**Supporting Information**

# Iodine Bonding Stabilizes Iodomethane in MIDAS Pesticide. Theoretical Study of Intermolecular Interactions between Iodomethane and Chloropicrin

Rainer Glaser* and Kaitlan Prugger

Department of Chemistry, University of Missouri, Columbia, Missouri 65211

Email: glaserr@missouri.edu

Table of Contents

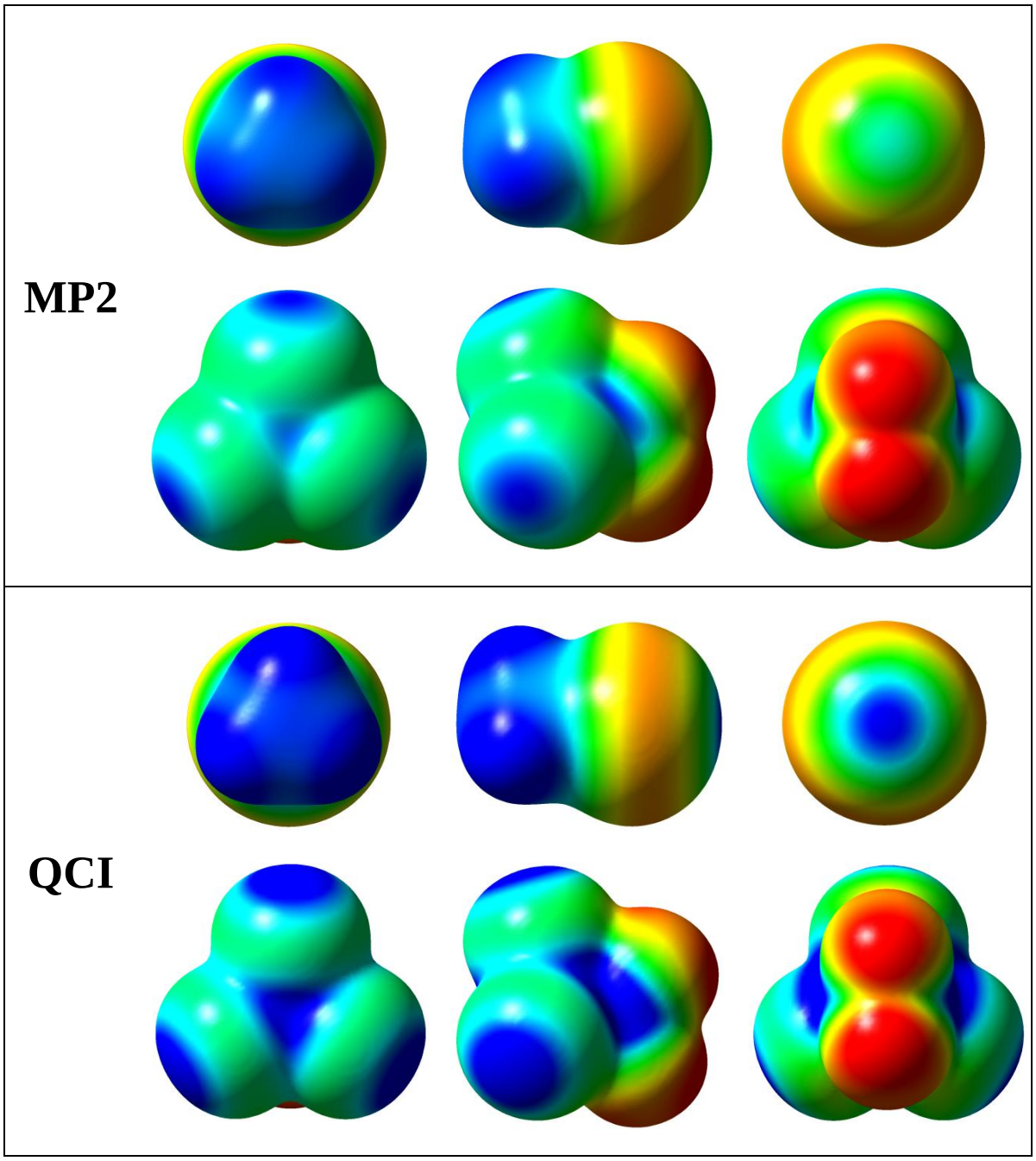


**Figure 3 (expanded).** Electrostatic potentials mapped on the total electron density surfaces of methyl iodide **1** (top row) and chloropicrin **2**, respectively, computed with the MP2/6-31G* (top panel) and QCI/6-31G* densities, respectively. Electrostatic potentials from -0.03 (red) to +0.03 (blue) and electron density surface computed for 0.002 e/a.u.[3]

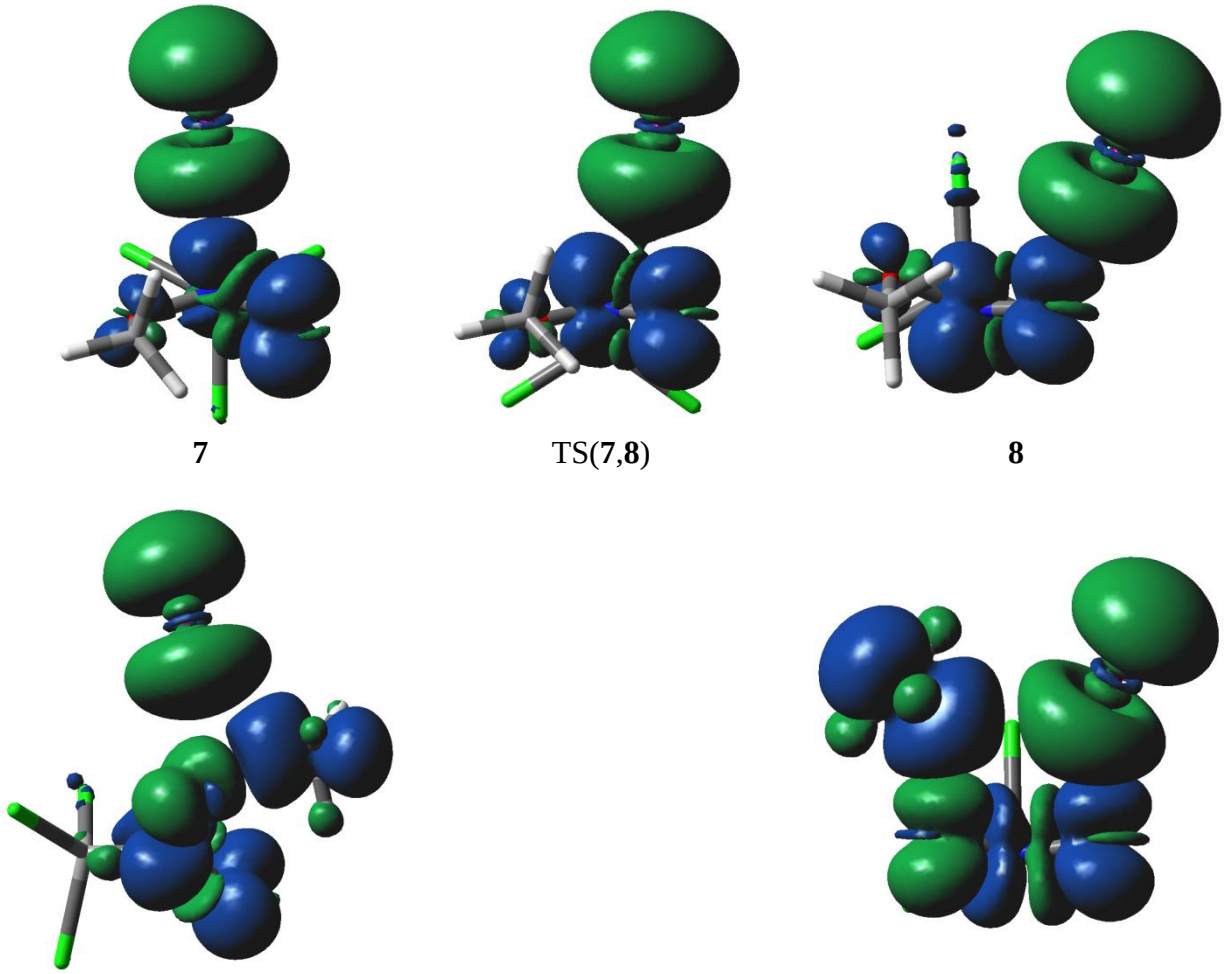


**Figure 9.** Spin density distributions of the unrestricted singlet wave functions of **7** and **8**, of the 1,2-iodine shift transition state structure TS(**7**,**8**), and of the reaction transition state structures TS(**5**,**7**) and TS(**5**,**8**) for the addition of iodomethane to chloropicrin. Surfaces are drawn for $\alpha$ and $\beta$ spin density values of 0.004 e/a.u.[3]

