# SUPPORTING INFORMATION

**for**

**Propagation of Polar Substituent Effects in 1-(Substituted Phenyl)-6,7-Dimethoxy- 3,4-Dihydro- and -1,2,3,4-Tetrahydroisoquinolines as Explained by Resonance Polarization Concept**

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**TABLE S1. Correlations of the atomic charges for 1-(*para*- and *meta*-substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines. DSP correlations were performed with four different resonance scales.**

**DHIQ *para*-substitution**

| | $\delta = \rho q + k$ | | $q = \rho\sigma + k$ | | | $q = \rho_F\sigma_F + \rho_R\sigma_R + k$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| | $\rho \pm s$ | *r* | | $\rho \pm s$ | *r* | $\rho_F \pm s$ | $\rho_R \pm s$ | Scale for $\sigma_R$ | $\rho_F/\rho_R$ | *r* |
| C1 | 55 ± 35 | 0.4842 | q1 | -0.0078 ± 0.0014 | 0.8956 | -0.0036 ± 0.0019 | -0.0152 ± 0.0019 | $\sigma_R^o$ | 0.24 | 0.9652 |
| N2 | 1110 ± 94 | 0.9723 | q2 | 0.00921 ± 9.7e-4 | 0.9587 | 0.0083 ± 0.0015 | 0.0141 ± 0.0015 | $\sigma_R^o$ | 0.59 | 0.9827 |
| C3 | -81 ± 8 | 0.9610 | q3 | -0.00389 ± 4.2e-4 | 0.9558 | -0.0056 ± 4e-4 | -0.0041 ± 4e-4 | $\sigma_R^o$ | 1.4 | 0.9934 |
| C4 | 158± 20 | 0.9414 | q4 | -0.00151 ±1.5e-4 | 0.9631 | -0.0020 ± 1e-4 | -0.0017 ± 1e-4 | $\sigma_R^o$ | 1.2 | 0.9952 |
| C4a | -273 ± 80 | 0.7706 | q4a | 6.1e-4 ± 6e-5 | 0.9633 | 8.9e-4 ± 8e-5 | 2.4e-4 ± 3e-5 | $\sigma_R^+$ | 3.7 | 0.9793 |
| C5 | 249 ± 13 | 0.9884 | q5 | 9.8e-4 ± 1.0e-4 | 0.9631 | 0.00142 ± 8e-5 | 9.9e-4 ± 9e-5 | $\sigma_R^o$ | 1.4 | 0.9948 |
| C6 | 245 ± 26 | 0.9575 | q6 | 0.00226 ± 2.9e-4 | 0.9390 | 0.0035 ± 3e-4 | 0.0016 ± 2e-4 | $\sigma_R^-$ | 2.2 | 0.9926 |
| C7 | 136 ± 15 | 0.9568 | q7 | 0.00207 ± 3.0e-4 | 0.9228 | 0.0037 ± 1 e-4 | 0.0015 ± 1e-4 | $\sigma_R^o$ | 2.5 | 0.9972 |
| C8 | 160 ± 255 | 0.2166 | q8 | -4.3e-5 ± 3.8e-4 | 0.04016 | -0.0021 ± 3e-4 | 0.0014 ± 2 e-4 | $\sigma_R^-$ | -1.5 | 0.9508 |
| C8a | -299 ± 51 | 0.9019 | q8a | 0.00217 ± 5.0e-4 | 0.8393 | 0.0020 ± 3e-4 | 0.0030 ± 2e-4 | $\sigma_R^-$ | 0.67 | 0.9892 |

