

# Supporting Information

## Asymmetric Imine *N*-Inversion in 3-Methyl-4-Pyrimidinimine. Molecular Dipole Analysis of Solvation Effects

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ITS-Structure of 3-Methyl-4-Pyrimidinimine ..... S34

SOSP-Structure of 3-Methyl-4-Pyrimidinimine ..... S44

**Table S1.** Results Computed at the MP2(full)/6-31G\* Level for the Gas-Phase Reaction and at the PCM(MP2(full)/6-31G\*) Level for the Reaction in Solution

| <b>Medium</b>          |          | $E_{tot}^a$ | $VZPE^b$ | $TE^b$ | $S^c$ | $NI$ | $\nu_1$ | $\nu_2$ |
|------------------------|----------|-------------|----------|--------|-------|------|---------|---------|
| Gas Phase              | <i>E</i> | -357.892662 | 77.81    | 82.06  | 81.18 | 0    | 123.3   | 179.8   |
|                        | <i>Z</i> | -357.886350 | 77.67    | 81.93  | 81.22 | 0    | 111.1   | 196.8   |
|                        | ITS      | -357.849175 | 75.93    | 80.28  | 81.80 | 1    | -1081.3 | 129.0   |
|                        | SOSP     | -357.847280 | 75.41    | 79.65  | 81.33 | 2    | -1120.6 | -390.5  |
| Heptane                | <i>E</i> | -357.897388 | 77.75    | 81.99  | 81.00 | 0    | 131.6   | 181.5   |
|                        | <i>Z</i> | -357.891841 | 77.70    | 81.93  | 80.97 | 0    | 119.6   | 201.4   |
|                        | ITS      | -357.853925 | 75.79    | 80.13  | 81.65 | 1    | -1088.3 | 135.4   |
|                        | SOSP     | -357.851924 | 75.24    | 79.47  | 81.22 | 2    | -1122.4 | -380.0  |
| Benzene                | <i>E</i> | -357.898435 | 77.71    | 81.94  | 80.98 | 0    | 132.1   | 182.1   |
|                        | <i>Z</i> | -357.893017 | 77.67    | 81.90  | 80.97 | 0    | 119.4   | 202.0   |
|                        | ITS      | -357.854966 | 75.73    | 80.06  | 81.65 | 1    | -1090.0 | 136.0   |
|                        | SOSP     | -357.852932 | 75.18    | 79.41  | 81.23 | 2    | -1123.2 | -380.7  |
| Diethyl<br>Ether       | <i>E</i> | -357.901961 | 77.56    | 81.79  | 80.95 | 0    | 134.0   | 183.0   |
|                        | <i>Z</i> | -357.896864 | 77.57    | 81.80  | 80.93 | 0    | 120.6   | 203.4   |
|                        | ITS      | -357.858440 | 75.51    | 79.85  | 81.64 | 1    | -1096.6 | 138.0   |
|                        | SOSP     | -357.856313 | 74.95    | 79.18  | 81.24 | 2    | -1126.2 | -378.1  |
| Chloro-<br>form        | <i>E</i> | -357.902513 | 77.53    | 81.76  | 80.94 | 0    | 133.6   | 183.5   |
|                        | <i>Z</i> | -357.897462 | 77.55    | 81.78  | 80.92 | 0    | 120.7   | 203.7   |
|                        | ITS      | -357.858983 | 75.48    | 79.82  | 81.64 | 1    | -1097.6 | 138.3   |
|                        | SOSP     | -357.856836 | 74.91    | 79.15  | 81.35 | 2    | -1127.0 | -380.4  |
| Aniline                | <i>E</i> | -357.903723 | 77.47    | 81.71  | 80.94 | 0    | 134.3   | 183.5   |
|                        | <i>Z</i> | -357.898731 | 77.52    | 81.74  | 80.92 | 0    | 121.0   | 204.3   |
|                        | ITS      | -357.860164 | 75.40    | 79.74  | 81.63 | 1    | -1099.4 | 139.1   |
|                        | SOSP     | -357.857986 | 74.83    | 79.06  | 81.25 | 2    | -1127.6 | -377.1  |
| THF                    | <i>E</i> | -357.904050 | 77.46    | 81.69  | 80.93 | 0    | 134.3   | 183.8   |
|                        | <i>Z</i> | -357.899076 | 77.50    | 81.73  | 80.91 | 0    | 121.0   | 204.2   |
|                        | ITS      | -357.860483 | 75.38    | 79.72  | 81.64 | 1    | -1100.1 | 139.1   |
|                        | SOSP     | -357.858290 | 74.80    | 79.04  | 81.26 | 2    | -1127.7 | -379.0  |
| Methylene-<br>chloride | <i>E</i> | -357.904549 | 77.43    | 81.67  | 80.93 | 0    | 133.9   | 184.0   |
|                        | <i>Z</i> | -357.899609 | 77.48    | 81.71  | 80.92 | 1    | 120.8   | 204.2   |
|                        | ITS      | -357.860959 | 75.35    | 79.69  | 81.63 | 2    | -1101.0 | 139.6   |
|                        | SOSP     | -357.858747 | 74.77    | 79.01  | 81.26 | 2    | -1128.1 | -378.8  |

|                     |          |             |       |       |       |   |         |        |
|---------------------|----------|-------------|-------|-------|-------|---|---------|--------|
| Dichloro-<br>Ethane | <i>E</i> | -357.904882 | 77.42 | 81.65 | 80.92 | 0 | 134.3   | 184.2  |
|                     | <i>Z</i> | -357.899947 | 77.47 | 81.70 | 80.91 | 0 | 121.1   | 204.3  |
|                     | ITS      | -357.861295 | 75.32 | 79.67 | 81.64 | 1 | -1101.5 | 139.6  |
|                     | SOSP     | -357.859074 | 74.74 | 78.98 | 81.27 | 2 | -1128.3 | -378.6 |
| Acetone             | <i>E</i> | -357.906123 | 77.36 | 81.59 | 80.93 | 0 | 133.8   | 184.6  |
|                     | <i>Z</i> | -357.901225 | 77.43 | 81.65 | 80.91 | 0 | 121.1   | 204.8  |
|                     | ITS      | -357.862490 | 75.24 | 79.58 | 81.63 | 1 | -1103.4 | 140.4  |
|                     | SOSP     | -357.860224 | 74.66 | 78.90 | 81.27 | 2 | -1129.5 | -378.5 |
| Ethanol             | <i>E</i> | -357.906368 | 77.34 | 81.57 | 80.92 | 0 | 134.7   | 184.4  |
|                     | <i>Z</i> | -357.901483 | 77.41 | 81.64 | 80.93 | 0 | 120.6   | 204.3  |
|                     | ITS      | -357.862708 | 75.23 | 79.57 | 81.61 | 1 | -1103.9 | 141.3  |
|                     | SOSP     | -357.860448 | 74.64 | 78.88 | 81.28 | 2 | -1129.9 | -378.4 |
| Methanol            | <i>E</i> | -357.906699 | 77.33 | 81.56 | 80.92 | 0 | 134.4   | 184.7  |
|                     | <i>Z</i> | -357.901837 | 77.40 | 81.62 | 80.91 | 0 | 121.1   | 204.7  |
|                     | ITS      | -357.863009 | 75.21 | 79.55 | 81.61 | 1 | -1104.4 | 141.2  |
|                     | SOSP     | -357.860743 | 74.61 | 78.85 | 81.27 | 2 | -1130.3 | -377.9 |
| Acetonitrile        | <i>E</i> | -357.906739 | 77.33 | 81.56 | 80.92 | 0 | 134.7   | 184.5  |
|                     | <i>Z</i> | -357.901862 | 77.40 | 81.63 | 80.93 | 0 | 120.6   | 204.4  |
|                     | ITS      | -357.863067 | 75.20 | 79.55 | 81.62 | 1 | -1104.5 | 141.0  |
|                     | SOSP     | -357.860790 | 74.61 | 78.85 | 81.28 | 2 | -1130.1 | -378.9 |
| DMSO                | <i>E</i> | -357.906828 | 77.32 | 81.55 | 80.92 | 0 | 134.1   | 184.6  |
|                     | <i>Z</i> | -357.901949 | 77.40 | 81.63 | 80.90 | 0 | 121.3   | 205.0  |
|                     | ITS      | -357.863186 | 75.19 | 79.54 | 81.63 | 1 | -1104.4 | 140.7  |
|                     | SOSP     | -357.860910 | 74.60 | 78.84 | 81.28 | 2 | -1132.1 | -382.5 |
| Water               | <i>E</i> | -357.907307 | 77.30 | 81.53 | 80.90 | 0 | 134.5   | 185.5  |
|                     | <i>Z</i> | -357.902505 | 77.37 | 81.59 | 80.89 | 0 | 121.8   | 204.9  |
|                     | ITS      | -357.863563 | 75.18 | 79.52 | 81.61 | 1 | -1105.3 | 141.3  |
|                     | SOSP     | -357.861268 | 74.58 | 78.82 | 81.28 | 2 | -1134.6 | -384.3 |

(a) Total energies in hartree.

(b) Thermochemical data *VZPE* and *TE* in kcal/mol.

(c) Entropies *S* in cal / (K mol).

**Table S2.** Results Computed at the SMD(MP2(full)/6-31G\*) Level for the Reaction in Solution

| Solvent           |          | $E_{tot}^a$ | VZPE <sup>b</sup> | TE <sup>b</sup> | S <sup>c</sup> | NI | $\nu_1$ | $\nu_2$ |
|-------------------|----------|-------------|-------------------|-----------------|----------------|----|---------|---------|
| Heptane           | <i>E</i> | -357.904695 | 78.00             | 82.24           | 81.14          | 0  | 115.9   | 184.8   |
|                   | <i>Z</i> | -357.899582 | 78.06             | 82.23           | 80.43          | 0  | 133.7   | 207.5   |
|                   | ITS      | -357.861208 | 76.13             | 80.41           | 81.26          | 1  | -1091.3 | 148.3   |
|                   | SOSP     | -357.858986 | 75.75             | 79.89           | 80.49          | 2  | -1138.7 | -394.5  |
| Benzene           | <i>E</i> | -357.906323 | 78.03             | 82.26           | 81.07          | 0  | 116.2   | 186.5   |
|                   | <i>Z</i> | -357.901486 | 78.09             | 82.25           | 80.35          | 0  | 135.1   | 208.9   |
|                   | ITS      | -357.862790 | 76.14             | 80.41           | 81.16          | 1  | -1093.8 | 151.6   |
|                   | SOSP     | -357.860474 | 75.76             | 79.90           | 80.44          | 2  | -1142.3 | -397.8  |
| Diethyl Ether     | <i>E</i> | -357.908940 | 78.08             | 82.29           | 80.82          | 0  | 122.1   | 192.6   |
|                   | <i>Z</i> | -357.904922 | 78.13             | 82.28           | 80.25          | 0  | 132.3   | 211.4   |
|                   | ITS      | -357.865190 | 76.14             | 80.39           | 80.94          | 1  | -1099.0 | 153.1   |
|                   | SOSP     | -357.862526 | 75.70             | 79.83           | 80.44          | 2  | -1150.3 | -406.0  |
| Chloroform        | <i>E</i> | -357.909341 | 78.12             | 82.32           | 80.73          | 0  | 124.6   | 195.8   |
|                   | <i>Z</i> | -357.905448 | 78.16             | 82.30           | 80.23          | 0  | 135.1   | 212.5   |
|                   | ITS      | -357.865537 | 76.15             | 80.39           | 80.95          | 1  | -1100.1 | 150.9   |
|                   | SOSP     | -357.862816 | 75.67             | 79.82           | 80.55          | 2  | -1151.3 | -406.3  |
| Aniline           | <i>E</i> | -357.907413 | 78.20             | 82.38           | 80.58          | 0  | 127.8   | 200.2   |
|                   | <i>Z</i> | -357.903835 | 78.20             | 82.34           | 80.23          | 0  | 131.9   | 213.2   |
|                   | ITS      | -357.863483 | 76.17             | 80.41           | 80.91          | 1  | -1102.6 | 148.2   |
|                   | SOSP     | -357.860604 | 75.65             | 79.81           | 80.60          | 2  | -1155.4 | -406.9  |
| THF               | <i>E</i> | -357.909944 | 78.11             | 82.31           | 80.73          | 0  | 123.1   | 195.2   |
|                   | <i>Z</i> | -357.906375 | 78.14             | 82.29           | 80.25          | 0  | 133.7   | 211.9   |
|                   | ITS      | -357.866098 | 76.16             | 80.39           | 80.80          | 1  | -1101.4 | 155.2   |
|                   | SOSP     | -357.863185 | 75.68             | 79.81           | 80.41          | 2  | -1155.7 | -409.0  |
| Methylenechloride | <i>E</i> | -357.911675 | 78.12             | 82.31           | 80.69          | 0  | 124.6   | 197.3   |
|                   | <i>Z</i> | -357.908229 | 78.15             | 82.29           | 80.24          | 0  | 133.8   | 212.9   |
|                   | ITS      | -357.867805 | 76.15             | 80.38           | 80.82          | 1  | -1102.0 | 154.6   |
|                   | SOSP     | -357.864813 | 75.65             | 79.79           | 80.49          | 2  | -1155.9 | -410.5  |
| Dichloroethane    | <i>E</i> | -357.911004 | 78.13             | 82.32           | 80.68          | 0  | 124.9   | 197.6   |
|                   | <i>Z</i> | -357.907621 | 78.15             | 82.29           | 80.25          | 0  | 132.8   | 212.9   |
|                   | ITS      | -357.867112 | 76.16             | 80.39           | 80.80          | 1  | -1102.4 | 154.6   |
|                   | SOSP     | -357.864080 | 75.65             | 79.79           | 80.48          | 2  | -1157.0 | -410.1  |
| Acetone           | <i>E</i> | -357.912011 | 78.12             | 82.31           | 80.65          | 0  | 125.2   | 198.6   |

|              |          |             |       |       |       |   |         |        |
|--------------|----------|-------------|-------|-------|-------|---|---------|--------|
|              | <i>Z</i> | -357.908865 | 78.13 | 82.28 | 80.31 | 0 | 130.2   | 212.7  |
|              | ITS      | -357.868087 | 76.15 | 80.37 | 80.79 | 1 | -1102.7 | 154.8  |
|              | SOSP     | -357.864875 | 75.62 | 79.76 | 80.46 | 2 | -1158.5 | -412.9 |
| Ethanol      | <i>E</i> | -357.909374 | 78.22 | 82.38 | 80.44 | 0 | 132.3   | 206.1  |
|              | <i>Z</i> | -357.906341 | 78.18 | 82.32 | 80.32 | 0 | 126.4   | 214.5  |
|              | ITS      | -357.865308 | 76.11 | 80.37 | 81.01 | 1 | -1104.5 | 143.4  |
|              | SOSP     | -357.862037 | 75.52 | 79.71 | 80.84 | 2 | -1158.0 | -412.5 |
| Methanol     | <i>E</i> | -357.908888 | 78.23 | 82.39 | 80.40 | 0 | 133.7   | 207.6  |
|              | <i>Z</i> | -357.905918 | 78.18 | 82.33 | 80.34 | 0 | 125.0   | 214.7  |
|              | ITS      | -357.864788 | 76.10 | 80.36 | 81.05 | 1 | -1104.4 | 141.0  |
|              | SOSP     | -357.861466 | 75.49 | 79.69 | 80.95 | 2 | -1158.3 | -412.6 |
| Acetonitrile | <i>E</i> | -357.911984 | 78.12 | 82.31 | 80.64 | 0 | 126.0   | 199.2  |
|              | <i>Z</i> | -357.908951 | 78.12 | 82.27 | 80.34 | 0 | 129.0   | 212.5  |
|              | ITS      | -357.868033 | 76.14 | 80.37 | 80.80 | 1 | -1103.1 | 154.3  |
|              | SOSP     | -357.864729 | 75.60 | 79.74 | 80.49 | 2 | -1159.6 | -412.9 |
| DMSO         | <i>E</i> | -357.909856 | 78.15 | 82.33 | 80.62 | 0 | 125.2   | 198.8  |
|              | <i>Z</i> | -357.906839 | 78.13 | 82.28 | 80.37 | 0 | 127.3   | 211.5  |
|              | ITS      | -357.865891 | 76.16 | 80.39 | 80.75 | 1 | -1103.5 | 154.7  |
|              | SOSP     | -357.862579 | 75.63 | 79.76 | 80.40 | 2 | -1161.0 | -411.6 |
| Solvent 60   | <i>E</i> | -357.908944 | 78.32 | 82.46 | 80.23 | 0 | 139.6   | 17.2   |
|              | <i>Z</i> | -357.906119 | 78.22 | 82.37 | 80.38 | 0 | 120.4   | 216.6  |
|              | ITS      | -357.864741 | 76.11 | 80.38 | 81.09 | 1 | -1104.1 | 131.9  |
|              | SOSP     | -357.861304 | 75.35 | 79.61 | 81.70 | 2 | -1156.8 | -414.8 |
| Solvent 70   | <i>E</i> | -357.909014 | 78.32 | 82.46 | 80.23 | 0 | 139.6   | 215.6  |
|              | <i>Z</i> | -357.906201 | 78.22 | 82.37 | 80.38 | 0 | 120.4   | 216.7  |
|              | ITS      | -357.864811 | 76.11 | 80.38 | 81.09 | 1 | -1104.0 | 132.0  |
|              | SOSP     | -357.861362 | 75.35 | 79.61 | 81.70 | 2 | -1156.9 | -414.9 |
| Water        | <i>E</i> | -357.909058 | 78.32 | 82.46 | 80.23 | 0 | 139.6   | 215.7  |
|              | <i>Z</i> | -357.906253 | 78.22 | 82.37 | 80.38 | 0 | 120.2   | 216.6  |
|              | ITS      | -357.864856 | 76.11 | 80.38 | 81.08 | 1 | -1103.9 | 132.1  |
|              | SOSP     | -357.861399 | 75.34 | 79.61 | 81.70 | 2 | -1157.0 | -414.9 |

(a) Total energies in hartree.

(b) Thermochemical data *VZPE* and *TE* in kcal/mol.

(c) Entropies *S* in cal / (K mol).

**Table S3.** Relative Isomer Stabilities and Activation Energies Computed at the MP2(full)/6-31G\* Level for the Gas-Phase Reaction and at the PCM and SMD Levels for the Reaction in Solution

| Medium                | Param. <sup>a</sup> | PCM(MP2(full)/6-31G*)       |                                       |                                       |                                  |
|-----------------------|---------------------|-----------------------------|---------------------------------------|---------------------------------------|----------------------------------|
|                       |                     | $\Delta E_r$<br>(Z) vs. (E) | $\Delta E_A$<br>(E) $\rightarrow$ ITS | $\Delta E_A$<br>(Z) $\rightarrow$ ITS | $\Delta E_{def}$<br>SOSP vs. ITS |
| Gas Phase<br>1.0      | $\Delta E$          | 3.96                        | 27.29                                 | 23.33                                 | 1.19                             |
|                       | $\Delta H_0$        | 3.83                        | 25.41                                 | 21.58                                 | 0.67                             |
|                       | $\Delta H_{298}$    | 3.83                        | 25.51                                 | 21.68                                 | 0.56                             |
|                       | $\Delta G_{298}$    | 3.82                        | 25.33                                 | 21.51                                 | 0.70                             |
| Heptane<br>1.92       | $\Delta E$          | 3.48                        | 27.27                                 | 23.79                                 | 1.26                             |
|                       | $\Delta H_0$        | 3.43                        | 25.31                                 | 21.89                                 | 0.71                             |
|                       | $\Delta H_{298}$    | 3.42                        | 25.41                                 | 21.99                                 | 0.60                             |
|                       | $\Delta G_{298}$    | 3.43                        | 25.22                                 | 21.79                                 | 0.73                             |
| Benzene<br>2.25       | $\Delta E$          | 3.40                        | 27.28                                 | 23.88                                 | 1.28                             |
|                       | $\Delta H_0$        | 3.36                        | 25.30                                 | 21.93                                 | 0.73                             |
|                       | $\Delta H_{298}$    | 3.36                        | 25.40                                 | 22.04                                 | 0.62                             |
|                       | $\Delta G_{298}$    | 3.36                        | 25.20                                 | 21.84                                 | 0.75                             |
| Diethyl Ether<br>4.34 | $\Delta E$          | 3.20                        | 27.31                                 | 24.11                                 | 1.33                             |
|                       | $\Delta H_0$        | 3.21                        | 25.26                                 | 22.05                                 | 0.77                             |
|                       | $\Delta H_{298}$    | 3.21                        | 25.37                                 | 22.16                                 | 0.67                             |
|                       | $\Delta G_{298}$    | 3.21                        | 25.16                                 | 21.95                                 | 0.79                             |
| Chloroform<br>4.90    | $\Delta E$          | 3.17                        | 27.32                                 | 24.15                                 | 1.35                             |
|                       | $\Delta H_0$        | 3.19                        | 25.26                                 | 22.07                                 | 0.78                             |
|                       | $\Delta H_{298}$    | 3.19                        | 25.37                                 | 22.18                                 | 0.68                             |
|                       | $\Delta G_{298}$    | 3.19                        | 25.16                                 | 21.97                                 | 0.77                             |
| Aniline<br>6.89       | $\Delta E$          | 3.13                        | 27.33                                 | 24.20                                 | 1.37                             |
|                       | $\Delta H_0$        | 3.17                        | 25.26                                 | 22.08                                 | 0.80                             |
|                       | $\Delta H_{298}$    | 3.17                        | 25.37                                 | 22.20                                 | 0.69                             |
|                       | $\Delta G_{298}$    | 3.17                        | 25.16                                 | 21.98                                 | 0.81                             |
| THF<br>7.58           | $\Delta E$          | 3.12                        | 27.34                                 | 24.22                                 | 1.38                             |
|                       | $\Delta H_0$        | 3.16                        | 25.26                                 | 22.09                                 | 0.80                             |
|                       | $\Delta H_{298}$    | 3.16                        | 25.37                                 | 22.21                                 | 0.70                             |
|                       | $\Delta G_{298}$    | 3.17                        | 25.16                                 | 21.99                                 | 0.81                             |