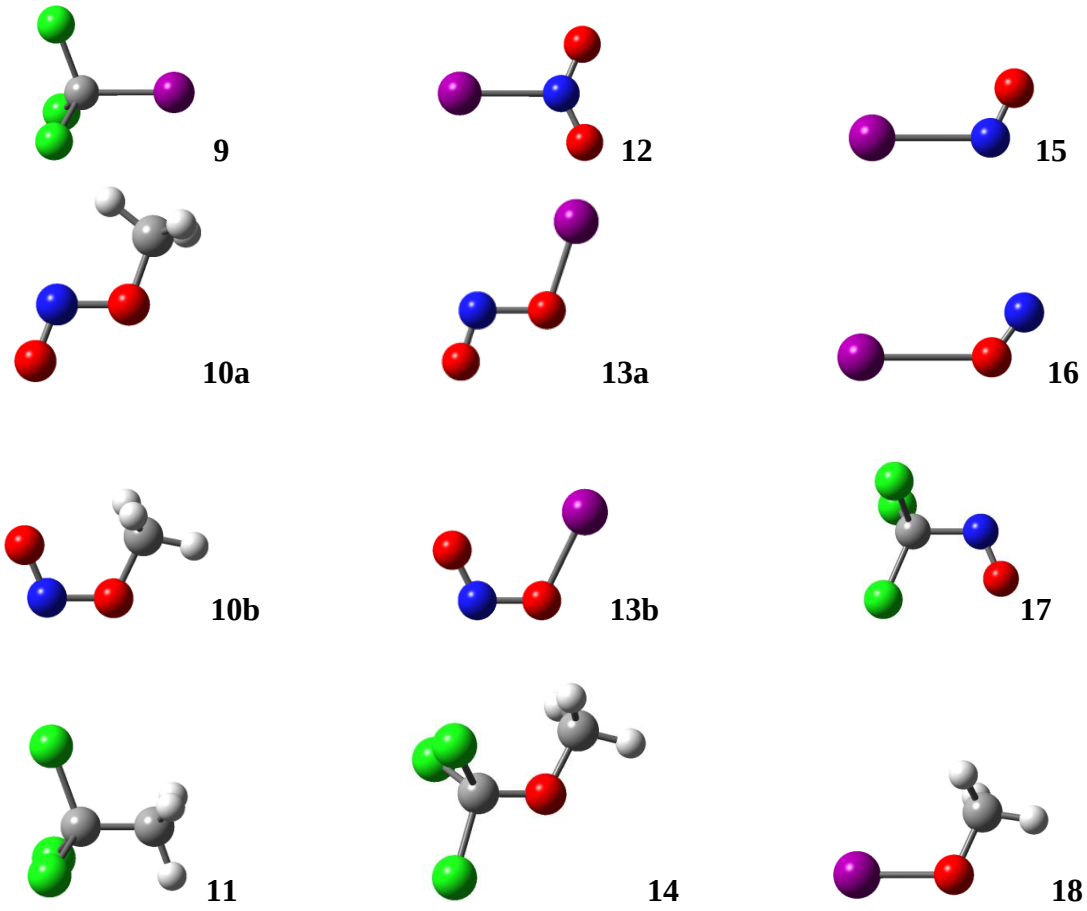


**Figure 10.** Models of the optimized structures of fragmentation products resulting from **7** and **8**.

**Table 3.** Mulliken Population Analysis of **3** - **6** at QCI/6-31G*//MP2/6-31G* Level

| | **3** | **4** | **5** | **6** | **1** | **2** |
|---|---|---|---|---|---|---|
| N | 0.503 | 0.486 | 0.503 | 0.505 | | 0.503 |
| C | -0.239 | -0.238 | -0.237 | -0.243 | | -0.239 |
| O | -0.332 | -0.328 | -0.333 | -0.337 | | -0.338 |
| O | -0.327 | -0.328 | -0.339 | -0.337 | | -0.339 |
| Cl | 0.135 | 0.130 | 0.147 | 0.146 | | 0.133 |
| Cl | 0.149 | 0.150 | 0.150 | 0.142 | | 0.146 |
| Cl | 0.135 | 0.135 | 0.130 | 0.128 | | 0.133 |
| C | -0.630 | -0.624 | -0.627 | -0.628 | -0.624 | |
| H | 0.209 | 0.214 | 0.209 | 0.213 | 0.215 | |
| H | 0.209 | 0.215 | 0.229 | 0.215 | 0.215 | |
| H | 0.209 | 0.215 | 0.213 | 0.217 | 0.215 | |
| I | -0.022 | -0.026 | -0.045 | -0.020 | -0.020 | |
| $CH_3$ | -0.003 | 0.020 | 0.025 | 0.016 | 0.020 | |
| $NO_2$ | -0.156 | -0.170 | -0.170 | -0.168 | | -0.173 |
| $CCl_3$ | 0.181 | 0.177 | 0.190 | 0.172 | | 0.173 |
| $CH_3I$ | -0.025 | -0.007 | -0.020 | -0.004 | | |

a) RQCISD for **1** and **4**, UQCISD for **2**, **3**, **5** & **6**.

## Cartesian Coordinates of Stationary Structures, MP2(full)/6-31G*

### Methyl Iodide, 1 CH3I.log

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | -1.830614 |
| 2 | 1 | 0 | 0.000000 | 1.034421 | -2.165018 |
| 3 | 1 | 0 | -0.895835 | -0.517211 | -2.165018 |
| 4 | 1 | 0 | 0.895835 | -0.517211 | -2.165018 |
| 5 | 53 | 0 | 0.000000 | 0.000000 | 0.329788 |

### Methyl Iodide, Cyclic Dimer $(1)_2$ CH3-I_DimerAntiP.log

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | -2.457263 | 0.204751 | -0.000657 |
| 2 | 53 | 0 | 2.457260 | -0.204753 | -0.000658 |
| 3 | 6 | 0 | 1.590798 | 1.777773 | 0.003651 |
| 4 | 1 | 0 | 0.510024 | 1.662907 | 0.000388 |
| 5 | 1 | 0 | 1.931994 | 2.284389 | 0.902861 |
| 6 | 1 | 0 | 1.936842 | 2.290364 | -0.890307 |
| 7 | 6 | 0 | -1.590785 | -1.777767 | 0.003652 |
| 8 | 1 | 0 | -1.933506 | -2.285074 | 0.901893 |
| 9 | 1 | 0 | -1.935248 | -2.289685 | -0.891300 |
| 10 | 1 | 0 | -0.510021 | -1.662798 | 0.002343 |

### Methyl Iodide, Open Dimer $(1)_2$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | 2.351874 | -0.242762 | 0.000000 |
| 2 | 53 | 0 | -1.951702 | -0.179143 | 0.000001 |
| 3 | 6 | 0 | -4.004474 | 0.500589 | -0.000002 |
| 4 | 1 | 0 | -4.158909 | 1.102851 | -0.891745 |
| 5 | 1 | 0 | -4.646039 | -0.377014 | -0.008334 |
| 6 | 1 | 0 | -4.163430 | 1.089146 | 0.900059 |
| 7 | 6 | 0 | 1.783163 | 1.842789 | 0.000002 |
| 8 | 1 | 0 | 0.696827 | 1.886370 | 0.000018 |
| 9 | 1 | 0 | 2.195173 | 2.299666 | 0.896270 |
| 10 | 1 | 0 | 2.195146 | 2.299661 | -0.896282 |