**DHIQ *meta*-substitution**

| | $\delta = \rho q + k$ | | $q = \rho\sigma + k$ | | | $q = \rho_F\sigma_F + \rho_R\sigma_R$[a] $+ k$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | $\rho \pm s$ | $r$ | | $\rho \pm s$ | $r$ | $\rho_F \pm s$ | $\rho_R \pm s$ | Scale for $\sigma_R$ | $\rho_F/\rho_R$ | $r$ |
| C1[b] | -187 ± 68 | 0.7195 | q1 | 0.0092 ± 0.0022 | 0.8265 | 0.0051 ± 0.0017 | 0.0097 ± 0.0017 | $\sigma_R^o$ | 0.53 | 0.9509 |
| C1_1[c] | -155 ± 48 | 0.7726 | q1_1 | 0.0108 ± 0.0028 | 0.8028 | 0.0060 ± 0.0023 | 0.0115 ± 0.0022 | $\sigma_R^o$ | 0.52 | 0.9403 |
| C1_2[d] | -298 ± 110 | 0.7151 | q1_2 | 0.0060 ± 0.0015 | 0.8179 | 0.0029 ± 9e-4 | 0.0069 ± 9e-4 | $\sigma_R^o$ | 0.42 | 0.9670 |
| N2[b] | 273 ± 436 | 0.2302 | q2 | -4e-4 ± 0,0029 | 0.0530 | 0.0031 ± 0.0037 | -0.0038 ± 0.0027 | $\sigma_R^-$ | -0.82 | 0.4714 |
| N2_1[c] | -597 ± 417 | 0.4761 | q2_1 | -0.0030 ± 0.0024 | 0.4052 | 0.0024 ± 0.0014 | -0.0068 ± 0.0010 | $\sigma_R^-$ | -0.35 | 0.9343 |
| N2_2[d] | 924 ± 214 | 0.8526 | q2_2 | 0.0076 ± 0.0019 | 0.8233 | 0.0069 ± 0.0025 | 0.0016 ± 0.0010 | $\sigma_R^+$ | 4.3 | 0.8414 |
| C3 | -46 ± 6 | 0.9498 | q3 | -0.00461 ± 5.3e-4 | 0.9515 | -0.0048 ± 6e-4 | -0.0011 ± 4e-4 | $\sigma_R^-$ | 4.4 | 0.9733 |
| C4 | 128 ± 14 | 0.9629 | q4 | -0.00163 ± 2.1e-4 | 0.9417 | -0.0018 ± 2e-4 | -1.5e-4 ± 1e-4 | $\sigma_R^+$ | 12 | 0.9592 |
| C4a | 125 ± 38 | 0.7779 | q4a | 0.00129 ± 1.8e-4 | 0.9281 | 0.0011 ± 2e-4 | 6.0e-4 ± 1.2e-4 | $\sigma_R^{BA}$ | 1.8 | 0.9679 |
| C5 | 235 ± 22 | 0.9699 | q5 | 0.00159 ± 3.3e-4 | 0.8616 | 0.0012 ± 3e-4 | 9.3e-4 ± 2.0e-4 | $\sigma_R^-$ | 1.3 | 0.9595 |
| C6 | 204 ± 9 | 0.9926 | q6 | 0.00387 ± 3.0e-4 | 0.9769 | 0.0036 ± 2e-4 | 0.0013 ± 2e-4 | $\sigma_R^-$ | 2.8 | 0.9929 |
| C7 | 66 ± 5 | 0.9819 | q7 | 0.0056 ± 0.0010 | 0.8880 | 0.0041 ± 4e-4 | 0.0035 ± 0.0003 | $\sigma_R^-$ | 1.2 | 0.9940 |
| C8[b] | 150 ± 110 | 0.4569 | q8 | -0.0013 ± 0.0012 | 0.3732 | -4.4e-4 ± 0.00140 | -0.0017 ± 0.0010 | $\sigma_R^{BA}$ | 0.26 | 0.6027 |
| C8_1[c] | 80 ± 143 | 0.2065 | q8_1 | -8e-4 ± 0.0010 | 0.2706 | -5.2e-4 ± 0.00142 | -0.0010 ± 0.0014 | $\sigma_R^o$ | 1.1 | 0.3662 |
| C8_2[d] | 209 ± 54 | 0.8271 | q8_2 | -0.0041 ± 0.0011 | 0.8065 | -0.0021 ± 5e-4 | -0.0048 ± 5e-4 | $\sigma_R^o$ | 0.52 | 0.9800 |
| C8a | -439 ± 84 | 0.8933 | q8a | 0.00313 ± 3.7e-4 | 0.9487 | 0.0031 ± 6e-4 | 0.00042 ± 2.4e-4 | $\sigma_R^+$ | 7.4 | 0.9299 |

[a]Resonance scales $\sigma_R^+$, $\sigma_R^o$, $\sigma_R^{BA}$ and $\sigma_R^-$ (from ref 22b) have been tested and the one which yields the best fit to the experimental data has been selected. [b]In each case for the minimum energy conformation. [c]For the X-*in* conformation. [d]For the X-*out* conformation.