|                |                  |      |       |       |      |
|----------------|------------------|------|-------|-------|------|
| Methylene      | $\Delta E$       | 3.10 | 27.35 | 24.25 | 1.39 |
| Chloride       | $\Delta H_0$     | 3.15 | 25.27 | 22.12 | 0.81 |
| 8.93           | $\Delta H_{298}$ | 3.14 | 25.38 | 22.23 | 0.71 |
|                | $\Delta G_{298}$ | 3.15 | 25.17 | 22.02 | 0.82 |
| Dichloroethane | $\Delta E$       | 3.10 | 27.35 | 24.25 | 1.39 |
| 10.36          | $\Delta H_0$     | 3.15 | 25.26 | 22.10 | 0.81 |
|                | $\Delta H_{298}$ | 3.15 | 25.37 | 22.22 | 0.71 |
|                | $\Delta G_{298}$ | 3.15 | 25.15 | 22.00 | 0.82 |
| Acetone        | $\Delta E$       | 3.07 | 27.40 | 24.31 | 1.42 |
| 20.70          | $\Delta H_0$     | 3.15 | 25.27 | 22.12 | 0.84 |
|                | $\Delta H_{298}$ | 3.14 | 25.38 | 22.24 | 0.73 |
|                | $\Delta G_{298}$ | 3.15 | 25.17 | 22.02 | 0.84 |
| Ethanol        | $\Delta E$       | 3.07 | 27.40 | 24.33 | 1.42 |
| 24.55          | $\Delta H_0$     | 3.13 | 25.28 | 22.15 | 0.82 |
|                | $\Delta H_{298}$ | 3.13 | 25.39 | 22.26 | 0.73 |
|                | $\Delta G_{298}$ | 3.13 | 25.19 | 22.06 | 0.82 |
| Methanol       | $\Delta E$       | 3.05 | 27.42 | 24.37 | 1.42 |
| 32.63          | $\Delta H_0$     | 3.12 | 25.30 | 22.18 | 0.82 |
|                | $\Delta H_{298}$ | 3.12 | 25.41 | 22.29 | 0.72 |
|                | $\Delta G_{298}$ | 3.12 | 25.20 | 22.09 | 0.82 |
| Acetonitrile   | $\Delta E$       | 3.06 | 27.40 | 24.34 | 1.43 |
| 36.64          | $\Delta H_0$     | 3.13 | 25.28 | 22.15 | 0.83 |
|                | $\Delta H_{298}$ | 3.13 | 25.39 | 22.26 | 0.73 |
|                | $\Delta G_{298}$ | 3.13 | 25.19 | 22.06 | 0.83 |
| DMSO           | $\Delta E$       | 3.06 | 27.38 | 24.32 | 1.43 |
| 46.70          | $\Delta H_0$     | 3.14 | 25.26 | 22.11 | 0.83 |
|                | $\Delta H_{298}$ | 3.14 | 25.37 | 22.23 | 0.73 |
|                | $\Delta G_{298}$ | 3.15 | 25.16 | 22.01 | 0.84 |
| Water          | $\Delta E$       | 3.01 | 27.45 | 24.44 | 1.44 |
| 78.39          | $\Delta H_0$     | 3.09 | 25.33 | 22.25 | 0.84 |
|                | $\Delta H_{298}$ | 3.08 | 25.44 | 22.36 | 0.74 |
|                | $\Delta G_{298}$ | 3.09 | 25.23 | 22.15 | 0.84 |

(a) All data in kcal/mol.

**Table S3, Continued.** [Editor: Attach the following table to the right of the table on the previous page without the first two columns.]

| Solvent       | Param. <sup>a</sup> | SMD(MP2(full)/6-31G*)       |                                       |                                       |   |
|---------------|---------------------|-----------------------------|---------------------------------------|---------------------------------------|---|
|               |                     | $\Delta E_r$<br>(Z) vs. (E) | $\Delta E_A$<br>(E) $\rightarrow$ ITS | $\Delta E_A$<br>(Z) $\rightarrow$ ITS | $\Delta E_{\text{def}}$<br>SOSP vs. ITS |
| Gas Phase     | $\Delta E$          |                             |                                       |                                       |   |
| 1.0           | $\Delta H_0$        |                             |                                       |                                       |   |
|               | $\Delta H_{298}$    |                             |                                       |                                       |   |
|               | $\Delta G_{298}$    |                             |                                       |                                       |   |
| Heptane       | $\Delta E$          | 3.21                        | 27.29                                 | 24.08                                 | 1.39                                    |
| 1.92          | $\Delta H_0$        | 3.27                        | 25.42                                 | 22.15                                 | 1.02                                    |
|               | $\Delta H_{298}$    | 3.20                        | 25.46                                 | 22.26                                 | 0.88                                    |
|               | $\Delta G_{298}$    | 3.41                        | 25.42                                 | 22.01                                 | 1.11                                    |
| Benzene       | $\Delta E$          | 3.04                        | 27.32                                 | 24.28                                 | 1.45                                    |
| 2.25          | $\Delta H_0$        | 3.10                        | 25.43                                 | 22.32                                 | 1.08                                    |
|               | $\Delta H_{298}$    | 3.03                        | 25.47                                 | 22.44                                 | 0.94                                    |
|               | $\Delta G_{298}$    | 3.24                        | 25.44                                 | 22.20                                 | 1.16                                    |
| Diethyl Ether | $\Delta E$          | 2.52                        | 27.45                                 | 24.93                                 | 1.67                                    |
| 4.34          | $\Delta H_0$        | 2.57                        | 25.51                                 | 22.94                                 | 1.22                                    |
|               | $\Delta H_{298}$    | 2.51                        | 25.56                                 | 23.04                                 | 1.11                                    |
|               | $\Delta G_{298}$    | 2.68                        | 25.52                                 | 22.84                                 | 1.26                                    |
| Chloroform    | $\Delta E$          | 2.44                        | 27.49                                 | 25.04                                 | 1.71                                    |
| 4.90          | $\Delta H_0$        | 2.48                        | 25.51                                 | 23.03                                 | 1.23                                    |
|               | $\Delta H_{298}$    | 2.43                        | 25.56                                 | 23.14                                 | 1.13                                    |
|               | $\Delta G_{298}$    | 2.58                        | 25.50                                 | 22.92                                 | 1.25                                    |
| Aniline       | $\Delta E$          | 2.25                        | 27.57                                 | 25.32                                 | 1.81                                    |
| 6.89          | $\Delta H_0$        | 2.24                        | 25.53                                 | 23.29                                 | 1.29                                    |
|               | $\Delta H_{298}$    | 2.21                        | 25.60                                 | 23.40                                 | 1.20                                    |
|               | $\Delta G_{298}$    | 2.31                        | 25.50                                 | 23.19                                 | 1.30                                    |
| THF           | $\Delta E$          | 2.24                        | 27.51                                 | 25.27                                 | 1.83                                    |
| 7.58          | $\Delta H_0$        | 2.27                        | 25.57                                 | 23.29                                 | 1.34                                    |
|               | $\Delta H_{298}$    | 2.22                        | 25.60                                 | 23.38                                 | 1.25                                    |
|               | $\Delta G_{298}$    | 2.36                        | 25.58                                 | 23.21                                 | 1.36                                    |
| Methylene     | $\Delta E$          | 2.16                        | 27.53                                 | 25.37                                 | 1.88                                    |



|                         |                  |      |       |       |      |
|-------------------------|------------------|------|-------|-------|------|
| Chloride<br>8.93        | $\Delta H_0$     | 2.19 | 25.56 | 23.37 | 1.37 |
|                         | $\Delta H_{298}$ | 2.14 | 25.60 | 23.46 | 1.28 |
|                         | $\Delta G_{298}$ | 2.28 | 25.56 | 23.29 | 1.38 |
| Dichloroethane<br>10.36 | $\Delta E$       | 2.12 | 27.54 | 25.42 | 1.90 |
|                         | $\Delta H_0$     | 2.15 | 25.57 | 23.43 | 1.39 |
|                         | $\Delta H_{298}$ | 2.10 | 25.61 | 23.51 | 1.30 |
|                         | $\Delta G_{298}$ | 2.23 | 25.58 | 23.35 | 1.40 |
| Acetone<br>20.70        | $\Delta E$       | 1.97 | 27.60 | 25.59 | 2.02 |
|                         | $\Delta H_0$     | 1.98 | 25.59 | 23.61 | 1.49 |
|                         | $\Delta H_{298}$ | 1.94 | 25.63 | 23.69 | 1.40 |
|                         | $\Delta G_{298}$ | 2.05 | 25.59 | 23.54 | 1.50 |
| Ethanol<br>24.55        | $\Delta E$       | 1.90 | 27.65 | 25.75 | 2.05 |
|                         | $\Delta H_0$     | 1.86 | 25.55 | 23.69 | 1.46 |
|                         | $\Delta H_{298}$ | 1.84 | 25.64 | 23.79 | 1.39 |
|                         | $\Delta G_{298}$ | 1.88 | 25.47 | 23.59 | 1.44 |
| Methanol<br>32.63       | $\Delta E$       | 1.86 | 27.67 | 25.81 | 2.08 |
|                         | $\Delta H_0$     | 1.81 | 25.54 | 23.74 | 1.47 |
|                         | $\Delta H_{298}$ | 1.80 | 25.64 | 23.84 | 1.41 |
|                         | $\Delta G_{298}$ | 1.82 | 25.45 | 23.63 | 1.44 |
| Acetonitrile<br>36.64   | $\Delta E$       | 1.90 | 27.58 | 25.68 | 2.07 |
|                         | $\Delta H_0$     | 1.90 | 25.60 | 23.70 | 1.53 |
|                         | $\Delta H_{298}$ | 1.87 | 25.64 | 23.77 | 1.45 |
|                         | $\Delta G_{298}$ | 1.96 | 25.59 | 23.63 | 1.54 |
| DMSO<br>46.70           | $\Delta E$       | 1.89 | 27.59 | 25.69 | 2.08 |
|                         | $\Delta H_0$     | 1.87 | 25.61 | 23.73 | 1.54 |
|                         | $\Delta H_{298}$ | 1.85 | 25.65 | 23.80 | 1.46 |
|                         | $\Delta G_{298}$ | 1.92 | 25.61 | 23.69 | 1.56 |
| Water<br>78.39          | $\Delta E$       | 1.76 | 27.74 | 25.98 | 2.17 |
|                         | $\Delta H_0$     | 1.67 | 25.54 | 23.87 | 1.40 |
|                         | $\Delta H_{298}$ | 1.67 | 25.66 | 23.98 | 1.40 |
|                         | $\Delta G_{298}$ | 1.63 | 25.40 | 23.78 | 1.22 |

**Table S4.** *N*-Inversion Saddle Point Geometries Computed at Levels PCM and SMD

| Medium             | PCM(MP2(full)/6-31G*) |         |        |          |          |
|--------------------|-----------------------|---------|--------|----------|----------|
|                    | ITS                   |         |        |          | SOSP     |
|                    | $\alpha$              | $\beta$ | $\eta$ | $\sigma$ | $\alpha$ |
| Gas Phase          | 140.69                | 93.81   | 140.59 | -171.00  | 179.55   |
| Heptane            | 139.24                | 93.11   | 139.34 | -170.88  | 179.95   |
| Benzene            | 138.80                | 87.81   | 138.85 | -170.82  | 179.84   |
| Diethyl Ether      | 137.55                | 90.17   | 137.55 | -170.76  | 179.51   |
| Chloroform         | 137.17                | 85.72   | 137.35 | -170.56  | 179.43   |
| Aniline            | 137.17                | 93.73   | 137.31 | -171.32  | 179.34   |
| THF                | 136.63                | 88.90   | 136.64 | -170.67  | 179.29   |
| Methylene Chloride | 136.49                | 90.45   | 136.49 | -170.66  | 179.26   |
| Dichloroethane     | 136.09                | 93.00   | 136.17 | -170.64  | 179.22   |
| Acetone            | 135.72                | 90.16   | 135.72 | -170.59  | 179.10   |
| Ethanol            | 135.43                | 88.46   | 135.45 | -170.64  | 179.07   |
| Methanol           | 135.15                | 92.73   | 135.21 | -170.54  | 179.06   |
| Acetonitrile       | 135.08                | 93.89   | 135.21 | -170.60  | 179.06   |
| DMSO               | 135.24                | 93.11   | 139.24 | -170.57  | 178.97   |
| Water              | 134.24                | 93.64   | 134.83 | -170.56  | 178.96   |
| AVERAGE            | 136.46                | 91.06   | 136.53 | -170.70  | 179.29   |
| STD. DEV.          | 1.40                  | 2.62    | 1.40   | 0.21     | 0.31     |

**Table S4, Continued.** [Attach to the right of the above Table and omitting the first column.]

|                    | SMD(MP2(full)/6-31G*) |         |        |          |          |
|--------------------|-----------------------|---------|--------|----------|----------|
|                    | ITS                   |         |        |          | SOSP     |
|                    | $\alpha$              | $\beta$ | $\eta$ | $\sigma$ | $\alpha$ |
| Gas Phase          | 140.69                | 93.81   | 140.59 | -171.00  | 179.55   |
| Heptane            | 137.54                | 92.42   | 137.59 | -170.59  | 179.95   |
| Benzene            | 137.21                | 90.65   | 137.22 | -170.54  | 179.84   |
| Diethyl Ether      | 135.42                | 92.47   | 135.47 | -170.42  | 179.55   |
| Chloroform         | 134.50                | 94.23   | 134.65 | -170.38  | 179.51   |
| Aniline            | 133.37                | 97.09   | 133.79 | -170.31  | 179.37   |
| THF                | 133.24                | 92.69   | 133.30 | -170.28  | 179.95   |
| Methylene Chloride | 132.87                | 93.12   | 132.95 | -170.28  | 179.95   |
| Dichloroethane     | 132.64                | 93.11   | 132.72 | -170.27  | 179.30   |
| Acetone            | 131.61                | 93.08   | 131.68 | -170.25  | 179.19   |
| Ethanol            | 131.00                | 93.03   | 131.06 | -170.33  | 179.14   |
| Methanol           | 130.63                | 93.01   | 130.70 | -170.36  | 179.11   |
| Acetonitrile       | 131.08                | 93.05   | 131.16 | -170.25  | 179.15   |
| DMSO               | 131.03                | 93.06   | 131.10 | -170.24  | 179.14   |
| Water              | 129.45                | 91.47   | 129.45 | -170.50  | 179.03   |
| AVERAGE            | 132.89                | 93.13   | 132.98 | -170.35  | 179.44   |
| STD. DEV.          | 2.60                  | 1.37    | 2.60   | 0.11     | 0.36     |

**Table S5.** Population Data Computed for Gas-Phase and Selected Solvents

| Medium             | Str.     | Natural Population (NBO) |         |          |        |
|--------------------|----------|--------------------------|---------|----------|--------|
|                    |          | C4                       | Imine-N | NH-group | CNH    |
| Gas-Phase          | <i>E</i> | 0.375                    | -0.734  | -0.371   | 0.004  |
|                    | <i>Z</i> | 0.373                    | -0.710  | -0.360   | 0.013  |
|                    | ITS      | 0.421                    | -0.864  | -0.445   | -0.024 |
|                    | SOSP     | 0.413                    | -0.851  | -0.393   | 0.020  |
| Heptane, PCM       | <i>E</i> | 0.378                    | -0.748  | -0.381   | -0.003 |
|                    | <i>Z</i> | 0.377                    | -0.726  | -0.371   | 0.006  |
|                    | ITS      | 0.424                    | -0.864  | -0.438   | -0.014 |
|                    | SOSP     | 0.430                    | -0.818  | -0.365   | 0.065  |
| Heptane, SMD       | <i>E</i> | 0.384                    | -0.794  | -0.408   | -0.024 |
|                    | <i>Z</i> | 0.378                    | -0.734  | -0.375   | 0.003  |
|                    | ITS      | 0.424                    | -0.871  | -0.442   | -0.018 |
|                    | SOSP     | 0.430                    | -0.823  | -0.366   | 0.064  |
| Benzene, PCM       | <i>E</i> | 0.379                    | -0.751  | -0.383   | -0.004 |
|                    | <i>Z</i> | 0.378                    | -0.730  | -0.373   | 0.005  |
|                    | ITS      | 0.424                    | -0.866  | -0.439   | -0.015 |
|                    | SOSP     | 0.430                    | -0.819  | -0.365   | 0.065  |
| Benzene, SMD       | <i>E</i> | 0.380                    | -0.760  | -0.388   | -0.008 |
|                    | <i>Z</i> | 0.379                    | -0.740  | -0.379   | 0.000  |
|                    | ITS      | 0.424                    | -0.876  | -0.446   | -0.022 |
|                    | SOSP     | 0.429                    | -0.824  | -0.366   | 0.063  |
| Diethyl Ether, PCM | <i>E</i> | 0.380                    | -0.760  | -0.389   | -0.009 |
|                    | <i>Z</i> | 0.380                    | -0.742  | -0.381   | -0.001 |
|                    | ITS      | 0.425                    | -0.874  | -0.445   | -0.020 |
|                    | SOSP     | 0.428                    | -0.820  | -0.363   | 0.065  |
| Diethyl Ether, SMD | <i>E</i> | 0.382                    | -0.774  | -0.397   | -0.015 |
|                    | <i>Z</i> | 0.380                    | -0.742  | -0.381   | -0.001 |
|                    | ITS      | 0.425                    | -0.887  | -0.452   | -0.027 |
|                    | SOSP     | 0.427                    | -0.828  | -0.365   | 0.062  |
| Aniline, PCM       | <i>E</i> | 0.381                    | -0.765  | -0.392   | -0.011 |
|                    | <i>Z</i> | 0.381                    | -0.748  | -0.385   | -0.004 |
|                    | ITS      | 0.425                    | -0.878  | -0.448   | -0.023 |
|                    | SOSP     | 0.428                    | -0.821  | -0.363   | 0.065  |

|              |          |       |        |        |        |
|--------------|----------|-------|--------|--------|--------|
| Aniline, SMD | <i>E</i> | 0.383 | -0.781 | -0.401 | -0.018 |
|              | <i>Z</i> | 0.382 | -0.766 | -0.394 | -0.012 |
|              | ITS      | 0.425 | -0.878 | -0.448 | -0.023 |
|              | SOSP     | 0.426 | -0.830 | -0.364 | 0.062  |
| Acetone, PCM | <i>E</i> | 0.382 | -0.771 | -0.396 | -0.014 |
|              | <i>Z</i> | 0.382 | -0.762 | -0.391 | -0.009 |
|              | ITS      | 0.426 | -0.884 | -0.452 | -0.026 |
|              | SOSP     | 0.424 | -0.833 | -0.364 | 0.060  |
| Acetone, SMD | <i>E</i> | 0.394 | -0.790 | -0.406 | -0.022 |
|              | <i>Z</i> | 0.383 | -0.776 | -0.399 | -0.016 |
|              | ITS      | 0.426 | -0.901 | -0.461 | -0.035 |
|              | SOSP     | 0.427 | -0.822 | -0.362 | 0.065  |
| Water, PCM   | <i>E</i> | 0.381 | -0.773 | -0.398 | -0.017 |
|              | <i>Z</i> | 0.381 | -0.761 | -0.393 | -0.048 |
|              | ITS      | 0.427 | -0.904 | -0.475 | -0.048 |
|              | SOSP     | 0.426 | -0.822 | -0.362 | 0.064  |
| Water, SMD   | <i>E</i> | 0.383 | -0.794 | -0.410 | -0.027 |
|              | <i>Z</i> | 0.381 | -0.782 | -0.406 | -0.025 |
|              | ITS      | 0.434 | -0.953 | -0.527 | -0.093 |
|              | SOSP     | 0.421 | -0.838 | -0.368 | 0.053  |

**Table S6.** Molecular Dipole Moments ( $\mu$ , Debye) of Isomers and Saddle-Point Structures Computed at the Levels PCM and SMD

| <b>Medium</b>      | <b>Method</b> | $\mu(\mathbf{Z})$ | $\mu(\mathbf{E})$ | $\mu(\mathbf{TS})$ | $\mu(\mathbf{SOSP})$ |
|--------------------|---------------|-------------------|-------------------|--------------------|----------------------|
| Gas Phase          |               | 3.2798            | 0.4506            | 2.3176             | 2.7623               |
| Heptane            | PCM           | 3.5722            | 0.4559            | 2.4892             | 3.0659               |
|                    | SMD           | 3.7172            | 0.5236            | 2.5265             | 3.0683               |
| Benzene            | PCM           | 3.6433            | 0.4542            | 2.5244             | 3.1302               |
|                    | SMD           | 3.8027            | 0.5399            | 2.5780             | 3.1379               |
| Diethyl Ether      | PCM           | 3.8530            | 0.4467            | 2.6430             | 3.3511               |
|                    | SMD           | 4.1246            | 0.5872            | 2.7474             | 3.3449               |
| Chloroform         | PCM           | 3.8859            | 0.4452            | 2.6605             | 3.3817               |
|                    | SMD           | 4.1663            | 0.5939            | 2.7734             | 3.1496               |
| Aniline            | PCM           | 3.9551            | 0.4415            | 2.7015             | 3.4605               |
|                    | SMD           | 4.2946            | 0.6128            | 2.8558             | 3.3481               |
| THF                | PCM           | 3.9744            | 0.4404            | 2.7117             | 3.4786               |
|                    | SMD           | 4.3117            | 0.6145            | 2.8675             | 3.2335               |
| Methylene Chloride | PCM           | 4.0046            | 0.4380            | 2.7265             | 3.5084               |
|                    | SMD           | 4.3581            | 0.6216            | 2.9016             | 3.4930               |
| Dichloroethane     | PCM           | 4.0225            | 0.4380            | 2.7389             | 3.5300               |
|                    | SMD           | 4.3887            | 0.6256            | 2.9216             | 3.5099               |
| Acetone            | PCM           | 4.0956            | 0.4327            | 2.7804             | 3.6029               |
|                    | SMD           | 4.4995            | 0.6418            | 3.0101             | 3.5770               |
| Ethanol            | PCM           | 4.1081            | 0.4313            | 2.7834             | 3.6173               |
|                    | SMD           | 4.5208            | 0.6474            | 3.0393             | 3.5904               |
| Methanol           | PCM           | 4.1297            | 0.4263            | 2.7999             | 3.6348               |
|                    | SMD           | 4.5436            | 0.6512            | 3.0634             | 3.6044               |
| Acetonitrile       | PCM           | 4.1293            | 0.4300            | 2.7977             | 3.6442               |
|                    | SMD           | 4.5483            | 0.6491            | 3.0531             | 3.6065               |
| DMSO               | PCM           | 4.1359            | 0.4325            | 2.8045             | 3.6464               |
|                    | SMD           | 4.5642            | 0.6512            | 3.0645             | 3.6145               |
| Water              | PCM           | 4.1717            | 0.4177            | 2.8176             | 3.6541               |
|                    | SMD           | 4.5875            | 0.6583            | 3.1285             | 3.6326               |

