3,D9,0\H,4,B
12,1,A11,3,D10,0\H,6,B13,2,A12,1,D11,0\H,6,B14,2,A13,1,D12,0\H,6,B15,2
,A14,1,D13,0\H,9,B16,3,A15,1,D14,0\H,9,B17,3,A16,1,D15,0\H,9,B18,3,A17
,1,D16,0\H,12,B19,4,A18,1,D17,0\H,12,B20,4,A19,1,D18,0\H,12,B21,4,A20,
1,D19,0\C,1,B22,4,A21,12,D20,0\H,23,B23,1,A22,4,D21,0\C,23,B24,1,A23,4
,D22,0\H,23,B25,1,A24,4,D23,0\H,25,B26,23,A25,1,D24,0\H,25,B27,23,A26,
1,D25,0\H,25,B28,23,A27,1,D26,0\I,23,B29,1,A28,4,D27,0\\B1=1.525\B2=1.
5316\B3=1.5224\B4=1.1009\B5=1.5546\B6=1.113\B7=1.1015\B8=1.5566\B9=1.1
129\B10=1.0993\B11=1.5559\B12=1.1137\B13=1.1024\B14=1.1016\B15=1.1051\
B16=1.1021\B17=1.1054\B18=1.1022\B19=1.1024\B20=1.1051\B21=1.102\B23=1
.0855\B24=1.5404\B25=1.0856\B26=1.1013\B27=1.103\B28=1.1013\A1=110.077
4\A2=109.1306\A3=106.8173\A4=114.7532\A5=108.3922\A6=106.6852\A7=115.4
462\A8=107.9897\A9=107.6001\A10=113.8864\A11=108.2579\A12=112.8697\A13
=111.264\A14=108.1145\A15=112.1498\A16=107.7637\A17=112.6318\A18=111.2
314\A19=108.6465\A20=112.3986\A21=115.4072\A22=87.4772\A23=104.6416\A2
4=86.685\A25=110.0875\A26=111.9979\A27=110.0633\A28=158.3365\D1=-121.6
153\D2=179.0532\D3=-60.8648\D4=62.5916\D5=62.9408\D6=-176.476\D7=-53.3
696\D8=178.7952\D9=-60.0609\D10=62.5038\D11=66.1587\D12=-56.8094\D13=-
175.0351\D14=-55.2308\D15=-173.2915\D16=68.4755\D17=-50.2009\D18=191.1

212\D19=72.1741\D20=55.6594\D21=-88.3133\D22=32.3237\D23=152.7732\D24=
120.0212\D25=-0.6543\D26=-121.5123\D27=-148.9837\B22=2.1132\B29=2.7308
\\Version=IA64L-G03RevD.01\State=1-A\HF=-380.0071288\MP2=-380.9525212\
RMSD=3.447e-09\RMSF=2.069e-05\ZeroPoint=0.2768394\Thermal=0.2909328\Di
pole=0.5677471,-4.351022,1.3198759\

Gaussian 03 Reference

Gaussian 03, Revision B.03,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
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