**TABLE S2. Correlations of the atomic charges for 1-(*para*- and *meta*-substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines. DSP correlations were performed in each case with substituent parameters $\sigma_F$ and $\sigma_R$.**

**DHIQ *para*-substitution**

| | $\delta = \rho q + k$ | | $q = \rho\sigma + k$ | | | $q = \rho_F\sigma_F + \rho_R\sigma_R{}^a + k$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | $\rho \pm s$ | $r$ | | $\rho \pm s$ | $r$ | $\rho_F \pm s$ | $\rho_R \pm s$ | $\rho_F/\rho_R$ | $r$ |
| C1 | 55 ± 35 | 0.4842 | q1 | -0.0078 ± 0.0014 | 0.8956 | -0.0030 ± 0.0027 | -0.0141 ± 0.0026 | 0.21 | 0.9317 |
| N2 | 1110 ± 94 | 0.9723 | q2 | 0.00921 ± 9.7e-4 | 0.9587 | 0.0077 ± 0.0021 | 0.0132 ± 0.0020 | 0.58 | 0.9667 |
| C3 | -81 ± 8 | 0.9610 | q3 | -0.00389 ± 4.2e-4 | 0.9558 | -0.0054 ± 6e-4 | -0.0038 ± 6e-4 | 1.4 | 0.9837 |
| C4 | 158± 20 | 0.9414 | q4 | -0.00151 ±1.5e-4 | 0.9631 | -0.0020 ± 2e-4 | -0.00161 ± 2.2e-4 | 1.2 | 0.9849 |
| C4a | -273 ± 80 | 0.7706 | q4a | 6.1e-4 ± 6e-5 | 0.9633 | 8.9e-4 ± 1.1e-4 | 5.5e-4 ± 1.0e-4 | 1.6 | 0.9801 |
| C5 | 249 ± 13 | 0.9884 | q5 | 9.8e-4 ± 1.0e-4 | 0.9631 | 0.0014 ± 1e-4 | 9.6e-4 ± 9e-5 | 1.5 | 0.9934 |
| C6 | 245 ± 26 | 0.9575 | q6 | 0.00226 ± 2.9e-4 | 0.9390 | 0.0035 ± 5e-4 | 0.0019 ± 4e-4 | 1.8 | 0.9836 |
| C7 | 136 ± 15 | 0.9568 | q7 | 0.00207 ± 3.0e-4 | 0.9228 | 0.0036 ± 2e-4 | 0.0014 ± 2e-4 | 2.6 | 0.9956 |
| C8 | 160 ± 255 | 0.2166 | q8 | -4.3e-5 ± 3.8e-4 | 0.04016 | -0.0019 ± 5e-4 | 0.00149 ± 4.7e-4 | -1.3 | 0.8429 |
| C8a | -299 ± 51 | 0.9019 | q8a | 0.00217 ± 5.0e-4 | 0.8393 | 0.0025 ± 0.0011 | 0.0027 ± 0.0010 | 0.93 | 0.8718 |