**Table S7.** Computed *N*-Lone Pair Dipole Moments: Magnitude and Directions at PCM Level

| Medium             | $\epsilon$ | $ \mu(\text{N}_{\text{lp}}, Z) $ | $\lambda(Z)$ | $ \mu(\text{N}_{\text{lp}}, E) $ | $\lambda(E)$ |
|--------------------|------------|----------------------------------|--------------|----------------------------------|--------------|
| Gas-Phase          | 1          | 2.813                            | 145.19       | 2.347                            | 146.66       |
| Heptane            | 1.92       | 3.186                            | 146.13       | 2.641                            | 147.50       |
| Benzene            | 2.25       | 3.270                            | 146.17       | 2.705                            | 147.61       |
| Diethyl ether      | 4.34       | 3.541                            | 146.65       | 2.926                            | 147.97       |
| Chloroform         | 4.90       | 3.578                            | 146.64       | 2.958                            | 148.00       |
| Aniline            | 6.89       | 3.674                            | 146.86       | 3.037                            | 148.10       |
| THF                | 7.58       | 3.695                            | 146.86       | 3.055                            | 148.10       |
| Methylene Chloride | 8.93       | 3.729                            | 146.83       | 3.087                            | 148.16       |
| Dichloroethane     | 10.36      | 3.757                            | 146.91       | 3.107                            | 148.14       |
| Acetone            | 20.70      | 3.847                            | 146.97       | 3.183                            | 148.19       |
| Ethanol            | 24.55      | 3.859                            | 146.92       | 3.199                            | 148.25       |
| Methanol           | 32.63      | 3.874                            | 146.89       | 3.222                            | 148.25       |
| Acetonitrile       | 36.64      | 3.888                            | 146.99       | 3.226                            | 148.29       |
| DMSO               | 46.70      | 3.904                            | 147.02       | 3.226                            | 148.27       |
| Water              | 78.39      | 3.895                            | 146.60       | 3.250                            | 148.15       |

**Table S7, Continued.** [Attach to the right of above Table omitting the left column.]

| Medium             | $\langle\mu(\text{N}_{\text{lp}})\rangle$ | $\Delta\mu(\text{N}_{\text{lp}})$ | $\mu(\text{N}_{\text{lp}}, \text{ITS})$ | $\lambda(\text{ITS})$ | $\omega(\text{ITS})$ |
|--------------------|---|-----------------------------------|---|-----------------------|----------------------|
| Gas-Phase          | 2.580                                     | 0.466                             | 1.583                                   | 137.01                | 27.64                |
| Heptanes           | 2.914                                     | 0.545                             | 1.880                                   | 140.01                | 28.88                |
| Benzene            | 2.988                                     | 0.565                             | 1.952                                   | 140.48                | 29.33                |
| Diethyl ether      | 3.234                                     | 0.615                             | 2.215                                   | 142.27                | 30.68                |
| Chloroform         | 3.268                                     | 0.620                             | 2.261                                   | 142.52                | 30.97                |
| Aniline            | 3.356                                     | 0.637                             | 2.368                                   | 143.10                | 31.57                |
| THF                | 3.375                                     | 0.640                             | 2.397                                   | 143.26                | 31.73                |
| Methylene chloride | 3.408                                     | 0.642                             | 2.447                                   | 143.56                | 32.02                |
| Dichloroethane     | 3.432                                     | 0.650                             | 2.475                                   | 143.66                | 32.18                |
| Acetone            | 3.515                                     | 0.664                             | 2.600                                   | 144.20                | 32.95                |
| Ethanol            | 3.529                                     | 0.660                             | 2.628                                   | 144.47                | 33.05                |
| Methanol           | 3.548                                     | 0.652                             | 2.668                                   | 144.53                | 33.35                |
| Acetonitrile       | 3.557                                     | 0.662                             | 2.670                                   | 144.65                | 33.29                |
| DMSO               | 3.565                                     | 0.678                             | 2.675                                   | 144.53                | 33.37                |
| Water              | 3.573                                     | 0.645                             | 2.731                                   | 144.83                | 33.71                |

**Cartesian Coordinates of Stationary Structures (*E*, *Z*, ITS, SOSP) Computed in Gas-Phase and for Various Solvents at PCM and SMD Levels**

**(*E*)-Isomer of 3-Methyl-4-Pyrimidinimine**

**Gas Phase**

MP2 (full) / 6-31G\*, E = -357.89266222

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.52904200  | -1.35994300 | -0.00027300 |
| C | 1.94449100  | 0.40319600  | 0.00024400  |
| C | 0.92054900  | 1.29642600  | 0.00021000  |
| C | -0.45621400 | 0.85072300  | -0.00014900 |
| H | 0.31577200  | -2.42720200 | -0.00060600 |
| H | 2.97820700  | 0.73985800  | 0.00059500  |
| H | 1.11485700  | 2.36507000  | 0.00060100  |
| N | -0.56656600 | -0.55375200 | -0.00020000 |
| N | 1.77178800  | -0.96658500 | -0.00017400 |
| N | -1.55939600 | 1.52767500  | -0.00034400 |
| H | -1.33652000 | 2.52652900  | -0.00017300 |
| C | -1.91304400 | -1.11196500 | 0.00042700  |
| H | -1.83937300 | -2.19968500 | -0.00000900 |
| H | -2.45074800 | -0.76362400 | 0.88330600  |
| H | -2.45192500 | -0.76293800 | -0.88143700 |

**Heptane**

PCM(MP2 (full) / 6-31G\*), E = -357.89738825

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.52236400 | -1.36259200 | 0.00116800  |
| C | -1.94557700 | 0.39768100  | -0.00045600 |
| C | -0.92436000 | 1.29362100  | -0.00221400 |
| C | 0.45358100  | 0.85182800  | 0.00001400  |
| H | -0.30558500 | -2.42995800 | 0.00209600  |
| H | -2.98100900 | 0.73189900  | -0.00124800 |
| H | -1.12187800 | 2.36257800  | -0.00406100 |
| N | 0.56922400  | -0.55196200 | -0.00157600 |
| N | -1.76719900 | -0.97240600 | 0.00197600  |
| N | 1.55145300  | 1.53810600  | 0.00279400  |
| H | 1.31575500  | 2.53669900  | 0.00233900  |
| C | 1.91648800  | -1.10984400 | -0.00136900 |
| H | 1.84372400  | -2.19744200 | -0.01189000 |
| H | 2.45694600  | -0.75367800 | -0.87942700 |
| H | 2.45108600  | -0.77043100 | 0.88697600  |

SMD(MP2 (full) / 6-31G\*), E = -357.90469517

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51649900  | -1.36466600 | -0.00007900 |
| C | 1.94715700  | 0.39097500  | 0.00008900  |
| C | 0.92927900  | 1.29019700  | -0.00007100 |
| C | -0.44956600 | 0.85251200  | -0.00004700 |
| H | 0.29198100  | -2.42867800 | -0.00009000 |
| H | 2.98338100  | 0.71996700  | 0.00016600  |
| H | 1.12919000  | 2.35787100  | -0.00007500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.57132600 | -0.54976200 | -0.00013600 |
| N | 1.76117800  | -0.97642800 | 0.00005400  |
| N | -1.54362600 | 1.54498900  | 0.00002700  |
| H | -1.30211700 | 2.54008600  | 0.00010800  |
| C | -1.91989300 | -1.10409600 | 0.00008400  |
| H | -1.85003600 | -2.19197900 | -0.00000200 |
| H | -2.45824700 | -0.75924400 | 0.88404600  |
| H | -2.45859400 | -0.75915500 | -0.88363100 |

### Benzene

PCM(MP2 (full)/6-31G\*), E = -357.89843522

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.52144500 | -1.36323200 | -0.00043600 |
| C | -1.94560700 | 0.39710900  | 0.00021700  |
| C | -0.92465800 | 1.29333200  | 0.00074300  |
| C | 0.45315900  | 0.85181100  | -0.00005600 |
| H | -0.30445100 | -2.43076600 | -0.00078700 |
| H | -2.98128000 | 0.73119300  | 0.00056000  |
| H | -1.12237900 | 2.36245500  | 0.00140700  |
| N | 0.56946700  | -0.55193100 | 0.00039200  |
| N | -1.76656000 | -0.97313800 | -0.00064200 |
| N | 1.55027300  | 1.53950000  | -0.00092700 |
| H | 1.31241700  | 2.53822300  | -0.00087300 |
| C | 1.91694700  | -1.10932400 | 0.00054800  |
| H | 1.84443200  | -2.19698500 | 0.00111500  |
| H | 2.45430500  | -0.76210700 | -0.88305200 |
| H | 2.45433200  | -0.76121700 | 0.88377600  |

SMD(MP2 (full)/6-31G\*), E = -357.90632281

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51422200  | -1.36548400 | -0.00007200 |
| C | 1.94747400  | 0.38883300  | 0.00008600  |
| C | 0.93067700  | 1.28912800  | -0.00007400 |
| C | -0.44848300 | 0.85278300  | -0.00004500 |
| H | 0.28797600  | -2.42902600 | -0.00008300 |
| H | 2.98406900  | 0.71681200  | 0.00015500  |
| H | 1.13163400  | 2.35664000  | -0.00008700 |
| N | -0.57222300 | -0.54903300 | -0.00013000 |
| N | 1.75947200  | -0.97835400 | 0.00005400  |
| N | -1.54074400 | 1.54846400  | 0.00003300  |
| H | -1.29496200 | 2.54266100  | 0.00010600  |
| C | -1.92112900 | -1.10297600 | 0.00007600  |
| H | -1.85179700 | -2.19085800 | -0.00001000 |
| H | -2.45934200 | -0.75878100 | 0.88442000  |
| H | -2.45967400 | -0.75868900 | -0.88402900 |

### Diethyl Ether

PCM(MP2 (full)/6-31G\*), E = -357.90196078

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51705700  | -1.36537200 | -0.00046000 |
| C | 1.94623800  | 0.39355200  | 0.00035100  |
| C | 0.92715000  | 1.29157700  | 0.00047500  |
| C | -0.45151900 | 0.85245700  | -0.00024400 |
| H | 0.29742100  | -2.43314200 | -0.00089700 |
| H | 2.98308100  | 0.72630300  | 0.00088300  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.12652500  | 2.36117400  | 0.00113600  |
| N | -0.57115800 | -0.55078600 | -0.00021400 |
| N | 1.76341900  | -0.97702600 | -0.00036000 |
| N | -1.54494800 | 1.54655000  | -0.00069000 |
| H | -1.29787300 | 2.54535600  | -0.00018200 |
| C | -1.91912600 | -1.10783700 | 0.00070700  |
| H | -1.84712800 | -2.19549500 | 0.00061700  |
| H | -2.45530700 | -0.76084700 | 0.88518500  |
| H | -2.45670600 | -0.76077600 | -0.88287100 |

SMD(MP2(full)/6-31G\*), E = -357.90894004

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50865700  | -1.36747500 | -0.00036800 |
| C | 1.94809400  | 0.38382900  | 0.00034000  |
| C | 0.93376600  | 1.28670800  | 0.00010200  |
| C | -0.44608900 | 0.85327100  | -0.00017000 |
| H | 0.27883000  | -2.43012100 | -0.00074700 |
| H | 2.98535900  | 0.71010000  | 0.00077900  |
| H | 1.13684100  | 2.35386800  | 0.00039300  |
| N | -0.57458500 | -0.54725000 | -0.00034400 |
| N | 1.75585700  | -0.98346700 | -0.00008700 |
| N | -1.53367600 | 1.55774800  | -0.00029300 |
| H | -1.27526900 | 2.54918800  | -0.00003100 |
| C | -1.92445100 | -1.10099300 | 0.00050300  |
| H | -1.85548700 | -2.18866000 | 0.00011100  |
| H | -2.46091700 | -0.75808600 | 0.88646900  |
| H | -2.46238900 | -0.75754000 | -0.88434400 |

### Chloroform

PCM(MP2(full)/6-31G\*), E = -357.90251279

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51626800  | -1.36583900 | -0.00063600 |
| C | 1.94640100  | 0.39282400  | 0.00047900  |
| C | 0.92769100  | 1.29122600  | 0.00088900  |
| C | -0.45106300 | 0.85244100  | -0.00020600 |
| H | 0.29615000  | -2.43366200 | -0.00131000 |
| H | 2.98342900  | 0.72537300  | 0.00107300  |
| H | 1.12721300  | 2.36091600  | 0.00180400  |
| N | -0.57149200 | -0.55063900 | 0.00009000  |
| N | 1.76282300  | -0.97774300 | -0.00077700 |
| N | -1.54379900 | 1.54758700  | -0.00122200 |
| H | -1.29512200 | 2.54636800  | -0.00067900 |
| C | -1.91984400 | -1.10708400 | 0.00094400  |
| H | -1.84817000 | -2.19478100 | 0.00083200  |
| H | -2.45577600 | -0.76010900 | 0.88557400  |
| H | -2.45716700 | -0.75994100 | -0.88275000 |

SMD(MP2(full)/6-31G\*), E = -357.90934087

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50816400  | -1.36753500 | -0.00031000 |
| C | 1.94791500  | 0.38351300  | 0.00028100  |
| C | 0.93381000  | 1.28649400  | 0.00009000  |
| C | -0.44582600 | 0.85329700  | -0.00013400 |
| H | 0.27867400  | -2.43017100 | -0.00060300 |
| H | 2.98504500  | 0.70990700  | 0.00064200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.13685300  | 2.35363600  | 0.00033900  |
| N | -0.57476700 | -0.54710100 | -0.00029200 |
| N | 1.75574800  | -0.98403400 | -0.00007400 |
| N | -1.53295500 | 1.55867500  | -0.00025500 |
| H | -1.27311200 | 2.54977100  | -0.00000500 |
| C | -1.92474800 | -1.10096600 | 0.00042200  |
| H | -1.85589500 | -2.18859400 | 0.00009600  |
| H | -2.46119500 | -0.75829900 | 0.88647100  |
| H | -2.46243400 | -0.75784800 | -0.88468900 |

### Aniline

PCM(MP2(full)/6-31G\*), E = -357.90372301

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51474500  | -1.36650800 | -0.00037900 |
| C | 1.94659600  | 0.39166600  | 0.00030800  |
| C | 0.92848600  | 1.29064400  | 0.00033000  |
| C | -0.45059000 | 0.85280600  | -0.00024000 |
| H | 0.29371900  | -2.43442800 | -0.00069000 |
| H | 2.98405100  | 0.72367900  | 0.00074200  |
| H | 1.12866700  | 2.36049900  | 0.00084500  |
| N | -0.57205600 | -0.55022400 | -0.00026900 |
| N | 1.76175200  | -0.97907300 | -0.00023400 |
| N | -1.54211400 | 1.55014100  | -0.00052900 |
| H | -1.29035100 | 2.54902900  | 0.00014700  |
| C | -1.92032900 | -1.10691400 | 0.00059300  |
| H | -1.84875400 | -2.19459400 | 0.00056700  |
| H | -2.45632300 | -0.76011300 | 0.88529000  |
| H | -2.45753100 | -0.76013800 | -0.88334900 |

SMD(MP2(full)/6-31G\*), E = -357.90741298

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50621900  | -1.36799200 | -0.00027300 |
| C | 1.94738600  | 0.38179900  | 0.00023800  |
| C | 0.93447600  | 1.28572300  | 0.00011100  |
| C | -0.44493400 | 0.85344000  | -0.00010700 |
| H | 0.27616000  | -2.43036900 | -0.00050600 |
| H | 2.98453000  | 0.70812000  | 0.00054300  |
| H | 1.13855700  | 2.35264900  | 0.00034600  |
| N | -0.57536000 | -0.54644200 | -0.00024800 |
| N | 1.75449400  | -0.98570800 | -0.00008400 |
| N | -1.53043600 | 1.56173200  | -0.00025700 |
| H | -1.26601100 | 2.55172000  | -0.00000100 |
| C | -1.92523400 | -1.10032700 | 0.00037900  |
| H | -1.85717400 | -2.18795900 | 0.00017200  |
| H | -2.46169200 | -0.75867000 | 0.88685200  |
| H | -2.46273000 | -0.75841800 | -0.88536000 |

### THF

PCM(MP2(full)/6-31G\*), E = -357.90405036

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51443500  | -1.36675700 | -0.00034600 |
| C | 1.94665100  | 0.39144300  | 0.00020600  |
| C | 0.92863200  | 1.29052800  | 0.00052100  |
| C | -0.45030100 | 0.85274900  | -0.00008200 |
| H | 0.29346100  | -2.43478700 | -0.00059700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.98419200  | 0.72335200  | 0.00050500  |
| H | 1.12876600  | 2.36045500  | 0.00101900  |
| N | -0.57216300 | -0.55031000 | 0.00008900  |
| N | 1.76154300  | -0.97935800 | -0.00042200 |
| N | -1.54157800 | 1.55043000  | -0.00067600 |
| H | -1.28921600 | 2.54940300  | -0.00041500 |
| C | -1.92074100 | -1.10639000 | 0.00049000  |
| H | -1.84950500 | -2.19409800 | 0.00143900  |
| H | -2.45717200 | -0.75876500 | 0.88457400  |
| H | -2.45720900 | -0.76033100 | -0.88419000 |

SMD(MP2(full)/6-31G\*), E = -357.90994391

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50496500  | -1.36888000 | -0.00033100 |
| C | 1.94852500  | 0.38043800  | 0.00030500  |
| C | 0.93595000  | 1.28510300  | 0.00009200  |
| C | -0.44428200 | 0.85357700  | -0.00014400 |
| H | 0.27241200  | -2.43073000 | -0.00065700 |
| H | 2.98623500  | 0.70528600  | 0.00068500  |
| H | 1.14014100  | 2.35200700  | 0.00033400  |
| N | -0.57602500 | -0.54612600 | -0.00030100 |
| N | 1.75314300  | -0.98663200 | -0.00008100 |
| N | -1.52895700 | 1.56327300  | -0.00027400 |
| H | -1.26344800 | 2.55302300  | 0.00002100  |
| C | -1.92651400 | -1.09915200 | 0.00044800  |
| H | -1.85838300 | -2.18670700 | 0.00018600  |
| H | -2.46234200 | -0.75666300 | 0.88695200  |
| H | -2.46360800 | -0.75633000 | -0.88515100 |

### Methylene Chloride

PCM(MP2(full)/6-31G\*), E = -357.90454891

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51359900 | -1.36711100 | -0.00089500 |
| C | -1.94680300 | 0.39067000  | 0.00029400  |
| C | -0.92916800 | 1.29014400  | 0.00169200  |
| C | 0.44992900  | 0.85278900  | -0.00004200 |
| H | -0.29195400 | -2.43515500 | -0.00155700 |
| H | -2.98457800 | 0.72215300  | 0.00110800  |
| H | -1.12954000 | 2.36012600  | 0.00313900  |
| N | 0.57254000  | -0.55006100 | 0.00126500  |
| N | -1.76088900 | -0.98012800 | -0.00146500 |
| N | 1.54045600  | 1.55173300  | -0.00202700 |
| H | 1.28612700  | 2.55058200  | -0.00224200 |
| C | 1.92126400  | -1.10593400 | 0.00099600  |
| H | 1.85021700  | -2.19365200 | 0.00051100  |
| H | 2.45761100  | -0.75863300 | -0.88327400 |
| H | 2.45763000  | -0.75957900 | 0.88563500  |

SMD(MP2(full)/6-31G\*), E = -357.91167540

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50419900  | -1.36914600 | -0.00027500 |
| C | 1.94866700  | 0.37983700  | 0.00025400  |
| C | 0.93635900  | 1.28477000  | 0.00007100  |
| C | -0.44387400 | 0.85367500  | -0.00011800 |
| H | 0.27153200  | -2.43092000 | -0.00054300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.98639600  | 0.70447000  | 0.00057200  |
| H | 1.14055100  | 2.35168100  | 0.00027500  |
| N | -0.57639700 | -0.54590300 | -0.00026000 |
| N | 1.75281100  | -0.98747800 | -0.00006300 |
| N | -1.52792200 | 1.56459800  | -0.00023100 |
| H | -1.26083000 | 2.55397300  | 0.00005900  |
| C | -1.92721900 | -1.09891200 | 0.00037500  |
| H | -1.85911000 | -2.18642300 | 0.00019000  |
| H | -2.46286100 | -0.75643000 | 0.88698400  |
| H | -2.46391400 | -0.75621100 | -0.88550600 |