### Chloropicrin, eclipsed, 2a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.345838 | -0.029349 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -0.229616 | 0.027086 | 0.000000 |
| 3 | 8 | 0 | 1.957722 | 1.038534 | 0.000000 |
| 4 | 8 | 0 | 1.808312 | -1.170191 | 0.000000 |
| 5 | 17 | 0 | -0.748460 | -0.811823 | 1.449913 |
| 6 | 17 | 0 | -0.748460 | 1.688128 | 0.000000 |
| 7 | 17 | 0 | -0.748460 | -0.811823 | -1.449913 |

**Chloropicrin, staggered, 2b**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.431570 | 1.274425 | 0.000000 |
| 2 | 6 | 0 | 0.046059 | -0.226748 | 0.000000 |
| 3 | 8 | 0 | -0.558062 | 1.798681 | 1.106555 |
| 4 | 8 | 0 | -0.558062 | 1.798681 | -1.106555 |
| 5 | 17 | 0 | 1.802809 | -0.135905 | 0.000000 |
| 6 | 17 | 0 | -0.558062 | -1.000853 | 1.442162 |
| 7 | 17 | 0 | -0.558062 | -1.000853 | -1.442162 |

**Chloropicrin, Cyclic Dimer (2a)$_2$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -2.720241 | 1.360630 | -0.031801 |
| 2 | 6 | 0 | -2.493072 | -0.196986 | 0.027960 |
| 3 | 8 | 0 | -3.850426 | 1.766336 | -0.302968 |
| 4 | 8 | 0 | -1.709960 | 2.030768 | 0.186183 |
| 5 | 17 | 0 | -1.386314 | -0.572552 | -1.279058 |
| 6 | 17 | 0 | -1.780318 | -0.538746 | 1.591353 |
| 7 | 17 | 0 | -4.020729 | -1.008218 | -0.170541 |
| 8 | 7 | 0 | 1.816126 | -1.075299 | -0.499658 |
| 9 | 6 | 0 | 2.652814 | 0.133582 | 0.061847 |
| 10 | 8 | 0 | 1.676985 | -1.121073 | -1.722959 |
| 11 | 8 | 0 | 1.303537 | -1.810062 | 0.345242 |
| 12 | 17 | 0 | 3.814331 | 0.616305 | -1.147401 |
| 13 | 17 | 0 | 1.462038 | 1.385057 | 0.363840 |
| 14 | 17 | 0 | 3.440950 | -0.384472 | 1.532242 |

**Chloropicrin•$CH_3I$,** IBMA(O), **3**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.127435 | -0.090453 | -0.000080 |
| 2 | 6 | 0 | 2.699867 | 0.021832 | 0.000015 |
| 3 | 8 | 0 | 0.478676 | 0.956724 | -0.000093 |
| 4 | 8 | 0 | 0.703479 | -1.245971 | -0.000105 |
| 5 | 17 | 0 | 3.246733 | -0.798567 | -1.450028 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 17 | 0 | 3.159235 | 1.700156 | 0.000061 |
| 7 | 17 | 0 | 3.246561 | -0.798597 | 1.450106 |
| 8 | 6 | 0 | -5.008969 | -0.172104 | 0.000138 |
| 9 | 1 | 0 | -5.238256 | -1.234726 | -0.015534 |
| 10 | 1 | 0 | -5.396073 | 0.293748 | 0.902963 |
| 11 | 1 | 0 | -5.399027 | 0.320790 | -0.886919 |
| 12 | 53 | 0 | -2.859515 | 0.051285 | -0.000031 |

**Chloropicrin•$CH_3I$,** IBMA(Cl), **4**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -3.526807 | -0.078445 | -0.117008 |
| 2 | 6 | 0 | -1.966369 | 0.064438 | 0.052519 |
| 3 | 8 | 0 | -4.177150 | 0.945560 | -0.326268 |
| 4 | 8 | 0 | -3.941212 | -1.233201 | -0.014440 |
| 5 | 17 | 0 | -1.245112 | -0.949392 | -1.185040 |
| 6 | 17 | 0 | -1.512828 | 1.732160 | -0.142770 |
| 7 | 17 | 0 | -1.595389 | -0.524000 | 1.661794 |
| 8 | 6 | 0 | 4.556689 | 0.336218 | 0.447433 |
| 9 | 1 | 0 | 4.527331 | 0.981418 | 1.321783 |
| 10 | 1 | 0 | 5.047303 | -0.606697 | 0.675126 |
| 11 | 1 | 0 | 5.040156 | 0.834957 | -0.388733 |
| 12 | 53 | 0 | 2.518574 | -0.097405 | -0.127187 |

**Chloropicrin•$CH_3I$, IHBMA(O), 5**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.025530 | 0.939804 | 0.062115 |
| 2 | 6 | 0 | -2.176324 | -0.132339 | 0.009727 |
| 3 | 8 | 0 | -0.569317 | 1.242615 | 1.164885 |
| 4 | 8 | 0 | -0.702995 | 1.392753 | -1.037779 |
| 5 | 17 | 0 | -1.668237 | -1.363433 | -1.123687 |
| 6 | 17 | 0 | -2.424279 | -0.785805 | 1.603174 |
| 7 | 17 | 0 | -3.595939 | 0.729602 | -0.564037 |
| 8 | 53 | 0 | 2.605966 | -0.373367 | -0.017911 |
| 9 | 6 | 0 | 2.558650 | 1.786422 | 0.091394 |
| 10 | 1 | 0 | 3.362812 | 2.165640 | -0.534013 |
| 11 | 1 | 0 | 1.585157 | 2.104238 | -0.269531 |
| 12 | 1 | 0 | 2.702781 | 2.066297 | 1.131782 |

**Chloropicrin•$CH_3I$,** HBMA(Cl), **6**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -3.486840 | -0.626627 | -0.167231 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -2.095570 | 0.091464 | 0.003337 |
| 3 | 8 | 0 | -4.193871 | -0.288513 | -1.116286 |
| 4 | 8 | 0 | -3.724630 | -1.471266 | 0.696099 |
| 5 | 17 | 0 | -0.876058 | -1.164243 | -0.031177 |
| 6 | 17 | 0 | -1.873073 | 1.235646 | -1.292412 |
| 7 | 17 | 0 | -2.151078 | 0.893278 | 1.564888 |
| 8 | 6 | 0 | 1.833726 | 1.379947 | 0.499425 |
| 9 | 1 | 0 | 1.102128 | 1.510951 | -0.293715 |
| 10 | 1 | 0 | 1.351638 | 1.091110 | 1.430086 |
| 11 | 1 | 0 | 2.431068 | 2.278636 | 0.632050 |
| 12 | 53 | 0 | 3.165013 | -0.219700 | -0.082169 |

**Addition Product, 7**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.364654 | 0.711930 | -0.427961 |
| 2 | 6 | 0 | 1.395286 | -0.390957 | 0.068603 |
| 3 | 8 | 0 | 0.492225 | 1.071168 | -1.590307 |
| 4 | 8 | 0 | 0.409894 | 1.725656 | 0.595394 |
| 5 | 17 | 0 | 1.069394 | -0.821921 | 1.718091 |
| 6 | 17 | 0 | 1.218913 | -1.734971 | -1.024347 |
| 7 | 17 | 0 | 2.974822 | 0.361109 | -0.101208 |
| 8 | 53 | 0 | -1.992304 | -0.282703 | -0.002110 |
| 9 | 6 | 0 | -0.177532 | 2.935584 | 0.094717 |
| 10 | 1 | 0 | -1.210768 | 2.744973 | -0.212775 |
| 11 | 1 | 0 | 0.404787 | 3.343422 | -0.732752 |
| 12 | 1 | 0 | -0.151131 | 3.597317 | 0.959335 |

**Transition State Structure for Methyl-Rotation about NO Bond in 7, MRTS(7)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.313998 | 0.448475 | -0.804096 |
| 2 | 6 | 0 | 1.286325 | -0.444430 | 0.133727 |
| 3 | 8 | 0 | 0.472657 | 0.225317 | -1.988070 |
| 4 | 8 | 0 | 0.210163 | 1.933680 | -0.549064 |
| 5 | 17 | 0 | 1.005147 | -0.143251 | 1.822228 |
| 6 | 17 | 0 | 0.921750 | -2.093830 | -0.293159 |
| 7 | 17 | 0 | 2.926555 | -0.038103 | -0.352363 |
| 8 | 53 | 0 | -2.048568 | -0.064675 | 0.031909 |
| 9 | 6 | 0 | 1.120111 | 2.632455 | 0.316789 |
| 10 | 1 | 0 | 0.887925 | 3.671042 | 0.069826 |
| 11 | 1 | 0 | 2.166684 | 2.436759 | 0.085578 |
| 12 | 1 | 0 | 0.911642 | 2.458636 | 1.372079 |