**DHIQ *meta*-substitution**

| | $\delta = \rho q + k$ | | $q = \rho\sigma + k$ | | | $q = \rho_F\sigma_F + \rho_R\sigma_R + k$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $\rho \pm s$ | $r$ | | $\rho \pm s$ | $r$ | $\rho_F \pm s$ | $\rho_R \pm s$ | $\rho_F/\rho_R$ | $r$ |
| C1[b] | -187 ± 68 | 0.7195 | q1 | 0.0092 ± 0.0022 | 0.8265 | 0.0046 ± 0.0019 | 0.0093 ± 0.0018 | 0.49 | 0.9406 |
| C1_1[c] | -155 ± 48 | 0.7726 | q1_1 | 0.0108 ± 0.0028 | 0.8028 | 0.0056 ± 0.0027 | 0.0107 ± 0.0026 | 0.52 | 0.9164 |
| C1_2[d] | -298 ± 110 | 0.7151 | q1_2 | 0.0060 ± 0.0015 | 0.8179 | 0.0025 ± 9e-4 | 0.0068 ± 8e-4 | 0.37 | 0.9688 |
| N2[b] | 273 ± 436 | 0.2302 | q2 | -4e-4 ± 0,0029 | 0.0530 | 0.0028 ± 0.0038 | -0.0042 ± 0.0035 | -0.67 | 0.4157 |
| N2_1[c] | -597 ± 417 | 0.4761 | q2_1 | -0.0030 ± 0.0024 | 0.4052 | 0.0019 ± 0.0019 | -0.0079 ± 0.0018 | -0.24 | 0.8645 |
| N2_2[d] | 924 ± 214 | 0.8526 | q2_2 | 0.0076 ± 0.0019 | 0.8233 | 0.0069 ± 0.0026 | 0.0035 ± 0.0025 | 2.0 | 0.8315 |
| C3 | -46 ± 6 | 0.9498 | q3 | -0.00461 ± 5.3e-4 | 0.9515 | -0.0049 ± 6e-4 | -0.0012 ± 6e-4 | 4.1 | 0.9675 |
| C4 | 128 ± 14 | 0.9629 | q4 | -0.00163 ± 2.1e-4 | 0.9417 | -0.0018 ± 3e-4 | -3.2e-4 ± 2.5e-4 | 5.6 | 0.9553 |
| C4a | 125 ± 38 | 0.7779 | q4a | 0.00129 ± 1.8e-4 | 0.9281 | 0.0011 ± 2e-4 | 7.8e-4 ± 1.9e-4 | 1.4 | 0.9603 |
| C5 | 235 ± 22 | 0.9699 | q5 | 0.00159 ± 3.3e-4 | 0.8616 | 0.0014 ± 4e-4 | 8.4e-4 ± 3.9e-4 | 1.7 | 0.8962 |
| C6 | 204 ± 9 | 0.9926 | q6 | 0.00387 ± 3.0e-4 | 0.9769 | 0.0037 ± 4e-4 | 0.00152 ± 3.4e-4 | 2.4 | 0.9837 |
| C7 | 66 ± 5 | 0.9819 | q7 | 0.0056 ± 0.0010 | 0.8880 | 0.0047 ± 0.0012 | 0.0033 ± 0.0011 | 1.4 | 0.9244 |
| C8[b] | 150 ± 110 | 0.4569 | q8 | -0.0013 ± 0.0012 | 0.3732 | -4.8e-4 ± 0.00153 | -0.0019 ± 0.0014 | 0.25 | 0.5306 |
| C8_1[c] | 80 ± 143 | 0.2065 | q8_1 | -8e-4 ± 0.0010 | 0.2706 | -5.8e-4 ± 0.00148 | -7.7e-4 ± 0.00140 | 0.75 | 0.3237 |
| C8_2[d] | 209 ± 54 | 0.8271 | q8_2 | -0.0041 ± 0.0011 | 0.8065 | -0.0020 ± 8e-4 | -0.0044 ± 8e-4 | 0.45 | 0.9505 |
| C8a | -439 ± 84 | 0.8933 | q8a | 0.00313 ± 3.7e-4 | 0.9487 | 0.0030 ± 6e-4 | 0.0011 ± 6e-4 | 2.7 | 0.9346 |

[a]Calculated with substituent parameters $\sigma_F$ and $\sigma_R$ (from re. 21 and 22a). [b]In each case for the minimum energy conformation. [c]For the X-*in* conformation. [d]For the X-*out* conformation.