### Dichloroethane

PCM(MP2(full)/6-31G\*), E = -357.90488193

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51327500  | -1.36733700 | -0.00026700 |
| C | 1.94685000  | 0.39046100  | 0.00020500  |
| C | 0.92934500  | 1.29004900  | 0.00031900  |
| C | -0.44976700 | 0.85288200  | -0.00012000 |
| H | 0.29160300  | -2.43544900 | -0.00046300 |
| H | 2.98469400  | 0.72198800  | 0.00046400  |
| H | 1.12982900  | 2.36011000  | 0.00068700  |
| N | -0.57262300 | -0.55005400 | -0.00010900 |
| N | 1.76069100  | -0.98039100 | -0.00024200 |
| N | -1.54009700 | 1.55211400  | -0.00042800 |
| H | -1.28544600 | 2.55112800  | -0.00019800 |
| C | -1.92145500 | -1.10574100 | 0.00041600  |
| H | -1.85053100 | -2.19347800 | -0.00012200 |
| H | -2.45722800 | -0.75933400 | 0.88539800  |
| H | -2.45820900 | -0.75852900 | -0.88363800 |

SMD(MP2(full)/6-31G\*), E = -357.91100443

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50368600  | -1.36931900 | -0.00027200 |
| C | 1.94863500  | 0.37936100  | 0.00025300  |
| C | 0.93661200  | 1.28455300  | 0.00007800  |
| C | -0.44362300 | 0.85369000  | -0.00012300 |
| H | 0.27063500  | -2.43096000 | -0.00054300 |
| H | 2.98638600  | 0.70385500  | 0.00056800  |
| H | 1.14093700  | 2.35140500  | 0.00029200  |
| N | -0.57656400 | -0.54574300 | -0.00025700 |
| N | 1.75240100  | -0.98787700 | -0.00006900 |
| N | -1.52725500 | 1.56532600  | -0.00023600 |
| H | -1.25910400 | 2.55442600  | 0.00006000  |
| C | -1.92739900 | -1.09865000 | 0.00037700  |
| H | -1.85945000 | -2.18613300 | 0.00023400  |
| H | -2.46295800 | -0.75624400 | 0.88704900  |
| H | -2.46398300 | -0.75609400 | -0.88561100 |

### Acetone

PCM(MP2(full)/6-31G\*), E = -357.90612317

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51174400 | -1.36819400 | -0.00015100 |
| C | -1.94704400 | 0.38921400  | 0.00005200  |
| C | -0.93017500 | 1.28944600  | 0.00032200  |
| C | 0.44913400  | 0.85307500  | -0.00000400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.28911900 | -2.43646500 | -0.00022500 |
| H | -2.98528800 | 0.72030700  | 0.00017800  |
| H | -1.13108200 | 2.35972300  | 0.00056300  |
| N | 0.57320300  | -0.54974100 | 0.00021800  |
| N | -1.75954900 | -0.98173900 | -0.00027800 |
| N | 1.53813600  | 1.55455300  | -0.00038500 |
| H | 1.28008000  | 2.55364200  | -0.00032600 |
| C | 1.92226400  | -1.10505400 | 0.00017700  |
| H | 1.85161200  | -2.19281500 | -0.00005300 |
| H | 2.45839800  | -0.75820000 | -0.88441700 |
| H | 2.45826600  | -0.75862800 | 0.88502500  |

SMD(MP2(full)/6-31G\*), E = -357.91201091

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50149600  | -1.37015000 | -0.00025100 |
| C | 1.94892500  | 0.37728600  | 0.00023300  |
| C | 0.93800100  | 1.28367100  | 0.00008100  |
| C | -0.44259300 | 0.85398300  | -0.00014500 |
| H | 0.26686200  | -2.43142600 | -0.00051400 |
| H | 2.98706900  | 0.70094000  | 0.00055200  |
| H | 1.14335300  | 2.35038100  | 0.00032200  |
| N | -0.57747900 | -0.54503000 | -0.00025000 |
| N | 1.75083900  | -0.98984400 | -0.00006400 |
| N | -1.52452100 | 1.56870000  | -0.00022000 |
| H | -1.25236300 | 2.55683300  | 0.00008600  |
| C | -1.92866500 | -1.09765800 | 0.00036400  |
| H | -1.86112300 | -2.18513200 | 0.00037600  |
| H | -2.46387500 | -0.75553600 | 0.88742500  |
| H | -2.46477000 | -0.75563900 | -0.88619300 |

### Ethanol

PCM(MP2(full)/6-31G\*), E = -357.90636781

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51108500  | -1.36827500 | -0.00017400 |
| C | 1.94716300  | 0.38855300  | 0.00010600  |
| C | 0.93061600  | 1.28913400  | 0.00029800  |
| C | -0.44895800 | 0.85330400  | -0.00002200 |
| H | 0.28784100  | -2.43649900 | -0.00033100 |
| H | 2.98559300  | 0.71919700  | 0.00024500  |
| H | 1.13191400  | 2.35938100  | 0.00056500  |
| N | -0.57352400 | -0.54943900 | 0.00005700  |
| N | 1.75905000  | -0.98233900 | -0.00024400 |
| N | -1.53742600 | 1.55571300  | -0.00036500 |
| H | -1.27786900 | 2.55461900  | -0.00034600 |
| C | -1.92245500 | -1.10510200 | 0.00025400  |
| H | -1.85166100 | -2.19281800 | 0.00045300  |
| H | -2.45850800 | -0.75839800 | 0.88499500  |
| H | -2.45871800 | -0.75871200 | -0.88448500 |

SMD(MP2(full)/6-31G\*), E = -357.90937438

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50255900  | -1.36914600 | -0.00039700 |
| C | 1.94755500  | 0.37851800  | 0.00035800  |
| C | 0.93637300  | 1.28428200  | 0.00038100  |
| C | -0.44327700 | 0.85386300  | -0.00031700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.27122200  | -2.43121100 | -0.00083600 |
| H | 2.98502400  | 0.70421100  | 0.00085400  |
| H | 1.14198500  | 2.35099300  | 0.00106000  |
| N | -0.57699100 | -0.54516900 | -0.00030200 |
| N | 1.75250400  | -0.98938900 | -0.00028800 |
| N | -1.52570500 | 1.56802400  | -0.00049900 |
| H | -1.25314400 | 2.55604800  | -0.00033400 |
| C | -1.92764400 | -1.09931200 | 0.00066500  |
| H | -1.85993300 | -2.18683000 | 0.00082600  |
| H | -2.46303000 | -0.75817400 | 0.88808300  |
| H | -2.46417600 | -0.75853100 | -0.88616900 |

### Methanol

PCM(MP2 (full) /6-31G\*), E = -357.90669869

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.51059000  | -1.36849700 | -0.00000200 |
| C | 1.94717500  | 0.38810400  | -0.00000700 |
| C | 0.93084200  | 1.28894700  | 0.00000400  |
| C | -0.44876100 | 0.85338600  | -0.00001000 |
| H | 0.28700300  | -2.43671600 | -0.00001200 |
| H | 2.98571600  | 0.71859200  | 0.00003100  |
| H | 1.13232300  | 2.35921700  | 0.00004400  |
| N | -0.57371900 | -0.54932300 | 0.00001600  |
| N | 1.75868900  | -0.98278400 | -0.00000500 |
| N | -1.53680400 | 1.55658000  | 0.00000100  |
| H | -1.27572200 | 2.55533500  | -0.00004400 |
| C | -1.92266900 | -1.10495300 | 0.00000400  |
| H | -1.85190800 | -2.19266700 | -0.00021400 |
| H | -2.45879100 | -0.75867700 | 0.88487800  |
| H | -2.45885000 | -0.75832300 | -0.88470100 |

SMD(MP2 (full) /6-31G\*), E = -357.90888799

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50240600  | -1.36909100 | -0.00035000 |
| C | 1.94733600  | 0.37846200  | 0.00032100  |
| C | 0.93625700  | 1.28427300  | 0.00034700  |
| C | -0.44324700 | 0.85388700  | -0.00026300 |
| H | 0.27148500  | -2.43125700 | -0.00073100 |
| H | 2.98471500  | 0.70440900  | 0.00073100  |
| H | 1.14197900  | 2.35096500  | 0.00093000  |
| N | -0.57705800 | -0.54510500 | -0.00025400 |
| N | 1.75260200  | -0.98964300 | -0.00027000 |
| N | -1.52549000 | 1.56848500  | -0.00046300 |
| H | -1.25209600 | 2.55630300  | -0.00027400 |
| C | -1.92766800 | -1.09952600 | 0.00058700  |
| H | -1.85985300 | -2.18702300 | 0.00093400  |
| H | -2.46311600 | -0.75847100 | 0.88800100  |
| H | -2.46398700 | -0.75911000 | -0.88652500 |

### Acetonitrile

PCM(MP2 (full) /6-31G\*), E = -357.90673932

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.51047900 | -1.36852200 | 0.00004400 |
| C | -1.94725400 | 0.38802700  | 0.00002800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.93097100 | 1.28888500  | -0.00016900 |
| C | 0.44869400  | 0.85344500  | -0.00002300 |
| H | -0.28686900 | -2.43677800 | 0.00005600  |
| H | -2.98583400 | 0.71844000  | -0.00002600 |
| H | -1.13251200 | 2.35917500  | -0.00030800 |
| N | 0.57376600  | -0.54929800 | -0.00012900 |
| N | -1.75861500 | -0.98286900 | 0.00013200  |
| N | 1.53669200  | 1.55662400  | 0.00017900  |
| H | 1.27599700  | 2.55552900  | 0.00018900  |
| C | 1.92276000  | -1.10487400 | -0.00005400 |
| H | 1.85208000  | -2.19259700 | -0.00143900 |
| H | 2.45929100  | -0.75727000 | -0.88414600 |
| H | 2.45842900  | -0.75946800 | 0.88544400  |

SMD(MP2(full)/6-31G\*), E = -357.91198407

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50060900  | -1.37047100 | -0.00022100 |
| C | 1.94902200  | 0.37650800  | 0.00020800  |
| C | 0.93848800  | 1.28329500  | 0.00007600  |
| C | -0.44214800 | 0.85404100  | -0.00014200 |
| H | 0.26546500  | -2.43156700 | -0.00046500 |
| H | 2.98719800  | 0.69988500  | 0.00050100  |
| H | 1.14388300  | 2.34994900  | 0.00031300  |
| N | -0.57785800 | -0.54476400 | -0.00023100 |
| N | 1.75026000  | -0.99066600 | -0.00005900 |
| N | -1.52334500 | 1.57009400  | -0.00019800 |
| H | -1.24935900 | 2.55775100  | 0.00008600  |
| C | -1.92925200 | -1.09728800 | 0.00033200  |
| H | -1.86174800 | -2.18468400 | 0.00037500  |
| H | -2.46417600 | -0.75517200 | 0.88752600  |
| H | -2.46497700 | -0.75532300 | -0.88643600 |

#### DMSO

PCM(MP2(full)/6-31G\*), E = -357.90682633

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51049400 | -1.36866500 | 0.00310500  |
| C | -1.94726300 | 0.38809500  | -0.00082000 |
| C | -0.93094100 | 1.28889400  | -0.00679500 |
| C | 0.44851300  | 0.85331100  | -0.00037100 |
| H | -0.28730500 | -2.43700400 | 0.00535400  |
| H | -2.98580100 | 0.71874600  | -0.00263400 |
| H | -1.13236400 | 2.35924000  | -0.01210000 |
| N | 0.57369400  | -0.54945400 | -0.00558900 |
| N | -1.75864200 | -0.98279200 | 0.00601500  |
| N | 1.53654700  | 1.55618800  | 0.00815300  |
| H | 1.27669600  | 2.55536100  | 0.00834400  |
| C | 1.92302700  | -1.10435900 | -0.00337400 |
| H | 1.85288200  | -2.19178900 | -0.03158800 |
| H | 2.46776200  | -0.73542900 | -0.87345600 |
| H | 2.44988600  | -0.78037300 | 0.89556100  |

SMD(MP2(full)/6-31G\*), E = -357.90985640

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.50023200 | -1.37057400 | -0.00026000 |
| C | 1.94880200 | 0.37604700  | 0.00024400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.93866900  | 1.28315400  | 0.00009800  |
| C | -0.44197500 | 0.85404700  | -0.00016400 |
| H | 0.26449000  | -2.43149400 | -0.00054400 |
| H | 2.98705300  | 0.69930900  | 0.00058000  |
| H | 1.14454400  | 2.34969200  | 0.00036600  |
| N | -0.57785300 | -0.54460800 | -0.00026100 |
| N | 1.74972300  | -0.99075600 | -0.00007600 |
| N | -1.52291800 | 1.57038600  | -0.00023400 |
| H | -1.24840400 | 2.55788500  | 0.00006600  |
| C | -1.92896700 | -1.09694200 | 0.00038700  |
| H | -1.86193500 | -2.18438600 | 0.00046300  |
| H | -2.46403800 | -0.75516800 | 0.88764900  |
| H | -2.46494200 | -0.75538400 | -0.88640900 |

### Water

PCM(MP2 (full)/6-31G\*), E = -357.90730727

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50995700 | -1.36899900 | 0.00018500  |
| C | -1.94724000 | 0.38743700  | -0.00013500 |
| C | -0.93125700 | 1.28865400  | -0.00017100 |
| C | 0.44852600  | 0.85329500  | 0.00014000  |
| H | -0.28549600 | -2.43720000 | 0.00013800  |
| H | -2.98596700 | 0.71775800  | -0.00028000 |
| H | -1.13275700 | 2.35904200  | -0.00043300 |
| N | 0.57401100  | -0.54909400 | 0.00005900  |
| N | -1.75811400 | -0.98342600 | 0.00013800  |
| N | 1.53581600  | 1.55784500  | 0.00025200  |
| H | 1.27200100  | 2.55630000  | -0.00014700 |
| C | 1.92315600  | -1.10448800 | -0.00023700 |
| H | 1.85244200  | -2.19221900 | -0.00121300 |
| H | 2.45918400  | -0.75741400 | -0.88488700 |
| H | 2.45923000  | -0.75893500 | 0.88498900  |

SMD(MP2 (full)/6-31G\*), E = -357.9090584

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50301400  | -1.36833300 | -0.00001100 |
| C | 1.94604500  | 0.37947300  | 0.00001300  |
| C | 0.93494400  | 1.28476400  | -0.00001600 |
| C | -0.44361600 | 0.85401100  | -0.00001300 |
| H | 0.27545200  | -2.43141400 | 0.00000800  |
| H | 2.98290100  | 0.70722100  | 0.00002300  |
| H | 1.14101800  | 2.35159400  | -0.00000800 |
| N | -0.57692400 | -0.54522300 | -0.00004300 |
| N | 1.75411600  | -0.98990000 | 0.00001800  |
| N | -1.52608600 | 1.56873200  | 0.00001700  |
| H | -1.25153200 | 2.55632200  | 0.00001500  |
| C | -1.92705700 | -1.10104400 | 0.00001600  |
| H | -1.85899400 | -2.18864000 | -0.00006200 |
| H | -2.46322700 | -0.76183800 | 0.88792000  |
| H | -2.46333500 | -0.76172800 | -0.88777900 |



**(Z)-Isomer of 3-Methyl-4-Pyrimidinimine**

**Gas Phase**

MP2 (full) /6-31G\*, E = -357.88634952

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51935200 | -1.36456100 | 0.00007300  |
| N | -1.76028300 | -0.98332100 | 0.00022700  |
| C | -1.95167800 | 0.38968500  | -0.00006000 |
| C | 0.44530900  | 0.86824700  | -0.00004300 |
| N | 0.57683200  | -0.54224300 | -0.00036500 |
| H | -2.98935900 | 0.71163000  | -0.00019400 |
| H | -0.29437000 | -2.42983500 | 0.00022800  |
| N | 1.41143500  | 1.72697300  | 0.00020700  |
| H | 2.33208600  | 1.28259400  | 0.00029000  |
| C | -0.93786900 | 1.29018300  | -0.00011200 |
| H | -1.11693100 | 2.35958400  | -0.00007800 |
| C | 1.91506500  | -1.10989800 | -0.00001800 |
| H | 1.83942400  | -2.19691100 | -0.00028700 |
| H | 2.46253700  | -0.78924100 | -0.89076600 |
| H | 2.46188800  | -0.78961800 | 0.89128500  |

**Heptane**

PCM(MP2 (full) /6-31G\*), E = -357.89184103

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51324500 | -1.36591500 | 0.00007700  |
| N | -1.75660800 | -0.98765600 | 0.00013200  |
| C | -1.95434600 | 0.38476100  | -0.00000900 |
| C | 0.44119600  | 0.86903000  | 0.00000300  |
| N | 0.57818400  | -0.53954200 | -0.00018600 |
| H | -2.99378300 | 0.70454300  | -0.00005400 |
| H | -0.28343000 | -2.43094600 | 0.00013700  |
| N | 1.40744200  | 1.72879000  | 0.00017200  |
| H | 2.32952600  | 1.28595700  | 0.00021100  |
| C | -0.94302700 | 1.28785700  | -0.00015400 |
| H | -1.12775200 | 2.35752500  | -0.00020700 |
| C | 1.91898200  | -1.10441600 | -0.00005100 |
| H | 1.84622800  | -2.19163100 | -0.00036000 |
| H | 2.46450900  | -0.78202800 | -0.89127100 |
| H | 2.46421500  | -0.78246700 | 0.89151600  |

SMD(MP2 (full) /6-31G\*), E = -357.89958154

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50773300 | -1.36689800 | 0.00003700  |
| N | -1.75150600 | -0.99127600 | 0.00007900  |
| C | -1.95576200 | 0.37833700  | -0.00000400 |
| C | 0.43722400  | 0.87004500  | -0.00001600 |
| N | 0.57959700  | -0.53699300 | -0.00009800 |
| H | -2.99582900 | 0.69303700  | -0.00001000 |
| H | -0.27125200 | -2.42854100 | 0.00007200  |
| N | 1.40067700  | 1.73287000  | 0.00009600  |
| H | 2.32159400  | 1.28895800  | 0.00018000  |
| C | -0.94773500 | 1.28484600  | -0.00008800 |
| H | -1.13600300 | 2.35306400  | -0.00010700 |
| C | 1.92266800  | -1.09897000 | -0.00002800 |
| H | 1.85156700  | -2.18629500 | -0.00027700 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 2.46838800 | -0.77810800 | -0.89149500 |
| H | 2.46818300 | -0.77847800 | 0.89170000  |

**Benzene**

PCM(MP2 (full)/6-31G\*), E = -357.89301648

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.51304000 | -1.36557600 | -0.00006200 |
| N | -1.75692200 | -0.98747700 | -0.00003900 |
| C | -1.95399300 | 0.38478500  | 0.00006400  |
| C | 0.44123000  | 0.86891400  | -0.00005200 |
| N | 0.57773800  | -0.53905800 | -0.00010600 |
| H | -2.99350500 | 0.70500800  | 0.00013800  |
| H | -0.28410000 | -2.43091000 | -0.00010800 |
| N | 1.40789500  | 1.72873300  | -0.00007000 |
| H | 2.32981100  | 1.28541900  | -0.00007800 |
| C | -0.94246000 | 1.28799200  | 0.00006300  |
| H | -1.12834500 | 2.35775200  | 0.00018200  |
| C | 1.91879700  | -1.10513400 | 0.00012900  |
| H | 1.84437400  | -2.19216500 | -0.00015000 |
| H | 2.46400700  | -0.78300100 | -0.89126000 |
| H | 2.46357300  | -0.78337600 | 0.89192600  |

SMD(MP2 (full)/6-31G\*), E = -357.90148613

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50582200 | -1.36713700 | 0.00003600  |
| N | -1.75032700 | -0.99259100 | 0.00007700  |
| C | -1.95638600 | 0.37657700  | -0.00000300 |
| C | 0.43589500  | 0.87029400  | -0.00001600 |
| N | 0.57995200  | -0.53605800 | -0.00009500 |
| H | -2.99677800 | 0.69046500  | -0.00000700 |
| H | -0.26768300 | -2.42826700 | 0.00006800  |
| N | 1.39929800  | 1.73354400  | 0.00009300  |
| H | 2.31995100  | 1.28901600  | 0.00017700  |
| C | -0.94928100 | 1.28406900  | -0.00008700 |
| H | -1.13950100 | 2.35204800  | -0.00010500 |
| C | 1.92392800  | -1.09723000 | -0.00002700 |
| H | 1.85350400  | -2.18459300 | -0.00026900 |
| H | 2.46912000  | -0.77600100 | -0.89162400 |
| H | 2.46892200  | -0.77636100 | 0.89182300  |

**Diethyl Ether**

PCM(MP2 (full)/6-31G\*), E = -357.89686432

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50976300 | -1.36630700 | -0.00007900 |
| N | -1.75515100 | -0.98947400 | -0.00006900 |
| C | -1.95518000 | 0.38239400  | 0.00007900  |
| C | 0.43919800  | 0.86910800  | -0.00004600 |
| N | 0.57811600  | -0.53751800 | -0.00010000 |
| H | -2.99569400 | 0.70208300  | 0.00015400  |
| H | -0.27877100 | -2.43194800 | -0.00016800 |
| N | 1.40603200  | 1.72963000  | -0.00011300 |
| H | 2.32943900  | 1.28832700  | -0.00014700 |
| C | -0.94473200 | 1.28686800  | 0.00009600  |
| H | -1.13446600 | 2.35685400  | 0.00024000  |
| C | 1.92061000  | -1.10276900 | 0.00016000  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 1.84667000 | -2.18984700 | -0.00012000 |
| H | 2.46476400 | -0.77966800 | -0.89143900 |
| H | 2.46428500 | -0.78003700 | 0.89219400  |