**Addition Product, 8**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.817394 | 0.752082 | -0.545451 |
| 2 | 6 | 0 | 1.690233 | -0.335599 | 0.011854 |
| 3 | 8 | 0 | -0.225991 | 0.493486 | -1.185803 |
| 4 | 8 | 0 | 0.826748 | 1.821041 | 0.330041 |
| 5 | 17 | 0 | 1.057268 | -0.856627 | 1.569850 |
| 6 | 17 | 0 | 1.667991 | -1.641350 | -1.148541 |
| 7 | 17 | 0 | 3.303536 | 0.344596 | 0.175529 |
| 8 | 53 | 0 | -2.329744 | -0.235052 | 0.052900 |
| 9 | 6 | 0 | 0.086958 | 2.942899 | -0.226840 |
| 10 | 1 | 0 | -0.968987 | 2.697598 | -0.312395 |
| 11 | 1 | 0 | 0.513172 | 3.217225 | -1.193806 |
| 12 | 1 | 0 | 0.251786 | 3.725828 | 0.510440 |

**Transition State Structure for Methyl-Rotation about NO Bond in 8, MRTS(8)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.728458 | 0.376288 | -0.921592 |
| 2 | 6 | 0 | 1.608541 | -0.365713 | 0.041757 |
| 3 | 8 | 0 | -0.298289 | -0.191396 | -1.352640 |
| 4 | 8 | 0 | 0.570901 | 1.760690 | -0.892225 |
| 5 | 17 | 0 | 0.943935 | -0.317806 | 1.683511 |
| 6 | 17 | 0 | 1.664321 | -2.021151 | -0.525901 |
| 7 | 17 | 0 | 3.217253 | 0.346361 | -0.027620 |
| 8 | 53 | 0 | -2.389967 | -0.062810 | 0.058285 |
| 9 | 6 | 0 | 1.154411 | 2.611665 | 0.132107 |
| 10 | 1 | 0 | 2.195529 | 2.834253 | -0.092526 |
| 11 | 1 | 0 | 1.038186 | 2.197033 | 1.129644 |
| 12 | 1 | 0 | 0.543081 | 3.507661 | 0.030829 |

**Transition State Structure TS(5,7) for Formation of Addition Product 7**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.995480 | 1.098512 | -0.234990 |
| 2 | 6 | 0 | -1.750335 | -0.209831 | -0.025381 |
| 3 | 8 | 0 | -1.290121 | 2.049545 | 0.539842 |
| 4 | 8 | 0 | 0.137537 | 1.003794 | -0.874395 |
| 5 | 17 | 0 | -1.368040 | -1.309558 | -1.325427 |
| 6 | 17 | 0 | -1.266547 | -0.855833 | 1.535797 |
| 7 | 17 | 0 | -3.456978 | 0.207473 | -0.033307 |
| 8 | 53 | 0 | 2.207167 | -0.364846 | 0.072024 |
| 9 | 6 | 0 | 1.441474 | 2.347714 | -0.266082 |
| 10 | 1 | 0 | 2.053703 | 2.297245 | 0.622558 |
| 11 | 1 | 0 | 0.586969 | 3.002864 | -0.173927 |
| 12 | 1 | 0 | 1.978297 | 2.377727 | -1.205812 |

**Transition State Structure TS(5,8) for Formation of Addition Product 8**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.724749 | 0.187727 | -0.958267 |
| 2 | 6 | 0 | 1.810254 | -0.145099 | 0.064770 |
| 3 | 8 | 0 | -0.140212 | -0.722408 | -1.218882 |
| 4 | 8 | 0 | 0.472729 | 1.401680 | -1.148695 |
| 5 | 17 | 0 | 1.114633 | 0.065043 | 1.670903 |
| 6 | 17 | 0 | 2.306206 | -1.797533 | -0.199282 |
| 7 | 17 | 0 | 3.137677 | 0.969566 | -0.198085 |
| 8 | 53 | 0 | -2.285490 | -0.273006 | 0.040175 |
| 9 | 6 | 0 | -0.973019 | 2.327836 | 0.136264 |
| 10 | 1 | 0 | -1.282263 | 2.074611 | 1.140339 |
| 11 | 1 | 0 | -1.761350 | 2.587522 | -0.557923 |
| 12 | 1 | 0 | -0.076974 | 2.932222 | 0.080457 |

**Transition State Structure TS(7,8) for Isomerization of 8 to 7**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.510306 | 0.671065 | 0.213486 |
| 2 | 6 | 0 | -1.653854 | -0.316574 | -0.024221 |
| 3 | 8 | 0 | 0.000420 | 0.759972 | 1.395911 |
| 4 | 8 | 0 | -0.717009 | 1.840649 | -0.521673 |
| 5 | 17 | 0 | -2.947097 | 0.407719 | -0.973216 |
| 6 | 17 | 0 | -0.991083 | -1.698547 | -0.893817 |
| 7 | 17 | 0 | -2.275185 | -0.828785 | 1.537932 |
| 8 | 53 | 0 | 2.329629 | -0.275424 | -0.053650 |
| 9 | 6 | 0 | 0.093008 | 2.914723 | -0.021777 |
| 10 | 1 | 0 | 1.151162 | 2.658191 | -0.101883 |
| 11 | 1 | 0 | -0.163208 | 3.141718 | 1.013934 |
| 12 | 1 | 0 | -0.161137 | 3.739636 | -0.686198 |

**Trichloroiodomethane, 9**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.789919 | 0.000007 | -0.000002 |
| 2 | 53 | 0 | -1.411904 | 0.000001 | -0.000003 |
| 3 | 17 | 0 | 1.374347 | -1.214906 | -1.141398 |
| 4 | 17 | 0 | 1.374347 | 1.595942 | -0.481425 |
| 5 | 17 | 0 | 1.374330 | -0.381040 | 1.622833 |

**Methylnitrite, *Z*-isomer, 10a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.366127 | -0.526984 | 0.000041 |
| 2 | 6 | 0 | 1.640019 | 0.140777 | -0.000022 |
| 3 | 1 | 0 | 2.187037 | -0.161961 | -0.894232 |
| 4 | 1 | 0 | 1.485710 | 1.222029 | -0.000664 |
| 5 | 1 | 0 | 2.186669 | -0.161276 | 0.894564 |
| 6 | 7 | 0 | -0.667919 | 0.446247 | 0.000123 |
| 7 | 8 | 0 | -1.744139 | -0.081414 | -0.000090 |

**Methylnitrite, *E*-isomer, 10b**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | -0.474166 | -0.762161 | -0.000034 |
| 2 | 6 | 0 | -1.281496 | 0.432387 | 0.000003 |
| 3 | 1 | 0 | -1.082833 | 1.031881 | 0.890791 |
| 4 | 1 | 0 | -1.082967 | 1.031926 | -0.890759 |
| 5 | 1 | 0 | -2.302637 | 0.058909 | 0.000111 |
| 6 | 7 | 0 | 0.900363 | -0.532523 | 0.000035 |
| 7 | 8 | 0 | 1.206025 | 0.638489 | -0.000017 |

**1,1,1-Trichloroethane, 11**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.202194 | 0.104169 | 0.080416 |
| 2 | 17 | 0 | -0.610397 | -1.315904 | -0.908765 |
| 3 | 17 | 0 | 0.717158 | 1.260901 | -0.908765 |
| 4 | 17 | 0 | 0.797240 | -0.410733 | 1.457995 |
| 5 | 6 | 0 | -1.471427 | 0.758071 | 0.585210 |
| 6 | 1 | 0 | -2.080403 | 1.071812 | -0.264239 |
| 7 | 1 | 0 | -2.031154 | 0.043775 | 1.191293 |
| 8 | 1 | 0 | -1.214722 | 1.628482 | 1.191293 |