**TABLE S3. NMR Chemical shifts of 1-(substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines [$CDCl_3$, ppm $(CH_3)_4Si$ (0 ppm) as internal standard]**

| X | C–1 | N–2 | C–3 | C–4 | C–4a | C–5 | C-6 | C–7 | C–8 | C–8a |
|---|---|---|---|---|---|---|---|---|---|---|
| *p*-$NO_2$ | 165.15 | -68.4 | 48.00 | 25.84 | 132.59 | 110.56 | 151.47 | 147.39 | 110.77 | 120.74 |
| *m*-$NO_2$ | 164.75 | -70.3 | 47.88 | 25.88 | 132.74 | 110.60 | 151.47 | 147.40 | 110.77 | 120.61 |
| *p*-CN | 165.39 | -70.3 | 47.93 | 25.85 | 132.62 | 110.52 | 151.40 | 147.33 | 110.82 | 120.73 |
| *m*-CN | 164.94 | -71.3 | 47.85 | 25.87 | 132.71 | 110.57 | 151.44 | 147.36 | 110.82 | 120.68 |
| *p*-$CF_3$ | 165.70 | -72.2 | 47.85 | 25.91 | 132.60 | 110.44 | 151.25 | 147.29 | 111.07 | 121.08 |
| *m*-$CF_3$ | 165.58 | -74.2 | 47.77 | 25.91 | 132.69 | 110.46 | 151.25 | 147.28 | 111.03 | 120.98 |
| *p*-F | 165.70 | -77.1 | 47.67 | 25.99 | 132.68 | 110.34 | 151.10 | 147.15 | 111.34 | 121.40 |
| *m*-F | 165.61 | -74.2 | 47.75 | 25.94 | 132.60 | 110.35 | 151.10 | 147.18 | 111.24 | 121.17 |
| *p*-Cl | 165.70 | -76.1 | 47.72 | 25.95 | 132.63 | 110.37 | 151.07 | 147.18 | 111.21 | 121.23 |
| *m*-Cl | 165.54 | -74.2 | 47.77 | 25.93 | 132.60 | 110.37 | 151.14 | 147.21 | 111.21 | 121.14 |
| *p*-Br | 165.76 | -75.1 | 47.74 | 25.93 | 132.62 | 110.35 | 151.07 | 147.17 | 111.16 | 121.17 |
| *m*-Br | 165.42 | -74.2 | 47.77 | 25.92 | 132.59 | 110.35 | 151.12 | 147.20 | 111.15 | 121.11 |
| H | 166.69 | -77.0 | 47.72 | 26.03 | 132.61 | 110.28 | 150.91 | 147.09 | 111.60 | 121.62 |
| *p*-Me | 166.54 | -79.9 | 47.64 | 26.07 | 132.65 | 110.24 | 150.80 | 147.04 | 111.67 | 121.71 |
| *m*-Me | 166.80 | -78.0 | 47.69 | 26.04 | 132.59 | 110.24 | 150.86 | 147.06 | 111.69 | 121.70 |
| *p*-MeO | 166.06 | -81.9 | 47.57 | 26.09 | 132.77 | 110.26 | 150.77 | 147.02 | 111.64 | 121.70 |
| *m*-MeO | 166.59 | -78.0 | 47.68 | 26.01 | 132.59 | 110.25 | 150.94 | 147.09 | 111.62 | 121.59 |
| *p*-$N(Me)_2$ | 166.15 | -85.7 | 47.45 | 26.26 | 132.94 | 110.18 | 150.51 | 146.89 | 111.91 | 121.92 |

**TABLE S4. NMR Chemical shifts of 1-(substituted phenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines [$CDCl_3$, ppm $(CH_3)_4Si$ (0 ppm) as internal standard]**