SMD(MP2(full)/6-31G\*), E = -357.90492224

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50129300 | -1.36744200 | 0.00003600  |
| N | -1.74826300 | -0.99577100 | 0.00005200  |
| C | -1.95794800 | 0.37276800  | 0.00000300  |
| C | 0.43279600  | 0.87077200  | -0.00000700 |
| N | 0.58064400  | -0.53375600 | -0.00004300 |
| H | -2.99885600 | 0.68566200  | 0.00001000  |
| H | -0.25969600 | -2.42754500 | 0.00004500  |
| N | 1.39700200  | 1.73455800  | 0.00007600  |
| H | 2.31624700  | 1.28685100  | 0.00016500  |
| C | -0.95276600 | 1.28251200  | -0.00008600 |
| H | -1.14851100 | 2.34975400  | -0.00011700 |
| C | 1.92715400  | -1.09344700 | -0.00003800 |
| H | 1.85752900  | -2.18071100 | -0.00025800 |
| H | 2.47002400  | -0.76993800 | -0.89194400 |
| H | 2.46992100  | -0.77026900 | 0.89205300  |

### Chloroform

PCM(MP2(full)/6-31G\*), E = -357.89746233

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50927100 | -1.36646000 | -0.00014200 |
| N | -1.75487500 | -0.98975300 | -0.00014500 |
| C | -1.95535300 | 0.38205600  | 0.00011500  |
| C | 0.43892200  | 0.86912500  | -0.00004700 |
| N | 0.57816400  | -0.53731000 | -0.00007100 |
| H | -2.99601300 | 0.70172800  | 0.00022500  |
| H | -0.27789600 | -2.43218300 | -0.00026100 |
| N | 1.40571300  | 1.72981100  | -0.00022000 |
| H | 2.32966500  | 1.28928900  | -0.00030500 |
| C | -0.94505200 | 1.28670500  | 0.00018600  |
| H | -1.13543400 | 2.35672600  | 0.00039000  |
| C | 1.92085200  | -1.10249500 | 0.00023800  |
| H | 1.84690600  | -2.18957800 | -0.00007100 |
| H | 2.46487100  | -0.77919700 | -0.89135400 |
| H | 2.46431000  | -0.77960200 | 0.89233000  |

SMD(MP2(full)/6-31G\*), E = -357.90544757

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50095500 | -1.36727300 | 0.00002000  |
| N | -1.74836700 | -0.99607600 | -0.00002000 |
| C | -1.95787400 | 0.37262000  | -0.00008400 |
| C | 0.43245800  | 0.87079100  | 0.00001200  |
| N | 0.58059300  | -0.53350400 | -0.00001500 |
| H | -2.99860700 | 0.68579200  | -0.00012500 |
| H | -0.25969900 | -2.42734500 | 0.00004400  |
| N | 1.39698900  | 1.73439500  | 0.00013400  |
| H | 2.31585900  | 1.28593500  | 0.00026300  |
| C | -0.95283900 | 1.28240000  | -0.00013200 |
| H | -1.14910500 | 2.34955000  | -0.00017700 |
| C | 1.92742000  | -1.09317500 | 0.00004400  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 1.85791800 | -2.18041300 | -0.00016900 |
| H | 2.47002100 | -0.76954400 | -0.89191600 |
| H | 2.46985300 | -0.76985900 | 0.89222300  |

**Aniline**

PCM(MP2(full)/6-31G\*), E = -357.89873076

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50821400 | -1.36670800 | -0.00011900 |
| N | -1.75430000 | -0.99038100 | -0.00012400 |
| C | -1.95574400 | 0.38130300  | 0.00010700  |
| C | 0.43827200  | 0.86917800  | -0.00004200 |
| N | 0.57827800  | -0.53681800 | -0.00007500 |
| H | -2.99674100 | 0.70084200  | 0.00020600  |
| H | -0.27622800 | -2.43257700 | -0.00025400 |
| N | 1.40513800  | 1.73006700  | -0.00018700 |
| H | 2.32954400  | 1.29019800  | -0.00026100 |
| C | -0.94578000 | 1.28634000  | 0.00015200  |
| H | -1.13745400 | 2.35643300  | 0.00033200  |
| C | 1.92142600  | -1.10171400 | 0.00021100  |
| H | 1.84762700  | -2.18881800 | -0.00008100 |
| H | 2.46510300  | -0.77808500 | -0.89145100 |
| H | 2.46457700  | -0.77846800 | 0.89234300  |

SMD(MP2(full)/6-31G\*), E = -357.90383521

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50078000 | -1.36675500 | 0.00001400  |
| N | -1.74898600 | -0.99569300 | 0.00003100  |
| C | -1.95715100 | 0.37274800  | -0.00000400 |
| C | 0.43225000  | 0.87053400  | 0.00000400  |
| N | 0.57969600  | -0.53296600 | -0.00001300 |
| H | -2.99744400 | 0.68758000  | -0.00000700 |
| H | -0.26092600 | -2.42701400 | 0.00001800  |
| N | 1.39836700  | 1.73295300  | 0.00003600  |
| H | 2.31584600  | 1.28141500  | 0.00008100  |
| C | -0.95218800 | 1.28276000  | -0.00004100 |
| H | -1.15052800 | 2.34948100  | -0.00006900 |
| C | 1.92704500  | -1.09309200 | -0.00002400 |
| H | 1.85746700  | -2.18026100 | -0.00013700 |
| H | 2.46852100  | -0.76912200 | -0.89230500 |
| H | 2.46847800  | -0.76930400 | 0.89235000  |

**THF**

PCM(MP2(full)/6-31G\*), E = -357.89907580

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50803200 | -1.36681800 | -0.00018200 |
| N | -1.75421000 | -0.99045700 | -0.00018700 |
| C | -1.95581100 | 0.38121300  | 0.00014200  |
| C | 0.43817500  | 0.86915200  | -0.00005400 |
| N | 0.57826400  | -0.53676000 | -0.00006100 |
| H | -2.99686700 | 0.70082000  | 0.00028100  |
| H | -0.27587100 | -2.43275900 | -0.00034000 |
| N | 1.40503000  | 1.73010900  | -0.00028000 |
| H | 2.32983600  | 1.29080900  | -0.00040400 |
| C | -0.94588100 | 1.28629300  | 0.00023400  |
| H | -1.13784400 | 2.35641600  | 0.00047900  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.92151200 | -1.10161400 | 0.00029100  |
| H | 1.84769700 | -2.18872400 | -0.00001000 |
| H | 2.46514800 | -0.77788300 | -0.89134800 |
| H | 2.46453200 | -0.77827000 | 0.89245700  |

SMD(MP2(full)/6-31G\*), E = -357.90637453

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49856700 | -1.36769700 | 0.00003800  |
| N | -1.74678800 | -0.99746700 | 0.00005600  |
| C | -1.95882200 | 0.37046800  | 0.00000100  |
| C | 0.43095400  | 0.87095900  | -0.00000800 |
| N | 0.58096700  | -0.53245400 | -0.00004600 |
| H | -2.99999100 | 0.68264200  | 0.00000600  |
| H | -0.25454500 | -2.42698400 | 0.00005000  |
| N | 1.39550200  | 1.73504800  | 0.00008000  |
| H | 2.31414500  | 1.28597100  | 0.00017100  |
| C | -0.95482700 | 1.28150800  | -0.00008800 |
| H | -1.15362500 | 2.34826500  | -0.00011900 |
| C | 1.92884900  | -1.09105600 | -0.00004000 |
| H | 1.85986300  | -2.17824300 | -0.00026200 |
| H | 2.47048200  | -0.76614600 | -0.89193400 |
| H | 2.47037500  | -0.76648000 | 0.89204300  |

### Methylene Chloride

PCM(MP2(full)/6-31G\*), E = -357.89960877

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50760800 | -1.36689400 | -0.00003500 |
| N | -1.75397300 | -0.99071700 | -0.00009500 |
| C | -1.95593800 | 0.38090000  | 0.00003700  |
| C | 0.43799300  | 0.86919700  | -0.00002100 |
| N | 0.57834800  | -0.53659900 | -0.00005700 |
| H | -2.99712700 | 0.70039600  | 0.00003400  |
| H | -0.27503100 | -2.43289800 | -0.00010100 |
| N | 1.40466200  | 1.73041900  | -0.00012700 |
| H | 2.33009200  | 1.29204100  | -0.00020200 |
| C | -0.94614900 | 1.28614500  | 0.00014300  |
| H | -1.13857200 | 2.35628500  | 0.00025700  |
| C | 1.92166500  | -1.10154100 | 0.00012200  |
| H | 1.84775800  | -2.18864800 | -0.00012100 |
| H | 2.46511300  | -0.77770500 | -0.89158600 |
| H | 2.46473300  | -0.77803700 | 0.89219400  |

SMD(MP2(full)/6-31G\*), E = -357.90822883

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49808100 | -1.36769600 | 0.00003900  |
| N | -1.74679300 | -0.99792300 | 0.00005900  |
| C | -1.95905800 | 0.37016800  | 0.00000000  |
| C | 0.43054700  | 0.87100200  | -0.00000800 |
| N | 0.58105600  | -0.53220800 | -0.00004900 |
| H | -3.00017400 | 0.68240100  | 0.00000400  |
| H | -0.25406600 | -2.42691600 | 0.00005400  |
| N | 1.39530800  | 1.73511400  | 0.00008400  |
| H | 2.31367500  | 1.28542900  | 0.00017700  |
| C | -0.95515900 | 1.28131800  | -0.00009100 |
| H | -1.15451200 | 2.34801500  | -0.00012400 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.92946000 | -1.09065500 | -0.00004200 |
| H | 1.86050300 | -2.17781200 | -0.00026200 |
| H | 2.47071600 | -0.76524700 | -0.89193900 |
| H | 2.47060900 | -0.76557800 | 0.89204400  |

**Dichloroethane**

PCM(MP2 (full)/6-31G\*), E = -357.89994701

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50734100 | -1.36700000 | -0.00018800 |
| N | -1.75382700 | -0.99085100 | -0.00019400 |
| C | -1.95604500 | 0.38073200  | 0.00014300  |
| C | 0.43780500  | 0.86919100  | -0.00005300 |
| N | 0.57834700  | -0.53647400 | -0.00006600 |
| H | -2.99732200 | 0.70027000  | 0.00027500  |
| H | -0.27469100 | -2.43306300 | -0.00034400 |
| N | 1.40457900  | 1.73041400  | -0.00029400 |
| H | 2.33002600  | 1.29209300  | -0.00042400 |
| C | -0.94632700 | 1.28605500  | 0.00025100  |
| H | -1.13915400 | 2.35622500  | 0.00050500  |
| C | 1.92182900  | -1.10126700 | 0.00030200  |
| H | 1.84799800  | -2.18839100 | -0.00000600 |
| H | 2.46529100  | -0.77731700 | -0.89134600 |
| H | 2.46464600  | -0.77771300 | 0.89250000  |

SMD(MP2 (full)/6-31G\*), E = -357.90762131

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49893100 | -1.36747700 | 0.00001600  |
| N | -1.74769400 | -0.99692600 | 0.00003200  |
| C | -1.95851100 | 0.37105200  | -0.00000300 |
| C | 0.43107200  | 0.87063600  | 0.00000500  |
| N | 0.58025900  | -0.53231400 | -0.00001700 |
| H | -2.99923200 | 0.68468000  | -0.00000900 |
| H | -0.25649600 | -2.42705000 | 0.00001700  |
| N | 1.39681800  | 1.73397900  | 0.00003800  |
| H | 2.31439500  | 1.28248100  | 0.00008500  |
| C | -0.95400000 | 1.28195200  | -0.00004400 |
| H | -1.15351700 | 2.34848200  | -0.00007300 |
| C | 1.92890700  | -1.09147800 | -0.00002400 |
| H | 1.85920200  | -2.17849000 | -0.00015800 |
| H | 2.46940000  | -0.76558800 | -0.89203800 |
| H | 2.46934000  | -0.76579800 | 0.89210300  |

**Acetone**

PCM(MP2 (full)/6-31G\*), E = -357.90122543

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50666100 | -1.36716900 | -0.00039700 |
| N | -1.75365200 | -0.99107000 | -0.00046000 |
| C | -1.95608900 | 0.38042000  | 0.00021000  |
| C | 0.43753400  | 0.86912200  | -0.00014900 |
| N | 0.57815300  | -0.53608100 | 0.00023300  |
| H | -2.99754900 | 0.70034800  | 0.00057800  |
| H | -0.27425600 | -2.43362200 | -0.00058100 |
| N | 1.40445900  | 1.73052600  | -0.00062400 |
| H | 2.33056800  | 1.29296700  | -0.00085200 |
| C | -0.94646200 | 1.28597000  | 0.00054000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.14102100 | 2.35611100  | 0.00106000  |
| C | 1.92210600  | -1.10119200 | 0.00048500  |
| H | 1.84751100  | -2.18824300 | 0.00069700  |
| H | 2.46481200  | -0.77724700 | -0.89155900 |
| H | 2.46464800  | -0.77684200 | 0.89249100  |

SMD(MP2(full)/6-31G\*), E = -357.900886483

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49760400 | -1.36758100 | 0.00001900  |
| N | -1.74712200 | -0.99773100 | 0.00003500  |
| C | -1.95895000 | 0.36994400  | -0.00000500 |
| C | 0.43023300  | 0.87073700  | 0.00000600  |
| N | 0.58035000  | -0.53164900 | -0.00001700 |
| H | -2.99987300 | 0.68344000  | -0.00001400 |
| H | -0.25413100 | -2.42687800 | 0.00002300  |
| N | 1.39635800  | 1.73413500  | 0.00004100  |
| H | 2.31350400  | 1.28157300  | 0.00009200  |
| C | -0.95499500 | 1.28156500  | -0.00004600 |
| H | -1.15659000 | 2.34783000  | -0.00007800 |
| C | 1.92976800  | -1.09039100 | -0.00002800 |
| H | 1.86021500  | -2.17739700 | -0.00017100 |
| H | 2.46956100  | -0.76363500 | -0.89207300 |
| H | 2.46950100  | -0.76386000 | 0.89213600  |

### Ethanol

PCM(MP2(full)/6-31G\*), E = -357.90148274

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50602000 | -1.36728400 | -0.00008100 |
| N | -1.75306400 | -0.99165300 | -0.00008600 |
| C | -1.95650400 | 0.37974600  | 0.00006000  |
| C | 0.43714600  | 0.86931000  | -0.00005000 |
| N | 0.57859900  | -0.53595400 | -0.00010400 |
| H | -2.99820000 | 0.69898300  | 0.00007600  |
| H | -0.27230600 | -2.43355300 | -0.00010900 |
| N | 1.40351800  | 1.73117900  | -0.00013300 |
| H | 2.33047500  | 1.29509800  | -0.00024200 |
| C | -0.94722200 | 1.28555800  | 0.00016200  |
| H | -1.14156500 | 2.35577100  | 0.00028300  |
| C | 1.92244000  | -1.10073100 | 0.00016800  |
| H | 1.84854800  | -2.18786200 | -0.00000200 |
| H | 2.46555300  | -0.77641300 | -0.89154100 |
| H | 2.46508800  | -0.77662500 | 0.89225000  |

SMD(MP2(full)/6-31G\*), E = -357.90634054

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49897500 | -1.36643300 | 0.00002300  |
| N | -1.74912800 | -0.99695000 | 0.00004100  |
| C | -1.95757100 | 0.37165300  | -0.00000900 |
| C | 0.43098200  | 0.87061400  | 0.00000500  |
| N | 0.57954400  | -0.53185800 | -0.00002000 |
| H | -2.99779500 | 0.68731100  | -0.00002000 |
| H | -0.25905500 | -2.42660800 | 0.00003400  |
| N | 1.39869800  | 1.73238000  | 0.00005000  |
| H | 2.31460000  | 1.27728800  | 0.00010200  |
| C | -0.95319200 | 1.28245500  | -0.00005200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.15528000 | 2.34869400  | -0.00008900 |
| C | 1.92850600  | -1.09177700 | -0.00003400 |
| H | 1.85879000  | -2.17884200 | -0.00016500 |
| H | 2.46824200  | -0.76585300 | -0.89247200 |
| H | 2.46819500  | -0.76606100 | 0.89250900  |

### Methanol

PCM(MP2(full)/6-31G\*), E = -357.90183720

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50588800 | -1.36726500 | 0.00000800  |
| N | -1.75305900 | -0.99170100 | 0.00004900  |
| C | -1.95659400 | 0.37970600  | 0.00003200  |
| C | 0.43717000  | 0.86932700  | -0.00003300 |
| N | 0.57860300  | -0.53585400 | -0.00011300 |
| H | -2.99830900 | 0.69916700  | 0.00005100  |
| H | -0.27204200 | -2.43358800 | 0.00001100  |
| N | 1.40348800  | 1.73131300  | 0.00009100  |
| H | 2.33113300  | 1.29601200  | -0.00006200 |
| C | -0.94726800 | 1.28545600  | -0.00007200 |
| H | -1.14188700 | 2.35570600  | -0.00006500 |
| C | 1.92242200  | -1.10093200 | 0.00002400  |
| H | 1.84818900  | -2.18802800 | -0.00013600 |
| H | 2.46543700  | -0.77656500 | -0.89172200 |
| H | 2.46520900  | -0.77675600 | 0.89198500  |

SMD(MP2(full)/6-31G\*), E = -357.90591810

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49909100 | -1.36620900 | 0.00002500  |
| N | -1.74950300 | -0.99688000 | 0.00004300  |
| C | -1.95736900 | 0.37189500  | -0.00001000 |
| C | 0.43103000  | 0.87058100  | 0.00000500  |
| N | 0.57937400  | -0.53181900 | -0.00002200 |
| H | -2.99745100 | 0.68801200  | -0.00002200 |
| H | -0.25975800 | -2.42652000 | 0.00003800  |
| N | 1.39918300  | 1.73198100  | 0.00005300  |
| H | 2.31471800  | 1.27612400  | 0.00010600  |
| C | -0.95293900 | 1.28260400  | -0.00005400 |
| H | -1.15537500 | 2.34879100  | -0.00009400 |
| C | 1.92838500  | -1.09193100 | -0.00003600 |
| H | 1.85857800  | -2.17897900 | -0.00016900 |
| H | 2.46792900  | -0.76591000 | -0.89253200 |
| H | 2.46788200  | -0.76612200 | 0.89256700  |

### Acetonitrile

PCM(MP2(full)/6-31G\*), E = -357.90186178

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50571900 | -1.36734800 | -0.00007000 |
| N | -1.75289700 | -0.99182700 | -0.00007600 |
| C | -1.95660700 | 0.37953200  | 0.00005000  |
| C | 0.43700000  | 0.86933500  | -0.00004900 |
| N | 0.57864600  | -0.53583000 | -0.00010800 |
| H | -2.99840100 | 0.69872800  | 0.00005000  |
| H | -0.27178000 | -2.43367400 | -0.00008700 |
| N | 1.40330400  | 1.73134100  | -0.00011800 |
| H | 2.33059600  | 1.29576200  | -0.00023000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.94741600 | 1.28544800  | 0.00015700  |
| H | -1.14212900 | 2.35567600  | 0.00026600  |
| C | 1.92256400  | -1.10061900 | 0.00015500  |
| H | 1.84864200  | -2.18775100 | -0.00000600 |
| H | 2.46561500  | -0.77620800 | -0.89155300 |
| H | 2.46516300  | -0.77640800 | 0.89222500  |

SMD(MP2(full)/6-31G\*), E = -357.90895103

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49722600 | -1.36754400 | 0.00002100  |
| N | -1.74708300 | -0.99791700 | 0.00003700  |
| C | -1.95907000 | 0.36973200  | -0.00000600 |
| C | 0.42995100  | 0.87069200  | 0.00000700  |
| N | 0.58028200  | -0.53143400 | -0.00001800 |
| H | -2.99991600 | 0.68335000  | -0.00001700 |
| H | -0.25354900 | -2.42671700 | 0.00002600  |
| N | 1.39642100  | 1.73390500  | 0.00004400  |
| H | 2.31322200  | 1.28060500  | 0.00009700  |
| C | -0.95519500 | 1.28148000  | -0.00004900 |
| H | -1.15733700 | 2.34761700  | -0.00008300 |
| C | 1.93005500  | -1.09004900 | -0.00003000 |
| H | 1.86043200  | -2.17697500 | -0.00018000 |
| H | 2.46938600  | -0.76269200 | -0.89202400 |
| H | 2.46932400  | -0.76292800 | 0.89208900  |

#### DMSO

PCM(MP2(full)/6-31G\*), E = -357.90194898

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50624100 | -1.36727600 | -0.00061400 |
| N | -1.75348700 | -0.99123900 | -0.00068200 |
| C | -1.95617400 | 0.38019000  | 0.00035100  |
| C | 0.43734500  | 0.86911300  | -0.00025300 |
| N | 0.57810400  | -0.53587400 | 0.00025000  |
| H | -2.99776800 | 0.70023400  | 0.00098600  |
| H | -0.27379100 | -2.43390100 | -0.00105800 |
| N | 1.40432200  | 1.73065200  | -0.00095900 |
| H | 2.33078200  | 1.29359900  | -0.00126800 |
| C | -0.94662900 | 1.28587100  | 0.00080700  |
| H | -1.14199100 | 2.35602500  | 0.00168500  |
| C | 1.92226000  | -1.10107800 | 0.00080500  |
| H | 1.84744000  | -2.18811800 | 0.00111200  |
| H | 2.46495000  | -0.77707600 | -0.89120000 |
| H | 2.46444300  | -0.77645200 | 0.89290300  |