**$INO_2$, 12**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.520050 | 0.000039 | 0.000044 |
| 2 | 8 | 0 | 2.006762 | -1.107561 | -0.000016 |
| 3 | 8 | 0 | 2.006266 | 1.107728 | -0.000016 |
| 4 | 53 | 0 | -0.806501 | -0.000030 | -0.000001 |

**IO–NO, s-trans, 13a**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | 0.881616 | -0.037637 | -0.000001 |
| 2 | 8 | 0 | -1.020670 | 0.697733 | 0.000005 |
| 3 | 7 | 0 | -1.986082 | -0.469232 | 0.000010 |
| 4 | 8 | 0 | -3.082214 | -0.037811 | -0.000008 |

**IO–NO, s-cis, 13b**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | -0.755750 | -0.055170 | -0.000003 |
| 2 | 8 | 0 | 1.031636 | 1.030056 | 0.000045 |
| 3 | 7 | 0 | 2.187249 | 0.281534 | -0.000067 |
| 4 | 8 | 0 | 2.061365 | -0.910894 | 0.000033 |

**$Cl_3C–O–CH_3$, 14**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.107196 | -0.000008 | 0.108581 |
| 2 | 17 | 0 | 1.759856 | -0.000481 | 0.724322 |
| 3 | 17 | 0 | -0.143445 | -1.451492 | -0.919383 |
| 4 | 17 | 0 | -0.142552 | 1.451725 | -0.919177 |
| 5 | 8 | 0 | -0.697831 | 0.000198 | 1.202441 |
| 6 | 6 | 0 | -2.120363 | 0.000290 | 0.973494 |
| 7 | 1 | 0 | -2.420499 | -0.897220 | 0.430237 |
| 8 | 1 | 0 | -2.553126 | 0.001227 | 1.971153 |
| 9 | 1 | 0 | -2.420308 | 0.896932 | 0.428674 |

**I–N=O, 15**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | 0.000000 | 0.621223 | 0.000000 |
| 2 | 7 | 0 | 0.490747 | -1.821251 | 0.000000 |
| 3 | 8 | 0 | -0.429404 | -2.522009 | 0.000000 |

**I–O=N, 16**

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 53 | 0 | 0.000000 | 0.681380 | 0.000000 |
| 2 | 8 | 0 | -0.384650 | -2.028570 | 0.000000 |
| 3 | 7 | 0 | 0.439600 | -2.840656 | 0.000000 |

**$Cl_3C–N=O$, 17**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.085040 | -0.000018 | -0.010673 |
| 2 | 17 | 0 | 1.066869 | -1.454190 | -0.073261 |
| 3 | 17 | 0 | 1.062456 | 1.457274 | -0.070081 |
| 4 | 17 | 0 | -1.017993 | -0.003182 | 1.339323 |
| 5 | 7 | 0 | -0.649673 | 0.000194 | -1.403074 |
| 6 | 8 | 0 | -1.856896 | 0.000054 | -1.305764 |

**$H_3C–O-I$, 18**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 1.295900 | 0.699336 | 0.000021 |
| 2 | 6 | 0 | 2.286623 | -0.341094 | 0.000036 |
| 3 | 1 | 0 | 2.221565 | -0.968785 | 0.894460 |
| 4 | 1 | 0 | 2.221596 | -0.968782 | -0.894393 |
| 5 | 1 | 0 | 3.235218 | 0.200480 | 0.000053 |
| 6 | 53 | 0 | -0.599346 | -0.034170 | -0.000009 |

**Energies of Computed at UQCISD(full)//6-31G*//MP2(full)/6-31G***

**Iodomethane 1**

```
 Iteration Nr.  11
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      2852
 NAB=   961 NAA=   465 NBB=   465.
 DE(Corr)= -0.82690387     E(CORR)=     -6957.2528838     Delta=-7.46D-08
 NORM(A)=   0.10693707D+01
 Largest amplitude= 7.89D-02

 S**2, projected HF & approx projected MPn energies after annihilation of
 unwanted spin states (see manual for definitions):

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1         0.00000  0.00000-6956.425980-6957.262929-6957.239260
 s+1,s+2     0.00000  0.00000-6956.425980-6957.262929-6957.239260
 s+1 to s+3  0.00000  0.00000-6956.425980-6957.262929-6957.239260
 s+1 to s+4  0.00000  0.00000-6956.425980-6957.262929-6957.239260
 s+1 to s+5  0.00000  0.00000-6956.425980
 s+1 to s+6  0.00000  0.00000-6956.425980
```

**Chloropicrin 2a**

```
 Iteration Nr.  22
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      4760
 NAB=  1600 NAA=   780 NBB=   780.
 DE(Corr)=  -1.1088723     E(CORR)=     -1621.4094729     Delta=-2.40D-08
 NORM(A)=   0.12869787D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           36        41           -0.225447D+00
    AA           36        44           -0.103985D+00
    AA           38        41           -0.106145D+00
    BB           34        41            0.134120D+00
    BB           36        41           -0.108128D+00
    BB           39        41            0.192275D+00
 Largest amplitude= 2.25D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.01838  0.00091-1620.338594-1621.380072-1621.398077
 s+1,s+2     0.00011 -0.00010-1620.334187-1621.375966-1621.394478
 s+1 to s+3  0.00000  0.00000-1620.334212-1621.375988-1621.394496
 s+1 to s+4  0.00000  0.00000-1620.334212-1621.375986-1621.394491
 s+1 to s+5  0.00000  0.00000-1620.334212
 s+1 to s+6  0.00000  0.00000-1620.334212
```

**Chloropicrin 2b**

```
 Iteration Nr.  24
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      4760
 NAB=  1600 NAA=   780 NBB=   780.
 DE(Corr)=  -1.1088822     E(CORR)=     -1621.4093336     Delta=-4.63D-08
 NORM(A)=   0.12866888D+01
```

```
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           34        41           0.106300D+00
    AA           36        41          -0.150926D+00
    AA           38        41           0.103424D+00
    AA           39        41           0.112397D+00
    BB           34        41           0.106300D+00
    BB           36        41          -0.150926D+00
    BB           38        41           0.103424D+00
    BB           39        41           0.112397D+00
 Largest amplitude= 1.51D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.01827  0.00091-1620.338366-1621.379958-1621.397926
 s+1,s+2     0.00011 -0.00010-1620.333987-1621.375878-1621.394353
 s+1 to s+3  0.00000  0.00000-1620.334011-1621.375901-1621.394371
 s+1 to s+4  0.00000  0.00000-1620.334011-1621.375900-1621.394368
 s+1 to s+5  0.00000  0.00000-1620.334011
 s+1 to s+6  0.00000  0.00000-1620.334011
```

**Dimer of Chloropicrin**

```
 Iteration Nr.  30
 **********************
 DD1Dir will call FoFMem  13 times, MxPair=      1472
 NAB=  6400 NAA=  3160 NBB=  3160.
 DE(Corr)=  -2.2238293     E(CORR)=     -3242.8234953     Delta=-9.68D-09
 NORM(A)=   0.15205617D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           67        81           -0.120731D+00
    AA           71        82           -0.220992D+00
    AA           72        81           -0.155732D+00
    BB           67        82           -0.108253D+00
    BB           71        81            0.100183D+00
    BB           71        82           -0.103181D+00
    BB           78        81           -0.128033D+00
    BB           78        82           -0.113884D+00
 Largest amplitude= 2.21D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -1.62423 -0.99802-3240.726129-3242.818361-3242.855157
 s+1,s+2     0.04155 -0.00717-3240.649898-3242.743221-3242.782224
 s+1 to s+3 -0.00052  0.00054-3240.655270-3242.748204-3242.786422
 s+1 to s+4  0.00000 -0.00001-3240.655196-3242.747261-3242.783377
 s+1 to s+5  0.00000 -0.00001-3240.655196
 s+1 to s+6 -0.00010 -0.00001-3240.655196
```