| X | C–1 | N-2 | C–3 | C–4 | C–4a | C–5 | C–6 | C-7 | C–8 | C–8a |
|---|---|---|---|---|---|---|---|---|---|---|
| *p*-$NO_2$ | 60.67 | -331.9 | 41.63 | 29.11 | 127.76 | 111.71 | 148.04 | 147.30 | 110.57 | 128.21 |
| *m*-$NO_2$ | 60.67 | -331.2 | 41.61 | 29.13 | 127.90 | 111.78 | 148.08 | 147.32 | 110.64 | 128.24 |
| *p*-CN | 60.93 | -331.6 | 41.59 | 29.11 | 127.79 | 111.66 | 147.99 | 147.25 | 110.62 | 128.28 |
| *m*-CN | 60.58 | -331.4 | 41.48 | 29.10 | 127.85 | 111.74 | 148.04 | 147.29 | 110.64 | 128.27 |
| *p*-$CF_3$ | 60.93 | -330.7 | 41.68 | 29.21 | 127.78 | 111.60 | 147.89 | 147.21 | 110.75 | 128.82 |
| *m*-$CF_3$ | 61.06 | -330.7 | 41.82 | 29.18 | 127.80 | 111.63 | 147.92 | 147.22 | 110.77 | 128.84 |
| *p*-F | 60.81 | -329.7 | 41.97 | 29.29 | 127.67 | 111.47 | 147.70 | 147.09 | 110.81 | 129.77 |
| *m*-F | 60.93 | -330.7 | 41.70 | 29.22 | 127.68 | 111.52 | 147.79 | 147.13 | 110.81 | 129.14 |
| *p*-Cl | 60.80 | -330.2 | 41.85 | 29.24 | 127.68 | 111.49 | 147.74 | 147.12 | 110.75 | 129.36 |
| *m*-Cl | 60.94 | -330.7 | 41.68 | 29.21 | 127.72 | 111.53 | 147.80 | 147.15 | 110.80 | 129.00 |
| *p*-Br | 60.85 | -330.2 | 41.81 | 29.24 | 127.68 | 111.50 | 147.76 | 147.12 | 110.74 | 129.26 |
| *m*-Br | 60.93 | -330.6 | 41.67 | 29.20 | 127.72 | 111.53 | 147.81 | 147.15 | 110.80 | 128.95 |
| H | 61.47 | -330.1 | 41.89 | 29.34 | 127.68 | 111.42 | 147.60 | 147.04 | 110.96 | 129.88 |
| *p*-Me | 61.14 | -330.0 | 41.83 | 29.36 | 127.66 | 111.39 | 147.55 | 147.01 | 110.98 | 130.07 |
| *m*-Me | 61.49 | -329.7 | 41.97 | 29.37 | 127.67 | 111.39 | 147.57 | 147.02 | 111.02 | 129.99 |
| *p*-MeO | 60.88 | -329.4 | 41.98 | 29.36 | 127.64 | 111.39 | 147.54 | 147.00 | 110.93 | 130.29 |
| *m*-MeO | 61.44 | -330.2 | 41.86 | 29.30 | 127.63 | 111.41 | 147.62 | 147.04 | 110.93 | 129.70 |
| *p*-$N(Me)_2$ | 60.84 | -328.7 | 41.84 | 29.42 | 127.65 | 111.33 | 147.43 | 146.96 | 111.06 | 130.65 |

**TABLE S5. Correlation parameters ρ from eq 1 and $\rho_F$ and $\rho_R$ and from the DSP eq 2 (calculated with substituent parameters $\sigma_F$ and $\sigma_R$) for the NMR shift data of 1-(*para*- or *meta*-substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines.[a]**