SMD(MP2(full)/6-31G\*), E = -357.90683874

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49693300 | -1.36753300 | 0.00002100  |
| N | -1.74665200 | -0.99786500 | 0.00003600  |
| C | -1.95888100 | 0.36937000  | -0.00000700 |
| C | 0.42981600  | 0.87069300  | 0.00000600  |
| N | 0.58017600  | -0.53125800 | -0.00001600 |
| H | -2.99979900 | 0.68289200  | -0.00001700 |
| H | -0.25269300 | -2.42652800 | 0.00002700  |
| N | 1.39628500  | 1.73379900  | 0.00004300  |
| H | 2.31310700  | 1.28056400  | 0.00009600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.95535200 | 1.28140700  | -0.00004700 |
| H | -1.15806200 | 2.34741700  | -0.00008000 |
| C | 1.92970500  | -1.08971800 | -0.00003000 |
| H | 1.86041100  | -2.17669000 | -0.00017800 |
| H | 2.46914600  | -0.76273300 | -0.89205900 |
| H | 2.46908900  | -0.76296600 | 0.89212000  |

### Water

PCM(MP2(full)/6-31G\*), E = -357.90250528

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50588900  | -1.36722600 | -0.00002300 |
| N | 1.75332700  | -0.99147500 | -0.00011000 |
| C | 1.95634100  | 0.37989700  | -0.00002400 |
| C | -0.43749900 | 0.86924400  | 0.00006500  |
| N | -0.57834200 | -0.53580100 | -0.00020700 |
| H | 2.99795700  | 0.70010600  | -0.00048100 |
| H | 0.27272900  | -2.43382100 | 0.00016500  |
| N | -1.40356700 | 1.73172000  | -0.00019700 |
| H | -2.33232200 | 1.29765000  | -0.00046400 |
| C | 0.94678600  | 1.28550400  | 0.00038400  |
| H | 1.14252500  | 2.35566700  | 0.00026200  |
| C | -1.92227400 | -1.10191000 | 0.00014300  |
| H | -1.84658100 | -2.18888100 | 0.00036100  |
| H | -2.46459300 | -0.77729700 | 0.89213000  |
| H | -2.46510500 | -0.77758800 | -0.89163700 |

SMD(MP2(full)/6-31G\*), E = -357.90625337

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49980800 | -1.36524100 | -0.00016400 |
| N | -1.75130600 | -0.99675500 | -0.00017800 |
| C | -1.95624300 | 0.37297200  | 0.00021500  |
| C | 0.43142400  | 0.87085400  | 0.00002100  |
| N | 0.57879200  | -0.53187800 | 0.00012700  |
| H | -2.99573900 | 0.69124900  | 0.00033700  |
| H | -0.26372300 | -2.42643100 | -0.00056100 |
| N | 1.40087500  | 1.73092700  | -0.00018200 |
| H | 2.31542900  | 1.27305900  | -0.00046700 |
| C | -0.95173400 | 1.28323100  | 0.00003900  |
| H | -1.15569700 | 2.34932900  | 0.00002700  |
| C | 1.92782200  | -1.09302700 | 0.00018000  |
| H | 1.85783200  | -2.18019100 | 0.00047800  |
| H | 2.46723900  | -0.76813500 | -0.89296800 |
| H | 2.46736200  | -0.76766500 | 0.89304400  |

### ITS-Structure of 3-Methyl-4-Pyrimidinimine

#### Gas Phase

MP2(full)/6-31G\*, E = -357.84917495

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.59657400  | -1.34374800 | -0.01599200 |
| C | 1.93157200  | 0.47991100  | 0.01213300  |
| C | 0.86593000  | 1.33213800  | 0.02644000  |
| C | -0.49914700 | 0.85699400  | 0.01800700  |
| H | 0.43872000  | -2.42077100 | -0.04589400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.94985900  | 0.86239700  | 0.02059200  |
| H | 1.00696500  | 2.40791000  | 0.03382700  |
| N | -0.52775200 | -0.58111700 | 0.02682600  |
| N | 1.82141700  | -0.88876100 | -0.01900400 |
| N | -1.56155700 | 1.53129700  | -0.12348300 |
| H | -2.27610700 | 1.97134900  | 0.41921500  |
| C | -1.84709600 | -1.19654300 | 0.01605300  |
| H | -1.73611300 | -2.27579200 | -0.09030000 |
| H | -2.37321300 | -0.96744200 | 0.94483800  |
| H | -2.42186600 | -0.78009700 | -0.81249300 |

### Heptane

PCM(MP2 (full)/6-31G\*), E = -357.85392471

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.59207500  | -1.34522100 | -0.01788700 |
| C | 1.93321600  | 0.47677200  | 0.01372200  |
| C | 0.86864100  | 1.33058600  | 0.02857500  |
| C | -0.49673500 | 0.85769500  | 0.01583900  |
| H | 0.43204300  | -2.42260100 | -0.04811100 |
| H | 2.95278300  | 0.85837100  | 0.02431400  |
| H | 1.01391900  | 2.40681700  | 0.03896800  |
| N | -0.52855700 | -0.57912700 | 0.02487900  |
| N | 1.81910100  | -0.89174900 | -0.02006200 |
| N | -1.56005700 | 1.53390600  | -0.12857300 |
| H | -2.26186300 | 1.97699300  | 0.43596000  |
| C | -1.84952700 | -1.19412000 | 0.01947200  |
| H | -1.73838600 | -2.27464300 | -0.07182300 |
| H | -2.37536600 | -0.95093800 | 0.94454700  |
| H | -2.42256400 | -0.78948700 | -0.81589000 |

SMD(MP2 (full)/6-31G\*), E = -357.86120821

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58662500  | -1.34717600 | -0.01749300 |
| C | 1.93512800  | 0.47064600  | 0.01296600  |
| C | 0.87317100  | 1.32760800  | 0.02881600  |
| C | -0.49206600 | 0.85731500  | 0.01765000  |
| H | 0.41920300  | -2.42177800 | -0.04866400 |
| H | 2.95550300  | 0.84766700  | 0.02173800  |
| H | 1.02038600  | 2.40272000  | 0.03754900  |
| N | -0.53006200 | -0.57638900 | 0.02664700  |
| N | 1.81347800  | -0.89513600 | -0.02013400 |
| N | -1.55455800 | 1.53790400  | -0.13123900 |
| H | -2.24529200 | 1.97481200  | 0.44860300  |
| C | -1.85301200 | -1.18694600 | 0.01844700  |
| H | -1.74455600 | -2.26925300 | -0.05021800 |
| H | -2.38863400 | -0.92678700 | 0.93312500  |
| H | -2.41768200 | -0.80071200 | -0.83135800 |

### Benzene

PCM(MP2 (full)/6-31G\*), E = -357.85496555

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.59108300  | -1.34561300 | -0.01841900 |
| C | 1.93355400  | 0.47605800  | 0.01415400  |
| C | 0.86917600  | 1.33020700  | 0.02936100  |
| C | -0.49617700 | 0.85779800  | 0.01536300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.43049500  | -2.42309300 | -0.04872800 |
| H | 2.95340300  | 0.85745300  | 0.02537300  |
| H | 1.01537800  | 2.40652000  | 0.04086900  |
| N | -0.52871300 | -0.57864800 | 0.02434400  |
| N | 1.81851300  | -0.89233700 | -0.02053900 |
| N | -1.55975100 | 1.53455400  | -0.13024100 |
| H | -2.25802200 | 1.97775400  | 0.44045300  |
| C | -1.85002900 | -1.19353700 | 0.02051200  |
| H | -1.73886900 | -2.27421700 | -0.06880900 |
| H | -2.37507800 | -0.94837600 | 0.94546900  |
| H | -2.42329100 | -0.79049600 | -0.81540600 |

SMD(MP2(full)/6-31G\*), E = -357.90148613

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.50582200 | -1.36713700 | 0.00003600  |
| N | -1.75032700 | -0.99259100 | 0.00007700  |
| C | -1.95638600 | 0.37657700  | -0.00000300 |
| C | 0.43589500  | 0.87029400  | -0.00001600 |
| N | 0.57995200  | -0.53605800 | -0.00009500 |
| H | -2.99677800 | 0.69046500  | -0.00000700 |
| H | -0.26768300 | -2.42826700 | 0.00006800  |
| N | 1.39929800  | 1.73354400  | 0.00009300  |
| H | 2.31995100  | 1.28901600  | 0.00017700  |
| C | -0.94928100 | 1.28406900  | -0.00008700 |
| H | -1.13950100 | 2.35204800  | -0.00010500 |
| C | 1.92392800  | -1.09723000 | -0.00002700 |
| H | 1.85350400  | -2.18459300 | -0.00026900 |
| H | 2.46912000  | -0.77600100 | -0.89162400 |
| H | 2.46892200  | -0.77636100 | 0.89182300  |

### Diethyl Ether

PCM(MP2(full)/6-31G\*), E = -357.85843976

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58774000  | -1.34683700 | -0.01961200 |
| C | 1.93476600  | 0.47362400  | 0.01521800  |
| C | 0.87114200  | 1.32899600  | 0.03061100  |
| C | -0.49426400 | 0.85817500  | 0.01364600  |
| H | 0.42531500  | -2.42473500 | -0.04983800 |
| H | 2.95556200  | 0.85448500  | 0.02802700  |
| H | 1.02053900  | 2.40564700  | 0.04438900  |
| N | -0.52933800 | -0.57708500 | 0.02277000  |
| N | 1.81667100  | -0.89453700 | -0.02106400 |
| N | -1.55866600 | 1.53667400  | -0.13394600 |
| H | -2.24584400 | 1.98047900  | 0.45567800  |
| C | -1.85188500 | -1.19149300 | 0.02281600  |
| H | -1.74049200 | -2.27309500 | -0.05368700 |
| H | -2.37744200 | -0.93442100 | 0.94403600  |
| H | -2.42328900 | -0.79851200 | -0.81900000 |

SMD(MP2(full)/6-31G\*), E = -357.86518953

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57911200  | -1.34874900 | -0.01889000 |
| C | 1.93729200  | 0.46403000  | 0.01437400  |
| C | 0.87714700  | 1.32405900  | 0.03057400  |
| C | -0.48751500 | 0.85747000  | 0.01559300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.40578700  | -2.42203400 | -0.04956600 |
| H | 2.95864500  | 0.83882700  | 0.02488000  |
| H | 1.03051100  | 2.39850400  | 0.04222800  |
| N | -0.53240900 | -0.57198000 | 0.02423900  |
| N | 1.80912900  | -0.90032800 | -0.02086600 |
| N | -1.55061500 | 1.54596500  | -0.13831700 |
| H | -2.21245400 | 1.97637800  | 0.48324800  |
| C | -1.85720600 | -1.18336600 | 0.02149900  |
| H | -1.74586700 | -2.26632600 | -0.02209100 |
| H | -2.39542600 | -0.90232100 | 0.92797600  |
| H | -2.41691700 | -0.81929700 | -0.84097100 |

### Chloroform

PCM(MP2 (full)/6-31G\*), E = -357.85898335

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58726300  | -1.34713600 | -0.01987800 |
| C | 1.93492600  | 0.47328000  | 0.01542800  |
| C | 0.87138000  | 1.32881000  | 0.03108900  |
| C | -0.49393800 | 0.85814400  | 0.01341300  |
| H | 0.42447300  | -2.42510900 | -0.05016000 |
| H | 2.95585600  | 0.85407500  | 0.02852000  |
| H | 1.02120500  | 2.40550900  | 0.04549000  |
| N | -0.52938100 | -0.57685600 | 0.02259300  |
| N | 1.81633900  | -0.89478100 | -0.02138500 |
| N | -1.55852100 | 1.53694800  | -0.13493500 |
| H | -2.24362300 | 1.98054000  | 0.45825300  |
| C | -1.85216500 | -1.19104400 | 0.02335500  |
| H | -1.74079700 | -2.27276300 | -0.05159800 |
| H | -2.37754800 | -0.93247400 | 0.94422300  |
| H | -2.42342900 | -0.79926600 | -0.81908700 |

SMD(MP2 (full)/6-31G\*), E = -357.86553666

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57850100  | -1.34868500 | -0.01902800 |
| C | 1.93724000  | 0.46356000  | 0.01449200  |
| C | 0.87721300  | 1.32373100  | 0.03089000  |
| C | -0.48711500 | 0.85747900  | 0.01530500  |
| H | 0.40522900  | -2.42187400 | -0.04939600 |
| H | 2.95846900  | 0.83841900  | 0.02520500  |
| H | 1.03109400  | 2.39807600  | 0.04303400  |
| N | -0.53259300 | -0.57152200 | 0.02412100  |
| N | 1.80899800  | -0.90082000 | -0.02108800 |
| N | -1.55034300 | 1.54680900  | -0.13919200 |
| H | -2.20870500 | 1.97625500  | 0.48715900  |
| C | -1.85750300 | -1.18333400 | 0.02181900  |
| H | -1.74560900 | -2.26638200 | -0.01679400 |
| H | -2.39691700 | -0.89847400 | 0.92630000  |
| H | -2.41601500 | -0.82379100 | -0.84326400 |

### Aniline

PCM(MP2 (full)/6-31G\*), E = -357.86016426

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.58607000 | -1.34750100 | -0.02046700 |
| C | 1.93533000 | 0.47238100  | 0.01594800  |
| C | 0.87203100 | 1.32835100  | 0.03173800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.49327400 | 0.85829200  | 0.01272600  |
| H | 0.42270100  | -2.42564400 | -0.05073700 |
| H | 2.95659600  | 0.85299600  | 0.02983200  |
| H | 1.02303300  | 2.40514600  | 0.04729500  |
| N | -0.52962200 | -0.57624600 | 0.02191000  |
| N | 1.81568300  | -0.89555600 | -0.02175800 |
| N | -1.55816500 | 1.53778000  | -0.13660200 |
| H | -2.23890900 | 1.98106900  | 0.46403900  |
| C | -1.85277400 | -1.19038700 | 0.02445600  |
| H | -1.74126000 | -2.27237400 | -0.04615600 |
| H | -2.37799700 | -0.92777400 | 0.94421100  |
| H | -2.42373500 | -0.80208500 | -0.81974400 |

SMD(MP2(full)/6-31G\*), E = -357.86348339

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57646600  | -1.34872900 | -0.01962800 |
| C | 1.93721600  | 0.46179800  | 0.01516400  |
| C | 0.87775700  | 1.32261800  | 0.03165300  |
| C | -0.48575300 | 0.85724300  | 0.01447800  |
| H | 0.40210800  | -2.42151400 | -0.04957300 |
| H | 2.95847300  | 0.83651100  | 0.02667800  |
| H | 1.03351200  | 2.39672300  | 0.04508600  |
| N | -0.53300700 | -0.57004400 | 0.02329700  |
| N | 1.80789700  | -0.90199600 | -0.02165900 |
| N | -1.54962700 | 1.54872600  | -0.14186900 |
| H | -2.19720800 | 1.97454900  | 0.49931900  |
| C | -1.85803800 | -1.18223800 | 0.02307100  |
| H | -1.74566900 | -2.26553100 | -0.00462900 |
| H | -2.39931500 | -0.88896000 | 0.92358600  |
| H | -2.41462500 | -0.83273000 | -0.84727500 |

### THF

PCM(MP2(full)/6-31G\*), E = -357.86048317

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58565300  | -1.34768700 | -0.02044500 |
| C | 1.93549200  | 0.47202200  | 0.01595700  |
| C | 0.87231000  | 1.32816500  | 0.03186300  |
| C | -0.49300300 | 0.85831300  | 0.01262700  |
| H | 0.42191100  | -2.42586500 | -0.05063500 |
| H | 2.95688500  | 0.85246600  | 0.02986000  |
| H | 1.02366300  | 2.40497600  | 0.04761000  |
| N | -0.52973900 | -0.57606200 | 0.02187300  |
| N | 1.81538000  | -0.89583100 | -0.02183900 |
| N | -1.55790800 | 1.53815800  | -0.13696700 |
| H | -2.23733400 | 1.98135400  | 0.46578200  |
| C | -1.85304800 | -1.19008700 | 0.02454300  |
| H | -1.74155800 | -2.27213600 | -0.04506000 |
| H | -2.37843300 | -0.92647900 | 0.94390100  |
| H | -2.42369000 | -0.80252800 | -0.82020600 |

SMD(MP2(full)/6-31G\*), E = -357.86609804

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.57550700 | -1.34954300 | -0.01957200 |
| C | 1.93830100 | 0.46072100  | 0.01501800  |
| C | 0.87901100 | 1.32225300  | 0.03167300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.48508700 | 0.85727100  | 0.01477900  |
| H | 0.39908100  | -2.42198400 | -0.05001500 |
| H | 2.96005100  | 0.83436300  | 0.02619400  |
| H | 1.03521900  | 2.39629400  | 0.04489300  |
| N | -0.53346200 | -0.56979200 | 0.02312900  |
| N | 1.80680500  | -0.90263700 | -0.02143300 |
| N | -1.54880700 | 1.54952300  | -0.14206600 |
| H | -2.19547300 | 1.97553300  | 0.50015400  |
| C | -1.85920800 | -1.18112800 | 0.02307000  |
| H | -1.74711200 | -2.26415600 | -0.01176700 |
| H | -2.39743900 | -0.89233900 | 0.92684500  |
| H | -2.41723100 | -0.82482000 | -0.84352500 |

### Methylene Chloride

PCM(MP2 (full)/6-31G\*), E = -357.86095877

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58530200  | -1.34792600 | -0.02063600 |
| C | 1.93560800  | 0.47177900  | 0.01611900  |
| C | 0.87244300  | 1.32803500  | 0.03200800  |
| C | -0.49274600 | 0.85825000  | 0.01236500  |
| H | 0.42119700  | -2.42617900 | -0.05084200 |
| H | 2.95708300  | 0.85227400  | 0.03026600  |
| H | 1.02411100  | 2.40490500  | 0.04812500  |
| N | -0.52974400 | -0.57584200 | 0.02154300  |
| N | 1.81516200  | -0.89600600 | -0.02184200 |
| N | -1.55792500 | 1.53835000  | -0.13760500 |
| H | -2.23513400 | 1.98102200  | 0.46890200  |
| C | -1.85323900 | -1.18972700 | 0.02491000  |
| H | -1.74166800 | -2.27186600 | -0.04325800 |
| H | -2.37844900 | -0.92477200 | 0.94394900  |
| H | -2.42380700 | -0.80336800 | -0.82040300 |

SMD(MP2 (full)/6-31G\*), E = -357.86780539

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57460900  | -1.34966500 | -0.01962800 |
| C | 1.93856500  | 0.45992600  | 0.01508500  |
| C | 0.87939600  | 1.32178500  | 0.03185600  |
| C | -0.48451900 | 0.85731200  | 0.01442900  |
| H | 0.39787900  | -2.42198100 | -0.04961700 |
| H | 2.96033400  | 0.83336200  | 0.02644100  |
| H | 1.03627600  | 2.39572100  | 0.04554900  |
| N | -0.53386900 | -0.56923600 | 0.02272000  |
| N | 1.80645100  | -0.90339900 | -0.02145700 |
| N | -1.54826000 | 1.55099600  | -0.14281200 |
| H | -2.19073100 | 1.97571800  | 0.50500100  |
| C | -1.85991700 | -1.18101500 | 0.02335200  |
| H | -1.74713800 | -2.26403000 | -0.00800500 |
| H | -2.39850200 | -0.88937000 | 0.92592400  |
| H | -2.41717700 | -0.82800100 | -0.84502300 |

### Dichloroethane

PCM(MP2 (full)/6-31G\*), E = -357.86129458

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.58483400 | -1.34801800 | -0.02073300 |
| C | 1.93577600 | 0.47138700  | 0.01623200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.87275400  | 1.32783600  | 0.03223700  |
| C | -0.49249900 | 0.85835300  | 0.01218900  |
| H | 0.42055700  | -2.42632200 | -0.05084700 |
| H | 2.95739900  | 0.85169800  | 0.03057500  |
| H | 1.02488000  | 2.40471400  | 0.04870300  |
| N | -0.52989500 | -0.57563600 | 0.02145000  |
| N | 1.81488000  | -0.89634000 | -0.02203800 |
| N | -1.55765700 | 1.53875200  | -0.13807400 |
| H | -2.23370000 | 1.98147700  | 0.47033200  |
| C | -1.85350200 | -1.18952300 | 0.02516500  |
| H | -1.74193200 | -2.27174800 | -0.04148100 |
| H | -2.37888900 | -0.92314600 | 0.94367500  |
| H | -2.42378700 | -0.80431300 | -0.82085900 |

SMD(MP2(full)/6-31G\*), E = -357.86711244

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57416300  | -1.34972800 | -0.01965600 |
| C | 1.93861700  | 0.45953200  | 0.01517300  |
| C | 0.87955800  | 1.32155000  | 0.03187800  |
| C | -0.48418600 | 0.85719600  | 0.01426500  |
| H | 0.39700400  | -2.42190400 | -0.04947700 |
| H | 2.96038700  | 0.83289600  | 0.02661800  |
| H | 1.03678600  | 2.39541800  | 0.04573000  |
| N | -0.53393800 | -0.56892200 | 0.02246600  |
| N | 1.80614000  | -0.90361200 | -0.02145100 |
| N | -1.54813300 | 1.55131800  | -0.14318800 |
| H | -2.18834100 | 1.97508800  | 0.50772400  |
| C | -1.86005300 | -1.18066300 | 0.02350300  |
| H | -1.74721200 | -2.26367800 | -0.00644600 |
| H | -2.39868300 | -0.88776500 | 0.92558500  |
| H | -2.41702500 | -0.82886100 | -0.84550500 |

### Acetone

PCM(MP2(full)/6-31G\*), E = -357.86249000

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58359400  | -1.34849600 | -0.02169300 |
| C | 1.93618400  | 0.47040200  | 0.01701500  |
| C | 0.87337500  | 1.32731300  | 0.03304500  |
| C | -0.49173400 | 0.85838800  | 0.01129500  |
| H | 0.41845800  | -2.42698200 | -0.05213900 |
| H | 2.95814600  | 0.85050100  | 0.03259900  |
| H | 1.02665500  | 2.40427600  | 0.05102300  |
| N | -0.53013500 | -0.57495400 | 0.02059400  |
| N | 1.81411100  | -0.89708600 | -0.02250500 |
| N | -1.55727800 | 1.53973300  | -0.14023200 |
| H | -2.22787600 | 1.98131700  | 0.47728300  |
| C | -1.85415700 | -1.18869900 | 0.02671000  |
| H | -1.74243900 | -2.27115900 | -0.03572500 |
| H | -2.37881900 | -0.91835500 | 0.94442300  |
| H | -2.42457800 | -0.80689800 | -0.82069300 |