**Number 3**

```
 Iteration Nr.  23
 **********************
 DD1Dir will call FoFDir   7 times, MxPair=      2152
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  4.
 DE(Corr)=  -1.9386811     E(CORR)=     -8578.6652824     Delta=-5.54D-08
```

```
 NORM(A)=   0.13428230D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           62        72           0.137676D+00
    AA           64        72          -0.112356D+00
    AA           67        72          -0.192300D+00
    BB           64        72          -0.226358D+00
    BB           64        76          -0.101579D+00
    BB           66        72           0.102684D+00
 Largest amplitude= 2.26D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.01867  0.00081-8576.764647-8578.646436-8578.639911
 s+1,s+2     0.00011 -0.00010-8576.760212-8578.642304-8578.636290
 s+1 to s+3  0.00000  0.00000-8576.760238-8578.642326-8578.636308
 s+1 to s+4  0.00000  0.00000-8576.760238-8578.642279-8578.636146
 s+1 to s+5  0.00000  0.00000-8576.760238
 s+1 to s+6 -0.00010  0.00000-8576.760238
```

**Number 4**

```
 Iteration Nr.  24
 **********************
 DD1Dir will call FoFDir   7 times, MxPair=      2152
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  4.
 DE(Corr)=  -1.9537719     E(CORR)=     -8578.6661486     Delta=-3.54D-08
 NORM(A)=   0.12549961D+01
 Largest amplitude= 9.86D-02

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1         0.00000  0.00000-8576.712377-8578.655288-8578.629885
 s+1,s+2     0.00000  0.00000-8576.712377-8578.655288-8578.629885
 s+1 to s+3  0.00000  0.00000-8576.712377-8578.655288-8578.629885
 s+1 to s+4  0.00000  0.00000-8576.712377-8578.655288-8578.629885
 s+1 to s+5  0.00000  0.00000-8576.712377
 s+1 to s+6  0.00001  0.00000-8576.712377
```

**Number 5**

```
Iteration Nr.  28
 **********************
 DD1Dir will call FoFDir   7 times, MxPair=      2152
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  4.
 DE(Corr)=  -1.9401486     E(CORR)=     -8578.6676798     Delta= 2.61D-08
 NORM(A)=   0.13418105D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           64        72          -0.219387D+00
    BB           62        72          -0.134482D+00
    BB           64        72           0.114981D+00
    BB           67        72           0.172618D+00
 Largest amplitude= 2.19D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
```

```
 annihilated
 s+1        -0.01817  0.00082-8576.765205-8578.649426-8578.642337
 s+1,s+2     0.00011 -0.00009-8576.760889-8578.645406-8578.638820
 s+1 to s+3  0.00000  0.00000-8576.760913-8578.645428-8578.638838
 s+1 to s+4  0.00000  0.00000-8576.760913-8578.645322-8578.638475
 s+1 to s+5  0.00000  0.00000-8576.760913
 s+1 to s+6 -0.00005  0.00000-8576.760913
```

**Number 6**

```
 Iteration Nr.  24
 **********************
 DD1Dir will call FoFDir   7 times, MxPair=      2152
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  4.
 DE(Corr)=  -1.9385105     E(CORR)=     -8578.6638057     Delta=-3.62D-08
 NORM(A)=   0.13424331D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           62        72           -0.129553D+00
    AA           64        72           -0.104448D+00
    AA           67        72           -0.193177D+00
    BB           64        72            0.210750D+00
    BB           64        76           -0.103994D+00
    BB           66        72           -0.103641D+00
 Largest amplitude= 2.11D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.01860  0.00091-8576.763422-8578.644996-8578.638883
 s+1,s+2     0.00011 -0.00010-8576.758966-8578.640842-8578.635241
 s+1 to s+3  0.00000  0.00000-8576.758991-8578.640865-8578.635259
 s+1 to s+4  0.00000  0.00000-8576.758991-8578.640941-8578.635520
 s+1 to s+5  0.00000  0.00000-8576.758991
 s+1 to s+6  0.00005  0.00000-8576.758991
```

**Number 7**

```
 Iteration Nr.  38
 **********************
 DD1Dir will call FoFDir   4 times, MxPair=      3764
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  2.
 DE(Corr)=  -1.9374855     E(CORR)=     -8578.6275622     Delta=-5.01D-09
 NORM(A)=   0.13042374D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           69        72           -0.222568D+00
    BB           69        72           -0.180179D+00
 Largest amplitude= 2.23D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.06916 -0.01106-8576.719563-8578.618526-8578.610726
 s+1,s+2     0.00072 -0.00048-8576.709337-8578.608619-8578.601324
 s+1 to s+3  0.00000  0.00000-8576.709449-8578.608727-8578.601425
 s+1 to s+4  0.00000  0.00000-8576.709449-8578.608715-8578.601383
 s+1 to s+5  0.00000  0.00000-8576.709449
```

```
 s+1 to s+6 -0.00003  0.00000-8576.709449
```

**MRTS(7)**

```
 Iteration Nr.  38
 **********************
 DD1Dir will call FoFMem   2 times, MxPair=      7526
 NAB=  5041 NAA=  2485 NBB=  2485.
 DE(Corr)=  -1.9411417     E(CORR)=     -8578.5960131     Delta=-1.44D-08
 NORM(A)=   0.13036864D+01
 Dominant configurations:
 ************************
 Spin Case        I    J    A    B          Value
    AA           69        72           -0.187926D+00
    BB           69        72           -0.174295D+00
 Largest amplitude= 1.88D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.08108 -0.01950-8576.684949-8578.587347-8578.579312
 s+1,s+2     0.00093 -0.00051-8576.674220-8578.576940-8578.569415
 s+1 to s+3  0.00000  0.00001-8576.674354-8578.577069-8578.569536
 s+1 to s+4  0.00000  0.00000-8576.674353-8578.577071-8578.569543
 s+1 to s+5  0.00000  0.00000-8576.674353
 s+1 to s+6 -0.00006  0.00000-8576.674353
```

**Number 8**

```
 Iteration Nr.  42
 **********************
 DD1Dir will call FoFDir   4 times, MxPair=      3764
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  2.
 DE(Corr)=  -1.9243519     E(CORR)=     -8578.6341400     Delta=-6.24D-09
 NORM(A)=   0.12885914D+01
 Dominant configurations:
 ************************
 Spin Case        I    J    A    B          Value
    AA           69        72           -0.239277D+00
 Largest amplitude= 2.39D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.07002 -0.00598-8576.740319-8578.626155-8578.623231
 s+1,s+2     0.00075 -0.00056-8576.728842-8578.615023-8578.612569
 s+1 to s+3  0.00000  0.00000-8576.728963-8578.615140-8578.612680
 s+1 to s+4  0.00000  0.00000-8576.728962-8578.615140-8578.612681
 s+1 to s+5  0.00000  0.00000-8576.728962
 s+1 to s+6 -0.00001  0.00000-8576.728962
```

**MRTS(8)**

```
 Iteration Nr.  42
 **********************
 DD1Dir will call FoFMem   2 times, MxPair=      7526
 NAB=  5041 NAA=  2485 NBB=  2485.
 DE(Corr)=  -1.9266907     E(CORR)=     -8578.6108106     Delta=-9.11D-09
 NORM(A)=   0.12939101D+01
 Dominant configurations:
 ************************
```

```
 Spin Case        I    J    A    B          Value
    AA           68        72           0.124882D+00
    BB           69        72          -0.233584D+00
 Largest amplitude= 2.34D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.06853 -0.00677-8576.715011-8578.601255-8578.599117
 s+1,s+2     0.00074 -0.00053-8576.703921-8578.590511-8578.588842
 s+1 to s+3  0.00000  0.00000-8576.704039-8578.590625-8578.588949
 s+1 to s+4  0.00000  0.00000-8576.704038-8578.590637-8578.588987
 s+1 to s+5  0.00000  0.00000-8576.704038
 s+1 to s+6  0.00010  0.00000-8576.704038
```

**TS(7,8)**

```
 Iteration Nr. 170
 **********************
 DD1Dir will call FoFMem   2 times, MxPair=      7526
 NAB=  5041 NAA=  2485 NBB=  2485.
 DE(Corr)=  -1.9195714     E(CORR)=     -8578.6081316     Delta= 3.50D-09
 NORM(A)=   0.12744814D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           69        72           0.132141D+00
    BB           71        72           0.145638D+00
 Largest amplitude= 1.46D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.10816 -0.01915-8576.709335-8578.590824-8578.590822
 s+1,s+2     0.00129 -0.00085-8576.693214-8578.574824-8578.574914
 s+1 to s+3 -0.00001  0.00001-8576.693414-8578.575025-8578.575114
 s+1 to s+4  0.00000  0.00000-8576.693414-8578.575024-8578.575113
 s+1 to s+5  0.00000  0.00000-8576.693414
 s+1 to s+6  0.00003  0.00000-8576.693414
```

**TS(5,7)**

```
 Iteration Nr.  42
 **********************
 DD1Dir will call FoFDir   4 times, MxPair=      3764
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  2.
 DE(Corr)=  -1.9388463     E(CORR)=     -8578.5467799     Delta=-1.70D-08
 NORM(A)=   0.13495143D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           69        72          -0.120050D+00
    BB           62        73           0.139754D+00
    BB           69        72          -0.234270D+00
    BB           69        73           0.107293D+00
 Largest amplitude= 2.34D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -1.34080 -0.83870-8576.692531-8578.578277-8578.572509
```

```
 s+1,s+2     0.04038 -0.00364-8576.633205-8578.519967-8578.515924
 s+1 to s+3 -0.00052  0.00047-8576.637135-8578.523766-8578.519496
 s+1 to s+4  0.00000 -0.00001-8576.637079-8578.523700-8578.519407
 s+1 to s+5  0.00000 -0.00001-8576.637079
 s+1 to s+6 -0.00004 -0.00001-8576.637079
```

**TS(5,8)**

```
 Iteration Nr.  48
 **********************
 DD1Dir will call FoFDir   4 times, MxPair=      3764
 NAB=  5041 NAA=  2485 NBB=  2485 NumPrc=  2.
 DE(Corr)=  -1.9267067     E(CORR)=     -8578.5417814     Delta= 1.04D-08
 NORM(A)=   0.13611809D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           62        73           -0.129266D+00
    AA           69        72           -0.174283D+00
    AA           71        72           -0.134527D+00
    AA           71        73            0.107268D+00
    BB           62        72           -0.100691D+00
    BB           65        72           -0.126537D+00
 Largest amplitude= 1.74D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -3.94108 -2.51207-8576.775113-8578.634362-8578.634779
 s+1,s+2     0.09072 -0.00387-8576.648621-8578.508891-8578.511297
 s+1 to s+3 -0.00134  0.00114-8576.657742-8578.517645-8578.519400
 s+1 to s+4  0.00001 -0.00002-8576.657592-8578.517529-8578.519352
 s+1 to s+5  0.00000 -0.00002-8576.657593
 s+1 to s+6 -0.00001 -0.00002-8576.657593
```

**Number 9**

```
 Iteration Nr.  15
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      9020
 NAB=  3025 NAA=  1485 NBB=  1485.
 DE(Corr)=  -1.2569299     E(CORR)=     -8334.3239316     Delta=-4.13D-09
 NORM(A)=   0.11487540D+01
 Largest amplitude= 5.23D-02

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1         0.00000  0.00000-8333.067002-8334.320121-8334.306980
 s+1,s+2     0.00000  0.00000-8333.067002-8334.320121-8334.306980
 s+1 to s+3  0.00000  0.00000-8333.067002-8334.320121-8334.306980
 s+1 to s+4  0.00000  0.00000-8333.067002-8334.320121-8334.306980
 s+1 to s+5  0.00000  0.00000-8333.067002
 s+1 to s+6 -0.00001  0.00000-8333.067002
```

**Number 10a**

```
 Iteration Nr.  24
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=       752
 NAB=   256 NAA=   120 NBB=   120.
```

```
 DE(Corr)= -0.68485920     E(CORR)=     -244.34051703     Delta=-1.58D-08
 NORM(A)=   0.11682089D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           11        17           0.170722D+00
    BB           12        17          -0.104988D+00
    BB           15        17          -0.203363D+00
 Largest amplitude= 2.03D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.00185  0.00006 -243.674459 -244.314378 -244.319174
 s+1,s+2     0.00000  0.00000 -243.674035 -244.313997 -244.318866
 s+1 to s+3  0.00000  0.00000 -243.674035 -244.313998 -244.318866
 s+1 to s+4  0.00000  0.00000 -243.674035 -244.313998 -244.318866
 s+1 to s+5  0.00000  0.00000 -243.674035
 s+1 to s+6  0.00000  0.00000 -243.674035
```

**Number 10b**

```
 Iteration Nr.  22
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=       752
 NAB=   256 NAA=   120 NBB=   120.
 DE(Corr)= -0.68576428     E(CORR)=     -244.34387198     Delta=-1.17D-08
 NORM(A)=   0.11537206D+01
 Dominant configurations:
 **********************
 Spin Case        I    J    A    B          Value
    AA           11        17           0.140513D+00
    AA           12        17           0.109189D+00
    BB           15        17          -0.174836D+00
 Largest amplitude= 1.75D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.00085  0.00004 -243.671362 -244.319917 -244.322441
 s+1,s+2     0.00000  0.00000 -243.671166 -244.319743 -244.322303
 s+1 to s+3  0.00000  0.00000 -243.671167 -244.319743 -244.322303
 s+1 to s+4  0.00000  0.00000 -243.671167 -244.319743 -244.322303
 s+1 to s+5  0.00000  0.00000 -243.671167
 s+1 to s+6  0.00000  0.00000 -243.671167
```

**Number 11**

```
 Iteration Nr.  13
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      3234
 NAB=  1089 NAA=   528 NBB=   528.
 DE(Corr)= -0.72645596     E(CORR)=     -1456.6304628     Delta=-4.01D-08
 NORM(A)=   0.11347948D+01
 Largest amplitude= 2.86D-02

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1         0.00000  0.00000-1455.904007-1456.581623-1456.622518
 s+1,s+2     0.00000  0.00000-1455.904007-1456.581623-1456.622518
```

```
 s+1 to s+3  0.00000  0.00000-1455.904007-1456.581623-1456.622518
 s+1 to s+4  0.00000  0.00000-1455.904007-1456.581623-1456.622518
 s+1 to s+5  0.00000  0.00000-1455.904007
 s+1 to s+6  0.00000  0.00000-1455.904007
```

**Number 12**

```
 Iteration Nr.  30
 ***********************
 DD1Dir will call FoFMem   1 times, MxPair=      4294
 NAB=  1444 NAA=   703 NBB=   703.
 DE(Corr)=  -1.2236520     E(CORR)=     -7122.0405335     Delta=-1.54D-09
 NORM(A)=   0.12487195D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           35        40           -0.267576D+00
    AA           36        39            0.249288D+00
    BB           31        40            0.105872D+00
    BB           35        40            0.204266D+00
   ABAB          35   35   40   40       -0.159663D+00
   ABAB          36   36   39   39        0.140862D+00
 Largest amplitude= 2.68D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.31427 -0.18594-7120.870352-7122.085538-7122.032756
 s+1,s+2     0.00564 -0.00139-7120.854586-7122.070109-7122.017873
 s+1 to s+3 -0.00004  0.00004-7120.855272-7122.070710-7122.018318
 s+1 to s+4  0.00000  0.00000-7120.855267-7122.070705-7122.018314
 s+1 to s+5  0.00000  0.00000-7120.855267
 s+1 to s+6  0.00000  0.00000-7120.855267
```

**Number 13a**

```
 Iteration Nr.  26
 ***********************
 DD1Dir will call FoFMem   1 times, MxPair=      4294
 NAB=  1444 NAA=   703 NBB=   703.
 DE(Corr)=  -1.2272029     E(CORR)=     -7122.0413757     Delta=-4.26D-08
 NORM(A)=   0.11830565D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           33        40            0.179082D+00
    BB           34        40           -0.186966D+00
   ABAB          33   33   40   40        0.117071D+00
 Largest amplitude= 1.87D-01

spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.00114 -0.00002-7120.829455-7122.061094-7122.007613
 s+1,s+2     0.00000  0.00000-7120.829208-7122.060873-7122.007435
 s+1 to s+3  0.00000  0.00000-7120.829208-7122.060873-7122.007435
 s+1 to s+4  0.00000  0.00000-7120.829208-7122.060875-7122.007443
 s+1 to s+5  0.00000  0.00000-7120.829208
 s+1 to s+6  0.00000  0.00000-7120.829208
```