SMD(MP2(full)/6-31G\*), E = -357.86808709

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.57191700 | -1.35019400 | -0.01990300 |
| C | 1.93929200 | 0.45740000  | 0.01555400  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.88068800  | 1.32035200  | 0.03221000  |
| C | -0.48273000 | 0.85702000  | 0.01351500  |
| H | 0.39300300  | -2.42197900 | -0.04903500 |
| H | 2.96142200  | 0.83006600  | 0.02744900  |
| H | 1.03975800  | 2.39402700  | 0.04698400  |
| N | -0.53474800 | -0.56752300 | 0.02126700  |
| N | 1.80472600  | -0.90509700 | -0.02149500 |
| N | -1.54699900 | 1.55422000  | -0.14505300 |
| H | -2.17675200 | 1.97424000  | 0.51961700  |
| C | -1.86134600 | -1.17956900 | 0.02434100  |
| H | -1.74785600 | -2.26260400 | -0.00049000 |
| H | -2.39962200 | -0.88226900 | 0.92512000  |
| H | -2.41773000 | -0.83273400 | -0.84698300 |

### Ethanol

PCM(MP2 (full)/6-31G\*), E = -357.86270820

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58373300  | -1.34873100 | -0.02064300 |
| C | 1.93614100  | 0.47061000  | 0.01633500  |
| C | 0.87320500  | 1.32742100  | 0.03222300  |
| C | -0.49170700 | 0.85821300  | 0.01153400  |
| H | 0.41856600  | -2.42730700 | -0.05030500 |
| H | 2.95804800  | 0.85102500  | 0.03085900  |
| H | 1.02638500  | 2.40446300  | 0.04938600  |
| N | -0.52995100 | -0.57497900 | 0.02052300  |
| N | 1.81418900  | -0.89691600 | -0.02175000 |
| N | -1.55771400 | 1.53940500  | -0.13936600 |
| H | -2.22662800 | 1.98046800  | 0.48073800  |
| C | -1.85411700 | -1.18844300 | 0.02553700  |
| H | -1.74236500 | -2.27090500 | -0.03715000 |
| H | -2.37940400 | -0.91832500 | 0.94292900  |
| H | -2.42379400 | -0.80641600 | -0.82223300 |

SMD(MP2 (full)/6-31G\*), E = -357.86530839

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57224600  | -1.34916000 | -0.02038000 |
| C | 1.93815200  | 0.45795700  | 0.01630700  |
| C | 0.87925800  | 1.32029400  | 0.03215700  |
| C | -0.48316800 | 0.85695800  | 0.01209500  |
| H | 0.39579700  | -2.42141500 | -0.04857300 |
| H | 2.95972600  | 0.83196800  | 0.02974200  |
| H | 1.03854600  | 2.39398700  | 0.04805700  |
| N | -0.53467100 | -0.56714700 | 0.02018200  |
| N | 1.80592200  | -0.90502600 | -0.02165200 |
| N | -1.54786900 | 1.55522600  | -0.14588400 |
| H | -2.17127800 | 1.97166400  | 0.52749400  |
| C | -1.86050300 | -1.18125100 | 0.02523300  |
| H | -1.74539600 | -2.26445000 | 0.01545700  |
| H | -2.40250700 | -0.87315800 | 0.92008400  |
| H | -2.41448200 | -0.84875600 | -0.85324100 |

### Methanol

PCM(MP2 (full)/6-31G\*), E = -357.86300862

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.58308800 | -1.34867100 | -0.02239900 |
|---|------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.93629400  | 0.46997700  | 0.01761200  |
| C | 0.87354800  | 1.32707500  | 0.03378000  |
| C | -0.49139000 | 0.85829800  | 0.01087400  |
| H | 0.41718300  | -2.42720300 | -0.05317700 |
| H | 2.95837200  | 0.85003200  | 0.03402200  |
| H | 1.02729100  | 2.40406700  | 0.05274000  |
| N | -0.53021700 | -0.57457000 | 0.02042400  |
| N | 1.81380700  | -0.89739400 | -0.02317300 |
| N | -1.55708900 | 1.54023200  | -0.14176200 |
| H | -2.22522100 | 1.98085100  | 0.48006500  |
| C | -1.85438200 | -1.18836300 | 0.02776200  |
| H | -1.74235100 | -2.27098500 | -0.03114600 |
| H | -2.37920900 | -0.91498200 | 0.94443800  |
| H | -2.42451200 | -0.80954500 | -0.82114800 |

SMD(MP2(full)/6-31G\*), E = -357.86478779

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57192700  | -1.34902400 | -0.02055400 |
| C | 1.93805000  | 0.45770000  | 0.01658600  |
| C | 0.87912700  | 1.32006800  | 0.03212900  |
| C | -0.48299400 | 0.85688300  | 0.01155500  |
| H | 0.39567600  | -2.42129600 | -0.04845800 |
| H | 2.95954500  | 0.83187200  | 0.03056500  |
| H | 1.03873200  | 2.39371900  | 0.04844800  |
| N | -0.53479900 | -0.56680600 | 0.01961400  |
| N | 1.80594100  | -0.90526400 | -0.02163300 |
| N | -1.54792800 | 1.55596800  | -0.14639400 |
| H | -2.16753000 | 1.97053800  | 0.53199000  |
| C | -1.86059100 | -1.18140500 | 0.02562100  |
| H | -1.74495300 | -2.26457500 | 0.02029200  |
| H | -2.40320400 | -0.86983500 | 0.91884900  |
| H | -2.41387800 | -0.85304100 | -0.85482200 |

### Acetonitrile

PCM(MP2(full)/6-31G\*), E = -357.86306744

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58327300  | -1.34885500 | -0.02135700 |
| C | 1.93629700  | 0.47021300  | 0.01683100  |
| C | 0.87347200  | 1.32721800  | 0.03281600  |
| C | -0.49143200 | 0.85824800  | 0.01117000  |
| H | 0.41775200  | -2.42747500 | -0.05140200 |
| H | 2.95833500  | 0.85047700  | 0.03214100  |
| H | 1.02706800  | 2.40427200  | 0.05076500  |
| N | -0.53007500 | -0.57473800 | 0.02035800  |
| N | 1.81389700  | -0.89721700 | -0.02221400 |
| N | -1.55744100 | 1.53979400  | -0.14045500 |
| H | -2.22509500 | 1.98059700  | 0.48185100  |
| C | -1.85437300 | -1.18816200 | 0.02647600  |
| H | -1.74255900 | -2.27076900 | -0.03345500 |
| H | -2.37970900 | -0.91556100 | 0.94307500  |
| H | -2.42387900 | -0.80838900 | -0.82241400 |

SMD(MP2(full)/6-31G\*), E = -357.86803258

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.57100600 | -1.35034300 | -0.01995300 |
|---|------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.93952400  | 0.45656600  | 0.01569500  |
| C | 0.88103000  | 1.31985400  | 0.03229000  |
| C | -0.48208000 | 0.85685300  | 0.01311600  |
| H | 0.39144700  | -2.42190800 | -0.04867600 |
| H | 2.96166000  | 0.82903800  | 0.02781700  |
| H | 1.04073500  | 2.39339800  | 0.04749200  |
| N | -0.53504900 | -0.56690500 | 0.02070700  |
| N | 1.80421300  | -0.90568600 | -0.02146900 |
| N | -1.54666200 | 1.55535700  | -0.14587800 |
| H | -2.17102500 | 1.97322600  | 0.52574500  |
| C | -1.86191600 | -1.17911400 | 0.02466200  |
| H | -1.74797000 | -2.26208900 | 0.00257800  |
| H | -2.40004600 | -0.87924500 | 0.92456300  |
| H | -2.41770700 | -0.83468200 | -0.84789200 |

### DMSO

PCM(MP2 (full)/6-31G\*), E = -357.86318639

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58291000  | -1.34880600 | -0.02187200 |
| C | 1.93641700  | 0.46987200  | 0.01721500  |
| C | 0.87373100  | 1.32703300  | 0.03339200  |
| C | -0.49128700 | 0.85839400  | 0.01091900  |
| H | 0.41738500  | -2.42742100 | -0.05214500 |
| H | 2.95857800  | 0.84987200  | 0.03317300  |
| H | 1.02767300  | 2.40405300  | 0.05204800  |
| N | -0.53025000 | -0.57459400 | 0.02025900  |
| N | 1.81367700  | -0.89749300 | -0.02273000 |
| N | -1.55709900 | 1.54019400  | -0.14122500 |
| H | -2.22455000 | 1.98117200  | 0.48146400  |
| C | -1.85455500 | -1.18814700 | 0.02720600  |
| H | -1.74279800 | -2.27077800 | -0.03218000 |
| H | -2.37942200 | -0.91499500 | 0.94392500  |
| H | -2.42446000 | -0.80872900 | -0.82157800 |

SMD(MP2 (full)/6-31G\*), E = -357.86589119

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57080300  | -1.35037700 | -0.02000900 |
| C | 1.93939900  | 0.45635900  | 0.01580300  |
| C | 0.88111600  | 1.31973700  | 0.03231900  |
| C | -0.48184800 | 0.85666400  | 0.01315000  |
| H | 0.39072000  | -2.42179300 | -0.04877800 |
| H | 2.96158800  | 0.82879100  | 0.02791000  |
| H | 1.04106900  | 2.39325500  | 0.04750200  |
| N | -0.53489700 | -0.56674500 | 0.02067200  |
| N | 1.80383500  | -0.90555900 | -0.02155600 |
| N | -1.54667300 | 1.55491500  | -0.14606300 |
| H | -2.17059600 | 1.97240500  | 0.52622100  |
| C | -1.86162500 | -1.17848500 | 0.02476100  |
| H | -1.74832000 | -2.26155200 | 0.00288300  |
| H | -2.39987100 | -0.87853500 | 0.92457000  |
| H | -2.41751600 | -0.83424200 | -0.84782000 |

### Water

PCM(MP2 (full)/6-31G\*), E = -357.86356290

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58184000  | -1.34882200 | -0.02179000 |
| C | 1.93671300  | 0.46879200  | 0.01726600  |
| C | 0.87433400  | 1.32649300  | 0.03326800  |
| C | -0.49072400 | 0.85848800  | 0.01083300  |
| H | 0.41480400  | -2.42737800 | -0.05198300 |
| H | 2.95913600  | 0.84823900  | 0.03327000  |
| H | 1.02908600  | 2.40345000  | 0.05207700  |
| N | -0.53072200 | -0.57385800 | 0.02010200  |
| N | 1.81292600  | -0.89828800 | -0.02266000 |
| N | -1.55632800 | 1.54180200  | -0.14175200 |
| H | -2.22059000 | 1.98135000  | 0.48598000  |
| C | -1.85489400 | -1.18805900 | 0.02719800  |
| H | -1.74246300 | -2.27059500 | -0.03175600 |
| H | -2.37983900 | -0.91463500 | 0.94378700  |
| H | -2.42488500 | -0.80936800 | -0.82184600 |

SMD (MP2 (full) /6-31G\*), E = -357.86485627

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.57140400  | -1.34810100 | -0.02149100 |
| C | 1.93719900  | 0.45734700  | 0.01791700  |
| C | 0.87807100  | 1.31947600  | 0.03183000  |
| C | -0.48291700 | 0.85694900  | 0.00918600  |
| H | 0.39748800  | -2.42082100 | -0.04860500 |
| H | 2.95833300  | 0.83247700  | 0.03463700  |
| H | 1.03854500  | 2.39312900  | 0.04974600  |
| N | -0.53520900 | -0.56585800 | 0.01737100  |
| N | 1.80675700  | -0.90596400 | -0.02152500 |
| N | -1.54837100 | 1.55888800  | -0.14785500 |
| H | -2.15545900 | 1.96663300  | 0.54696300  |
| C | -1.86046500 | -1.18297400 | 0.02727100  |
| H | -1.74287400 | -2.26600400 | 0.04227300  |
| H | -2.40694800 | -0.85675100 | 0.91285800  |
| H | -2.41107300 | -0.87429800 | -0.86209000 |

### SOSP-Structure of 3-Methyl-4-Pyrimidinimine

#### Gas Phase

MP2 (full) /6-31G\*, E = -357.84727986

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34592700 | 0.59453000  | 0.00000000 |
| C | -1.10853300 | -1.65355900 | 0.00000000 |
| C | 0.24953300  | -1.57597100 | 0.00000000 |
| C | 0.94900700  | -0.30090900 | 0.00000000 |
| H | -1.95118800 | 1.50038200  | 0.00000000 |
| H | -1.60767500 | -2.62002100 | 0.00000000 |
| H | 0.86407800  | -2.47020500 | 0.00000000 |
| N | 0.00000000  | 0.79011800  | 0.00000000 |
| N | -1.95078400 | -0.56097200 | 0.00000000 |
| N | 2.17567600  | -0.09258000 | 0.00000000 |
| H | 3.15045000  | 0.08076800  | 0.00000000 |
| C | 0.56293700  | 2.12967300  | 0.00000000 |
| H | -0.24919100 | 2.85712000  | 0.00000000 |
| H | 1.18859000  | 2.26670500  | 0.88434000 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 1.18859000 | 2.26670500 | -0.88434000 |
|---|------------|------------|-------------|

### Heptane

PCM(MP2 (full)/6-31G\*), E = -357.85192403

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34456900 | 0.59755600  | 0.00000000  |
| C | -1.11025100 | -1.65332900 | 0.00000000  |
| C | 0.24778400  | -1.57726200 | 0.00000000  |
| C | 0.94952700  | -0.30293700 | 0.00000000  |
| H | -1.94961900 | 1.50444200  | 0.00000000  |
| H | -1.60993800 | -2.62054700 | 0.00000000  |
| H | 0.85965700  | -2.47455500 | 0.00000000  |
| N | 0.00000000  | 0.79007700  | 0.00000000  |
| N | -1.95145900 | -0.55883900 | 0.00000000  |
| N | 2.17611500  | -0.09380300 | 0.00000000  |
| H | 3.15677400  | 0.07257000  | 0.00000000  |
| C | 0.56402500  | 2.13027800  | 0.00000000  |
| H | -0.24782800 | 2.85795300  | 0.00000000  |
| H | 1.18963000  | 2.26613000  | 0.88445900  |
| H | 1.18963000  | 2.26613000  | -0.88445900 |

SMD(MP2 (full)/6-31G\*), E = -357.85898627

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34398300 | 0.59684300  | 0.00000000  |
| C | -1.10886900 | -1.65482900 | 0.00000000  |
| C | 0.24882000  | -1.57811000 | 0.00000000  |
| C | 0.94822200  | -0.30236400 | 0.00000000  |
| H | -1.94459200 | 1.50474300  | 0.00000000  |
| H | -1.60832400 | -2.62132900 | 0.00000000  |
| H | 0.86176400  | -2.47388600 | 0.00000000  |
| N | 0.00000000  | 0.78928400  | 0.00000000  |
| N | -1.94748300 | -0.56044600 | 0.00000000  |
| N | 2.17495600  | -0.09179900 | 0.00000000  |
| H | 3.15297200  | 0.07519200  | 0.00000000  |
| C | 0.56081300  | 2.13092600  | 0.00000000  |
| H | -0.25301600 | 2.85651600  | 0.00000000  |
| H | 1.18443500  | 2.27234200  | 0.88519200  |
| H | 1.18443500  | 2.27234200  | -0.88519200 |

### Benzene

PCM(MP2 (full)/6-31G\*), E = -357.85293152

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34431100 | 0.59810200  | 0.00000000 |
| C | -1.11049200 | -1.65338700 | 0.00000000 |
| C | 0.24752900  | -1.57753300 | 0.00000000 |
| C | 0.94963300  | -0.30325600 | 0.00000000 |
| H | -1.94933500 | 1.50521000  | 0.00000000 |
| H | -1.61027700 | -2.62078100 | 0.00000000 |
| H | 0.85890900  | -2.47542400 | 0.00000000 |
| N | 0.00000000  | 0.79003100  | 0.00000000 |
| N | -1.95153200 | -0.55850900 | 0.00000000 |
| N | 2.17620000  | -0.09388900 | 0.00000000 |
| H | 3.15818500  | 0.07095800  | 0.00000000 |
| C | 0.56406000  | 2.13045000  | 0.00000000 |
| H | -0.24787400 | 2.85801600  | 0.00000000 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 1.18960200 | 2.26616800 | 0.88450200  |
| H | 1.18960200 | 2.26616800 | -0.88450200 |

SMD (MP2 (full) /6-31G\*), E = -357.86047444

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34359900 | 0.59717000  | 0.00000000  |
| C | -1.10876700 | -1.65512300 | 0.00000000  |
| C | 0.24883700  | -1.57835400 | 0.00000000  |
| C | 0.94815600  | -0.30246500 | 0.00000000  |
| H | -1.94370900 | 1.50528700  | 0.00000000  |
| H | -1.60804600 | -2.62179000 | 0.00000000  |
| H | 0.86132400  | -2.47456100 | 0.00000000  |
| N | 0.00000000  | 0.78917500  | 0.00000000  |
| N | -1.94714500 | -0.56049200 | 0.00000000  |
| N | 2.17498600  | -0.09175900 | 0.00000000  |
| H | 3.15377100  | 0.07348800  | 0.00000000  |
| C | 0.56021300  | 2.13141500  | 0.00000000  |
| H | -0.25408700 | 2.85644800  | 0.00000000  |
| H | 1.18341000  | 2.27340400  | 0.88541000  |
| H | 1.18341000  | 2.27340400  | -0.88541000 |

**Diethyl Ether**

PCM (MP2 (full) /6-31G\*), E = -357.85631252

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34351500 | 0.60033000  | 0.00000000  |
| C | -1.11162700 | -1.65343900 | 0.00000000  |
| C | 0.24631900  | -1.57855000 | 0.00000000  |
| C | 0.94980200  | -0.30452500 | 0.00000000  |
| H | -1.94836300 | 1.50840000  | 0.00000000  |
| H | -1.61177900 | -2.62144300 | 0.00000000  |
| H | 0.85602200  | -2.47851300 | 0.00000000  |
| N | 0.00000000  | 0.79001100  | 0.00000000  |
| N | -1.95187000 | -0.55701800 | 0.00000000  |
| N | 2.17618700  | -0.09462400 | 0.00000000  |
| H | 3.16270000  | 0.06554500  | 0.00000000  |
| C | 0.56513600  | 2.13078700  | 0.00000000  |
| H | -0.24665800 | 2.85852600  | 0.00000000  |
| H | 1.19058200  | 2.26564500  | 0.88462400  |
| H | 1.19058200  | 2.26564500  | -0.88462400 |

SMD (MP2 (full) /6-31G\*), E = -357.86252636

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34246900 | 0.59815300  | 0.00000000 |
| C | -1.10860700 | -1.65570500 | 0.00000000 |
| C | 0.24893200  | -1.57878000 | 0.00000000 |
| C | 0.94842300  | -0.30282800 | 0.00000000 |
| H | -1.94196800 | 1.50653600  | 0.00000000 |
| H | -1.60684700 | -2.62311100 | 0.00000000 |
| H | 0.85956500  | -2.47653900 | 0.00000000 |
| N | 0.00000000  | 0.78904000  | 0.00000000 |
| N | -1.94722100 | -0.56055300 | 0.00000000 |
| N | 2.17571400  | -0.09240300 | 0.00000000 |
| H | 3.15670300  | 0.06793200  | 0.00000000 |
| C | 0.55860800  | 2.13338900  | 0.00000000 |
| H | -0.25747600 | 2.85613700  | 0.00000000 |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 1.18062500 | 2.27553800 | 0.88608800  |
| H | 1.18062500 | 2.27553800 | -0.88608800 |

**Chloroform**

PCM(MP2(full)/6-31G\*), E = -357.85683563

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34349300 | 0.60032400  | 0.00000000  |
| C | -1.11145800 | -1.65376500 | 0.00000000  |
| C | 0.24642500  | -1.57867300 | 0.00000000  |
| C | 0.94987200  | -0.30439900 | 0.00000000  |
| H | -1.94832500 | 1.50852500  | 0.00000000  |
| H | -1.61161000 | -2.62187800 | 0.00000000  |
| H | 0.85616700  | -2.47874600 | 0.00000000  |
| N | 0.00000000  | 0.78991200  | 0.00000000  |
| N | -1.95177300 | -0.55716400 | 0.00000000  |
| N | 2.17629800  | -0.09436000 | 0.00000000  |
| H | 3.16356300  | 0.06467900  | 0.00000000  |
| C | 0.56459900  | 2.13103500  | 0.00000000  |
| H | -0.24759300 | 2.85834900  | 0.00000000  |
| H | 1.19022700  | 2.26661000  | 0.88387000  |
| H | 1.19022700  | 2.26661000  | -0.88387000 |

SMD(MP2(full)/6-31G\*), E = -357.86281616

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34230000 | 0.59803100  | 0.00000000  |
| C | -1.10830900 | -1.65573100 | 0.00000000  |
| C | 0.24913800  | -1.57864900 | 0.00000000  |
| C | 0.94847700  | -0.30280500 | 0.00000000  |
| H | -1.94215900 | 1.50608300  | 0.00000000  |
| H | -1.60614300 | -2.62325200 | 0.00000000  |
| H | 0.85959000  | -2.47651900 | 0.00000000  |
| N | 0.00000000  | 0.78897100  | 0.00000000  |
| N | -1.94744600 | -0.56073000 | 0.00000000  |
| N | 2.17584300  | -0.09244900 | 0.00000000  |
| H | 3.15713500  | 0.06702100  | 0.00000000  |
| C | 0.55816300  | 2.13373400  | 0.00000000  |
| H | -0.25815200 | 2.85616000  | 0.00000000  |
| H | 1.17996600  | 2.27624400  | 0.88614000  |
| H | 1.17996600  | 2.27624400  | -0.88614000 |

**Aniline**

PCM(MP2(full)/6-31G\*), E = -357.85798601

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34314700 | 0.60146700  | 0.00000000 |
| C | -1.11220100 | -1.65345800 | 0.00000000 |
| C | 0.24571800  | -1.57907900 | 0.00000000 |
| C | 0.94989700  | -0.30517200 | 0.00000000 |
| H | -1.94789600 | 1.51007100  | 0.00000000 |
| H | -1.61255100 | -2.62176800 | 0.00000000 |
| H | 0.85455000  | -2.48009700 | 0.00000000 |
| N | 0.00000000  | 0.78999400  | 0.00000000 |
| N | -1.95203000 | -0.55625600 | 0.00000000 |
| N | 2.17620000  | -0.09497600 | 0.00000000 |
| H | 3.16507400  | 0.06283000  | 0.00000000 |
| C | 0.56566300  | 2.13093000  | 0.00000000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.24609400 | 2.85872800 | 0.00000000  |
| H | 1.19107900  | 2.26538700 | 0.88466900  |
| H | 1.19107900  | 2.26538700 | -0.88466900 |

SMD(MP2(full)/6-31G\*), E = -357.86060365

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34172100 | 0.59836700  | 0.00000000  |
| C | -1.10808300 | -1.65555500 | 0.00000000  |
| C | 0.24907100  | -1.57842900 | 0.00000000  |
| C | 0.94819500  | -0.30287000 | 0.00000000  |
| H | -1.94159300 | 1.50624300  | 0.00000000  |
| H | -1.60556900 | -2.62323800 | 0.00000000  |
| H | 0.85861800  | -2.47699200 | 0.00000000  |
| N | 0.00000000  | 0.78878000  | 0.00000000  |
| N | -1.94753000 | -0.56056600 | 0.00000000  |
| N | 2.17571700  | -0.09267600 | 0.00000000  |
| H | 3.15785400  | 0.06441000  | 0.00000000  |
| C | 0.55796700  | 2.13371700  | 0.00000000  |
| H | -0.25805900 | 2.85642600  | 0.00000000  |
| H | 1.17943300  | 2.27649700  | 0.88628000  |
| H | 1.17943300  | 2.27649700  | -0.88628000 |

**THF**

PCM(MP2(full)/6-31G\*), E = -357.85828999

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34307900 | 0.60157000  | 0.00000000  |
| C | -1.11221000 | -1.65348400 | 0.00000000  |
| C | 0.24572500  | -1.57915600 | 0.00000000  |
| C | 0.95002500  | -0.30525500 | 0.00000000  |
| H | -1.94778000 | 1.51027500  | 0.00000000  |
| H | -1.61258400 | -2.62185100 | 0.00000000  |
| H | 0.85432800  | -2.48040100 | 0.00000000  |
| N | 0.00000000  | 0.78993400  | 0.00000000  |
| N | -1.95203000 | -0.55622000 | 0.00000000  |
| N | 2.17634300  | -0.09489300 | 0.00000000  |
| H | 3.16569500  | 0.06228200  | 0.00000000  |
| C | 0.56539900  | 2.13101500  | 0.00000000  |
| H | -0.24651600 | 2.85862100  | 0.00000000  |
| H | 1.19075600  | 2.26559500  | 0.88469200  |
| H | 1.19075600  | 2.26559500  | -0.88469200 |

SMD(MP2(full)/6-31G\*), E = -357.86318530

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34188700 | 0.59889100  | 0.00000000 |
| C | -1.10862700 | -1.65608100 | 0.00000000 |
| C | 0.24880500  | -1.57911200 | 0.00000000 |
| C | 0.94814800  | -0.30294700 | 0.00000000 |
| H | -1.94050600 | 1.50760000  | 0.00000000 |
| H | -1.60642700 | -2.62375000 | 0.00000000 |
| H | 0.85852600  | -2.47755400 | 0.00000000 |
| N | 0.00000000  | 0.78894200  | 0.00000000 |
| N | -1.94693400 | -0.56044400 | 0.00000000 |
| N | 2.17569200  | -0.09254900 | 0.00000000 |
| H | 3.15793200  | 0.06473600  | 0.00000000 |
| C | 0.55821500  | 2.13408400  | 0.00000000 |



|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.25830800 | 2.85613600 | 0.00000000  |
| H | 1.17978100  | 2.27608900 | 0.88631200  |
| H | 1.17978100  | 2.27608900 | -0.88631200 |

**Methylene Chloride**

PCM(MP2(full)/6-31G\*), E = -357.85874659

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34297000 | 0.60207000  | 0.00000000  |
| C | -1.11259000 | -1.65325700 | 0.00000000  |
| C | 0.24536800  | -1.57935300 | 0.00000000  |
| C | 0.95024700  | -0.30574700 | 0.00000000  |
| H | -1.94748500 | 1.51106400  | 0.00000000  |
| H | -1.61297100 | -2.62173400 | 0.00000000  |
| H | 0.85348700  | -2.48107700 | 0.00000000  |
| N | 0.00000000  | 0.78985000  | 0.00000000  |
| N | -1.95221000 | -0.55580200 | 0.00000000  |
| N | 2.17637700  | -0.09506500 | 0.00000000  |
| H | 3.16631700  | 0.06187200  | 0.00000000  |
| C | 0.56587700  | 2.13088400  | 0.00000000  |
| H | -0.24592000 | 2.85867700  | 0.00000000  |
| H | 1.19090400  | 2.26536900  | 0.88490900  |
| H | 1.19090400  | 2.26536900  | -0.88490900 |

SMD(MP2(full)/6-31G\*), E = -357.86481255

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34180200 | 0.59879500  | 0.00000000  |
| C | -1.10836700 | -1.65631700 | 0.00000000  |
| C | 0.24906000  | -1.57914500 | 0.00000000  |
| C | 0.94829100  | -0.30290000 | 0.00000000  |
| H | -1.94068000 | 1.50728100  | 0.00000000  |
| H | -1.60572900 | -2.62418000 | 0.00000000  |
| H | 0.85865700  | -2.47769500 | 0.00000000  |
| N | 0.00000000  | 0.78895700  | 0.00000000  |
| N | -1.94708900 | -0.56072500 | 0.00000000  |
| N | 2.17595300  | -0.09261100 | 0.00000000  |
| H | 3.15855100  | 0.06379300  | 0.00000000  |
| C | 0.55761100  | 2.13474900  | 0.00000000  |
| H | -0.25944400 | 2.85613500  | 0.00000000  |
| H | 1.17891600  | 2.27711200  | 0.88642700  |
| H | 1.17891600  | 2.27711200  | -0.88642700 |

**Dichloroethane**

PCM(MP2(full)/6-31G\*), E = -357.85907397

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34290900 | 0.60216800  | 0.00000000 |
| C | -1.11254200 | -1.65342900 | 0.00000000 |
| C | 0.24538100  | -1.57941900 | 0.00000000 |
| C | 0.95013900  | -0.30563500 | 0.00000000 |
| H | -1.94749900 | 1.51118700  | 0.00000000 |
| H | -1.61301100 | -2.62194000 | 0.00000000 |
| H | 0.85350000  | -2.48121900 | 0.00000000 |
| N | 0.00000000  | 0.78993200  | 0.00000000 |
| N | -1.95213200 | -0.55578600 | 0.00000000 |
| N | 2.17640300  | -0.09516600 | 0.00000000 |
| H | 3.16688200  | 0.06095100  | 0.00000000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 0.56563800  | 2.13108300 | 0.00000000  |
| H | -0.24620300 | 2.85877500 | 0.00000000  |
| H | 1.19109700  | 2.26539100 | 0.88465500  |
| H | 1.19109700  | 2.26539100 | -0.88465500 |

SMD(MP2(full)/6-31G\*), E = -357.86408031

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34168700 | 0.59897100  | 0.00000000  |
| C | -1.10843400 | -1.65626900 | 0.00000000  |
| C | 0.24895200  | -1.57915200 | 0.00000000  |
| C | 0.94816600  | -0.30294200 | 0.00000000  |
| H | -1.94036400 | 1.50752400  | 0.00000000  |
| H | -1.60578600 | -2.62411400 | 0.00000000  |
| H | 0.85836800  | -2.47780200 | 0.00000000  |
| N | 0.00000000  | 0.78891500  | 0.00000000  |
| N | -1.94705400 | -0.56059700 | 0.00000000  |
| N | 2.17584900  | -0.09264000 | 0.00000000  |
| H | 3.15859700  | 0.06334400  | 0.00000000  |
| C | 0.55777000  | 2.13465100  | 0.00000000  |
| H | -0.25914300 | 2.85615200  | 0.00000000  |
| H | 1.17908100  | 2.27679700  | 0.88641100  |
| H | 1.17908100  | 2.27679700  | -0.88641100 |

### Acetone

PCM(MP2(full)/6-31G\*), E = -357.86022407

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34269900 | 0.60284200  | 0.00000000  |
| C | -1.11282100 | -1.65354800 | 0.00000000  |
| C | 0.24506900  | -1.57977000 | 0.00000000  |
| C | 0.95022300  | -0.30597800 | 0.00000000  |
| H | -1.94720200 | 1.51228100  | 0.00000000  |
| H | -1.61337300 | -2.62229900 | 0.00000000  |
| H | 0.85267400  | -2.48224100 | 0.00000000  |
| N | 0.00000000  | 0.78989900  | 0.00000000  |
| N | -1.95217200 | -0.55539900 | 0.00000000  |
| N | 2.17645600  | -0.09527300 | 0.00000000  |
| H | 3.16862800  | 0.05918500  | 0.00000000  |
| C | 0.56577600  | 2.13122800  | 0.00000000  |
| H | -0.24620700 | 2.85878900  | 0.00000000  |
| H | 1.19110000  | 2.26551900  | 0.88473500  |
| H | 1.19110000  | 2.26551900  | -0.88473500 |

SMD(MP2(full)/6-31G\*), E = -357.86487461

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34141600 | 0.59936400  | 0.00000000 |
| C | -1.10841400 | -1.65656400 | 0.00000000 |
| C | 0.24893800  | -1.57934800 | 0.00000000 |
| C | 0.94809600  | -0.30294100 | 0.00000000 |
| H | -1.93980400 | 1.50808500  | 0.00000000 |
| H | -1.60549500 | -2.62470700 | 0.00000000 |
| H | 0.85772300  | -2.47857200 | 0.00000000 |
| N | 0.00000000  | 0.78896700  | 0.00000000 |
| N | -1.94694500 | -0.56062600 | 0.00000000 |
| N | 2.17599900  | -0.09288200 | 0.00000000 |
| H | 3.15953300  | 0.06116600  | 0.00000000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 0.55741400  | 2.13525100 | 0.00000000  |
| H | -0.25982900 | 2.85634800 | 0.00000000  |
| H | 1.17839200  | 2.27744700 | 0.88666000  |
| H | 1.17839200  | 2.27744700 | -0.88666000 |

**Ethanol**

PCM(MP2(full)/6-31G\*), E = -357.86044838

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34268400 | 0.60321800  | 0.00000000  |
| C | -1.11304400 | -1.65338200 | 0.00000000  |
| C | 0.24481000  | -1.57987400 | 0.00000000  |
| C | 0.95032400  | -0.30624400 | 0.00000000  |
| H | -1.94693600 | 1.51295200  | 0.00000000  |
| H | -1.61365600 | -2.62214600 | 0.00000000  |
| H | 0.85217100  | -2.48259000 | 0.00000000  |
| N | 0.00000000  | 0.78997600  | 0.00000000  |
| N | -1.95226800 | -0.55503900 | 0.00000000  |
| N | 2.17654500  | -0.09569700 | 0.00000000  |
| H | 3.16907200  | 0.05816000  | 0.00000000  |
| C | 0.56597000  | 2.13118100  | 0.00000000  |
| H | -0.24583000 | 2.85891700  | 0.00000000  |
| H | 1.19149000  | 2.26531800  | 0.88460600  |
| H | 1.19149000  | 2.26531800  | -0.88460600 |

SMD(MP2(full)/6-31G\*), E = -357.86203697

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34113300 | 0.59849200  | 0.00000000  |
| C | -1.10736800 | -1.65621500 | 0.00000000  |
| C | 0.24966100  | -1.57839600 | 0.00000000  |
| C | 0.94841500  | -0.30261900 | 0.00000000  |
| H | -1.94167400 | 1.50590900  | 0.00000000  |
| H | -1.60357200 | -2.62471800 | 0.00000000  |
| H | 0.85802200  | -2.47800900 | 0.00000000  |
| N | 0.00000000  | 0.78888500  | 0.00000000  |
| N | -1.94801200 | -0.56120100 | 0.00000000  |
| N | 2.17650200  | -0.09319400 | 0.00000000  |
| H | 3.16033300  | 0.05940700  | 0.00000000  |
| C | 0.55624600  | 2.13564300  | 0.00000000  |
| H | -0.26110800 | 2.85670500  | 0.00000000  |
| H | 1.17681900  | 2.27892800  | 0.88681400  |
| H | 1.17681900  | 2.27892800  | -0.88681400 |

**Methanol**

PCM(MP2(full)/6-31G\*), E = -357.86074247

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34254600 | 0.60367100  | 0.00000000 |
| C | -1.11335500 | -1.65318800 | 0.00000000 |
| C | 0.24453700  | -1.58005000 | 0.00000000 |
| C | 0.95051600  | -0.30662400 | 0.00000000 |
| H | -1.94657800 | 1.51370300  | 0.00000000 |
| H | -1.61396800 | -2.62202100 | 0.00000000 |
| H | 0.85147300  | -2.48315200 | 0.00000000 |
| N | 0.00000000  | 0.78980800  | 0.00000000 |
| N | -1.95235100 | -0.55466900 | 0.00000000 |
| N | 2.17673400  | -0.09610300 | 0.00000000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 3.16969300  | 0.05763900 | 0.00000000  |
| C | 0.56619500  | 2.13140800 | 0.00000000  |
| H | -0.24587200 | 2.85890600 | 0.00000000  |
| H | 1.19124400  | 2.26519100 | 0.88492600  |
| H | 1.19124400  | 2.26519100 | -0.88492600 |

SMD(MP2(full)/6-31G\*), E = -357.86146635

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34103700 | 0.59837500  | 0.00000000  |
| C | -1.10715800 | -1.65620400 | 0.00000000  |
| C | 0.24981300  | -1.57823300 | 0.00000000  |
| C | 0.94847100  | -0.30254300 | 0.00000000  |
| H | -1.94196400 | 1.50554900  | 0.00000000  |
| H | -1.60310600 | -2.62482600 | 0.00000000  |
| H | 0.85800300  | -2.47798100 | 0.00000000  |
| N | 0.00000000  | 0.78888100  | 0.00000000  |
| N | -1.94824400 | -0.56133000 | 0.00000000  |
| N | 2.17663800  | -0.09328800 | 0.00000000  |
| H | 3.16065000  | 0.05870500  | 0.00000000  |
| C | 0.55596300  | 2.13584900  | 0.00000000  |
| H | -0.26150000 | 2.85677200  | 0.00000000  |
| H | 1.17642400  | 2.27923500  | 0.88686500  |
| H | 1.17642400  | 2.27923500  | -0.88686500 |

### Acetonitrile

PCM(MP2(full)/6-31G\*), E = -357.86079037

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34255300 | 0.60354600  | 0.00000000  |
| C | -1.11352400 | -1.65319300 | 0.00000000  |
| C | 0.24435900  | -1.58014700 | 0.00000000  |
| C | 0.95064700  | -0.30678100 | 0.00000000  |
| H | -1.94679500 | 1.51336700  | 0.00000000  |
| H | -1.61418900 | -2.62201400 | 0.00000000  |
| H | 0.85117200  | -2.48336700 | 0.00000000  |
| N | 0.00000000  | 0.78984800  | 0.00000000  |
| N | -1.95254700 | -0.55474900 | 0.00000000  |
| N | 2.17665500  | -0.09571500 | 0.00000000  |
| H | 3.16950000  | 0.05850700  | 0.00000000  |
| C | 0.56662400  | 2.13117800  | 0.00000000  |
| H | -0.24480900 | 2.85941000  | 0.00000000  |
| H | 1.19152500  | 2.26539200  | 0.88502900  |
| H | 1.19152500  | 2.26539200  | -0.88502900 |

SMD(MP2(full)/6-31G\*), E = -357.86472933

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.34129000 | 0.59952500  | 0.00000000 |
| C | -1.10841100 | -1.65664300 | 0.00000000 |
| C | 0.24892700  | -1.57938800 | 0.00000000 |
| C | 0.94803000  | -0.30295000 | 0.00000000 |
| H | -1.93955700 | 1.50823600  | 0.00000000 |
| H | -1.60527200 | -2.62485500 | 0.00000000 |
| H | 0.85748800  | -2.47872800 | 0.00000000 |
| N | 0.00000000  | 0.78895700  | 0.00000000 |
| N | -1.94701000 | -0.56061300 | 0.00000000 |
| N | 2.17602000  | -0.09295000 | 0.00000000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 3.15985300  | 0.06030100 | 0.00000000  |
| C | 0.55737900  | 2.13548100 | 0.00000000  |
| H | -0.25997600 | 2.85634400 | 0.00000000  |
| H | 1.17829200  | 2.27739600 | 0.88667600  |
| H | 1.17829200  | 2.27739600 | -0.88667600 |

**DMSO**

PCM(MP2 (full) /6-31G\*), E = -357.86091019

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.59405600 | -1.34650900 | 0.00005400  |
| C | -1.93376000 | 0.48412700  | 0.00000500  |
| C | -0.87534600 | 1.33803600  | -0.00019400 |
| C | 0.50128900  | 0.86337100  | -0.00009800 |
| H | -0.43444200 | -2.42703300 | 0.00013000  |
| H | -2.95409500 | 0.86919500  | 0.00006600  |
| H | -1.02801300 | 2.41542600  | -0.00030300 |
| N | 0.52847400  | -0.58684500 | -0.00006200 |
| N | -1.82230400 | -0.89376300 | 0.00011500  |
| N | 1.55401900  | 1.52656600  | 0.00038400  |
| H | 2.39453100  | 2.07741200  | -0.00060700 |
| C | 1.84664600  | -1.20494200 | -0.00009300 |
| H | 1.73013400  | -2.28895800 | -0.00207800 |
| H | 2.40151000  | -0.88452500 | -0.88395300 |
| H | 2.40040900  | -0.88772400 | 0.88564100  |

SMD(MP2 (full) /6-31G\*), E = -357.86257925

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34113300 | 0.59991100  | 0.00000000  |
| C | -1.10869600 | -1.65635100 | 0.00000000  |
| C | 0.24853700  | -1.57937300 | 0.00000000  |
| C | 0.94769500  | -0.30308700 | 0.00000000  |
| H | -1.93889200 | 1.50889400  | 0.00000000  |
| H | -1.60590700 | -2.62440800 | 0.00000000  |
| H | 0.85681100  | -2.47890800 | 0.00000000  |
| N | 0.00000000  | 0.78886200  | 0.00000000  |
| N | -1.94677800 | -0.56016900 | 0.00000000  |
| N | 2.17562700  | -0.09299700 | 0.00000000  |
| H | 3.15948500  | 0.06013100  | 0.00000000  |
| C | 0.55807400  | 2.13476800  | 0.00000000  |
| H | -0.25855000 | 2.85649100  | 0.00000000  |
| H | 1.17912600  | 2.27636100  | 0.88661200  |
| H | 1.17912600  | 2.27636100  | -0.88661200 |

**Water**

PCM(MP2 (full) /6-31G\*), E = -357.86126777

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.59338000  | -1.34672700 | 0.00025200  |
| C | 1.93393500  | 0.48348600  | -0.00015300 |
| C | 0.87585600  | 1.33775300  | -0.00027900 |
| C | -0.50096500 | 0.86354000  | 0.00011900  |
| H | 0.43253000  | -2.42725800 | 0.00011300  |
| H | 2.95447300  | 0.86815200  | -0.00022600 |
| H | 1.02917400  | 2.41510900  | -0.00049000 |
| N | -0.52879800 | -0.58652700 | -0.00016400 |
| N | 1.82178000  | -0.89433900 | 0.00023800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.55320300 | 1.52777000  | 0.00038200  |
| H | -2.39345400 | 2.07964300  | -0.00010100 |
| C | -1.84696800 | -1.20503600 | -0.00023500 |
| H | -1.72988600 | -2.28897800 | -0.00121400 |
| H | -2.40101300 | -0.88729900 | 0.88511500  |
| H | -2.40170800 | -0.88579000 | -0.88461100 |

SMD(MP2(full)/6-31G\*), E = -357.86139895

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.34076300 | 0.59722200  | 0.00000000  |
| C | -1.10571800 | -1.65615500 | 0.00000000  |
| C | 0.25092700  | -1.57733100 | 0.00000000  |
| C | 0.94909500  | -0.30214100 | 0.00000000  |
| H | -1.94433900 | 1.50283600  | 0.00000000  |
| H | -1.60040900 | -2.62543800 | 0.00000000  |
| H | 0.85860300  | -2.47769200 | 0.00000000  |
| N | 0.00000000  | 0.78886300  | 0.00000000  |
| N | -1.94940500 | -0.56235600 | 0.00000000  |
| N | 2.17754800  | -0.09367500 | 0.00000000  |
| H | 3.16211600  | 0.05634600  | 0.00000000  |
| C | 0.55384100  | 2.13702500  | 0.00000000  |
| H | -0.26437000 | 2.85728500  | 0.00000000  |
| H | 1.17354900  | 2.28255600  | 0.88722900  |
| H | 1.17354900  | 2.28255600  | -0.88722900 |