**Number 13b**

```
 Iteration Nr.  23
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      4294
 NAB=  1444 NAA=   703 NBB=   703.
 DE(Corr)=  -1.2256040     E(CORR)=     -7122.0499008     Delta=-3.99D-08
 NORM(A)=   0.11740031D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           33        40            0.157637D+00
    BB           35        40           -0.159007D+00
 Largest amplitude= 1.59D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.00084 -0.00016-7120.834692-7122.071827-7122.016966
 s+1,s+2     0.00000  0.00000-7120.834559-7122.071707-7122.016867
 s+1 to s+3  0.00000  0.00000-7120.834559-7122.071707-7122.016867
 s+1 to s+4  0.00000  0.00000-7120.834559-7122.071705-7122.016860
 s+1 to s+5  0.00000  0.00000-7120.834559
 s+1 to s+6  0.00000  0.00000-7120.834559
```

**Number 14**

```
 Iteration Nr.  15
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      4070
 NAB=  1369 NAA=   666 NBB=   666.
 DE(Corr)= -0.90507557     E(CORR)=     -1531.6444683     Delta=-7.66D-09
 NORM(A)=   0.11579358D+01
 Largest amplitude= 2.46D-02

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1         0.00000  0.00000-1530.739393-1531.594977-1531.632600
 s+1,s+2     0.00000  0.00000-1530.739393-1531.594977-1531.632600
 s+1 to s+3  0.00000  0.00000-1530.739393-1531.594977-1531.632600
 s+1 to s+4  0.00000  0.00000-1530.739393-1531.594977-1531.632600
 s+1 to s+5  0.00000  0.00000-1530.739393
 s+1 to s+6  0.00000  0.00000-1530.739393
```

**Number 15**

```
 Iteration Nr.  29
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      3434
 NAB=  1156 NAA=   561 NBB=   561.
 DE(Corr)=  -1.0108657     E(CORR)=     -7047.0539861     Delta=-2.93D-08
 NORM(A)=   0.11877804D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           32        35           -0.311915D+00
    BB           32        36           -0.104455D+00
    BB           30        35            0.125918D+00
   ABAB          32   32   35   36       0.174420D+00
   ABAB          31   30   36   35      -0.135158D+00
```

```
 Largest amplitude= 3.12D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.20571 -0.11404-7046.084336-7047.093743-7047.053891
 s+1,s+2     0.00338 -0.00104-7046.070417-7047.080276-7047.041203
 s+1 to s+3 -0.00002  0.00002-7046.070825-7047.080661-7047.041551
 s+1 to s+4  0.00000  0.00000-7046.070822-7047.080659-7047.041549
 s+1 to s+5  0.00000  0.00000-7046.070822
 s+1 to s+6  0.00000  0.00000-7046.070822
```

**Number 16**

```
 Iteration Nr.  34
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      3434
 NAB=  1156 NAA=   561 NBB=   561.
 DE(Corr)= -0.99058068     E(CORR)=     -7047.0399327     Delta=-3.00D-08
 NORM(A)=   0.11172578D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           32        35           0.146082D+00
    BB           29        35           0.115959D+00
   ABAB          31   29   36   35      -0.128187D+00
 Largest amplitude= 1.46D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.30792 -0.17844-7046.082618-7047.079915-7047.043760
 s+1,s+2     0.00594 -0.00162-7046.061419-7047.059041-7047.023407
 s+1 to s+3 -0.00004  0.00005-7046.062124-7047.059736-7047.024088
 s+1 to s+4  0.00000  0.00000-7046.062119-7047.059731-7047.024083
 s+1 to s+5  0.00000  0.00000-7046.062119
 s+1 to s+6  0.00000  0.00000-7046.062119
```

**Number 17**

```
 Iteration Nr.  22
 **********************
 DD1Dir will call FoFMem   1 times, MxPair=      3852
 NAB=  1296 NAA=   630 NBB=   630.
 DE(Corr)= -0.92427139     E(CORR)=     -1546.4083598     Delta=-2.63D-08
 NORM(A)=   0.12260738D+01
 Dominant configurations:
 ***********************
 Spin Case        I    J    A    B          Value
    AA           27        37           0.107895D+00
    AA           29        37           0.163896D+00
    BB           27        37           0.198099D+00
   ABAB          27   27   37   37       0.101989D+00
   ABAB          29   27   37   37       0.126742D+00
 Largest amplitude= 1.98D-01

 spins       (S**2,0) (S**2,1)    PUHF        PMP2        PMP3        PMP4
 annihilated
 s+1        -0.00384 -0.00019-1545.510577-1546.365777-1546.391371
 s+1,s+2     0.00001 -0.00001-1545.509740-1546.365019-1546.390745
```

```
 s+1 to s+3  0.00000  0.00000-1545.509742-1546.365021-1546.390746
 s+1 to s+4  0.00000  0.00000-1545.509742-1546.365020-1546.390744
 s+1 to s+5  0.00000  0.00000-1545.509742
 s+1 to s+6  0.00000  0.00000-1545.509742
```

**Number 18**

```
 Iteration Nr.  17
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      3640
 NAB=  1225 NAA=   595 NBB=   595.
 DE(Corr)=  -1.0129724     E(CORR)=     -7032.2414567     Delta= 5.82D-09
 NORM(A)=   0.10980250D+01
 Largest amplitude= 7.46D-02

 spins       (S**2,0) (S**2,1)    PUHF         PMP2         PMP3         PMP4
 annihilated
 s+1         0.00000  0.00000-7031.228484-7032.250398-7032.223027
 s+1,s+2     0.00000  0.00000-7031.228484-7032.250398-7032.223027
 s+1 to s+3  0.00000  0.00000-7031.228484-7032.250398-7032.223027
 s+1 to s+4  0.00000  0.00000-7031.228484-7032.250398-7032.223027
 s+1 to s+5  0.00000  0.00000-7031.228484
 s+1 to s+6  0.00000  0.00000-7031.228484
```

## Relative Stabilities of 12 and 13

The cis-preference of **13** agrees with previous studies. Papayannis and Kosmas reported a preference for **12** over **13** based on effective core potential computations at the levels MP2, B3LYP and CCSD(T)/B3LYP and these data agree with the present MP2(full)/6-31G* results. The reversal of the stabilities of **12** and **13** at the UQCISD(full)/6-31G* level may reflect the difference between the present all-electron computations and the ECP computations of Papayannis and Kosmas and/or the fact that our UQCISD computations are based on the symmetry-broken, unrestricted reference wave functions. The energies of **12** and the isomers of **13** were computed at the RQCISD(full)/6-31G*//MP2(full)/6-31G* level to clarify this issue and, at this level, s-cis **13b** is preferred over s-trans **13a** by $\Delta G''_{rel}$ = 4.7 kcal/mol and **13b** is preferred over **12** by $\Delta G''_{rel}$ = 4.9 kcal/mol. Hence, the use of the all-electron wave functions causes a large difference of about 7.5 kcal/mol between the relative energies $\Delta G$ and $\Delta G$' of nitryl iodide **12** and nitrosyl hypoiodite **13** and this is the principal reason for the reversal of the isomer preference. The use of the unrestricted reference wave function in the QCISD treatment enhances the reversal by another 2 kcal/mol.

**Energies of Computed at RQCISD(full)//6-31G*//MP2(full)/6-31G***

**Compound 12**

```
Iteration Nr.  20
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      1482
 NAB=   741 NAA=     0 NBB=     0.
 DE(Corr)=  -1.2342566     E(CORR)=     -7122.0436908     Delta=-2.62D-08
 NORM(A)=   0.11542735D+01
 Largest amplitude= 1.27D-01
```

**Compound 13a**

```
Iteration Nr.  23
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      1482
 NAB=   741 NAA=     0 NBB=     0.
 DE(Corr)=  -1.2281402     E(CORR)=     -7122.0411828     Delta=-4.21D-08
 NORM(A)=   0.11493167D+01
 Largest amplitude= 9.46D-02
```

**Compound 13b**

```
Iteration Nr.  23
 *********************
 DD1Dir will call FoFMem   1 times, MxPair=      1482
 NAB=   741 NAA=     0 NBB=     0.
 DE(Corr)=  -1.2258985     E(CORR)=     -7122.0497707     Delta=-1.18D-08
 NORM(A)=   0.11514699D+01
 Largest amplitude= 9.28D-02
```