| | ρ ± *s* | *r* | $\rho_F \pm s$ | $\rho_R \pm s$ | *r* | $\rho_F/\rho_R$ |
|---|---|---|---|---|---|---|
| ***para*-substituted series** | | | | | | |
| C1 | -0.70 ± 0.25 | 0.7008 | -2.22 ± 0.08 | 0.29 ± 0.12 | 0.9826 | -7.66 |
| N2 | 10.7 ± 0.5 | 0.9897 | 8.7 ± 0.3 | 15.6 ± 0.5 | 0.9972 | 0.56 |
| C3 | 0.33 ± 0.03 | 0.9773 | 0.24 ± 0.02 | 0.51 ± 0.03 | 0.9893 | 0.47 |
| C4 | -0.26 ± 0.01 | 0.9888 | -0.25 ± 0.02 | -0.33 ± 0.03 | 0.9797 | 0.76 |
| C4a | -0.19 ± 0.04 | 0.8602 | 0.01± 0.04 | -0.40± 0.05 | 0.9155 | -0.03 |
| C5 | 0.24 ± 0.03 | 0.9557 | 0.32 ± 0.02 | 0.25 ± 0.03 | 0.9850 | 1.28 |
| C6 | 0.61 ± 0.04 | 0.9834 | 0.68 ± 0.03 | 0.72 ± 0.04 | 0.9941 | 0.94 |
| C7 | 0.31 ± 0.02 | 0.9904 | 0.35 ± 0.09 | 0.38 ± 0.01 | 0.9972 | 0.92 |
| C8 | -0.76 ± 0.07 | 0.9638 | -1.12 ± 0.03 | -0.70 ± 0.04 | 0.9964 | 1.60 |
| C8a | -0.82 ± 0.09 | 0.9542 | -1.18 ± 0.05 | -0.77 ± 0.08 | 0.9884 | 1.53 |
| ***meta*-substituted series** | | | | | | |
| C1 | -2.90 ± 0.20 | 0.9830 | -2.77 ± 0.11 | -0.96 ± 0.24 | 0.9873 | 2.89 |
| N2 | 10.2 ± 1.1 | 0.9617 | 8.2 ± 0.5 | 6.1 ± 1.2 | 0.9771 | 1.34 |
| C3 | 0.24 ± 0.04 | 0.9276 | 0.17 ± 0.01 | 0.19 ± 0.03 | 0.9710 | 0.89 |
| C4 | -0.24 ± 0.02 | 0.9751 | -0.24 ± 0.02 | -0.07 ± 0.02 | 0.9870 | 3.43 |
| C4a | 0.18 ± 0.06 | 0.7646 | 0.12 ± 0.02 | 0.21 ± 0.05 | 0.9209 | 0.57 |
| C5 | 0.48 ± 0.07 | 0.9254 | 0.38 ± 0.02 | 0.37 ± 0.04 | 0.9858 | 1.03 |
| C6 | 0.83 ± 0.08 | 0.9657 | 0.73 ± 0.03 | 0.47 ± 0.06 | 0.9911 | 1.55 |
| C7 | 0.45 ± 0.05 | 0.9637 | 0.39 ± 0.01 | 0.28 ± 0.02 | 0.9949 | 1.39 |
| C8 | -1.30 ± 0.10 | 0.9784 | -1.16 ± 0.03 | -0.68 ± 0.06 | 0.9965 | 1.71 |
| C8a | -1.52 ± 0.11 | 0.9835 | -1.38 ±0.02 | -0.73 ± 0.04 | 0.9985 | 1.89 |

[a] *s*, standard deviation; *r*, correlation coefficient; $\sigma_F$ and $\sigma_R$ values are from ref 22a except those for Br which are from ref. 21.

**TABLE S6. Correlation parameters ρ from eq 1 and $\rho_F$ and $\rho_R$ and from the DSP eq 2 (calculated with substituent parameters $\sigma_F$ and $\sigma_R$) for the NMR shift data of 1-(*para*- or *meta*-substituted phenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines.[a]**

| | ρ ± *s* | *r* | $\rho_F \pm s$ | $\rho_R \pm s$ | *r* | $\rho_F/\rho_F$ |
|---|---|---|---|---|---|---|
| ***para*-substituted series** | | | | | | |
| C1 | -0.10 ± 0.16 | 0.2147 | -1.22 ± 0.10 | 0.73 ± 0.14 | 0.9077 | -1.67 |
| N2 | -1.88 ± 0.23 | 0.9453 | -1.55 ± 0.20 | -2.80 ± 0.30 | 0.9689 | 0.55 |
| C3 | -0.20 ± 0.07 | 0.7026 | -0.30 ± 0.08 | -0.21 ± 0.08 | 0.7205 | 1.43 |
| C4 | -0.21 ± 0.02 | 0.9546 | -0.30 ± 0.01 | -0.20 ± 0.02 | 0.9869 | 1.50 |
| C4a | 0.10 ± 0.02 | 0.8466 | 0.10 ± 0.02 | 0.13 ± 0.04 | 0.8610 | 0.77 |
| C5 | 0.25 ± 0.03 | 0.9508 | 0.33 ± 0.02 | 0.26 ± 0.03 | 0.9778 | 1.27 |
| C6 | 0.41 ± 0.04 | 0.9677 | 0.50 ± 0.02 | 0.40 ± 0.04 | 0.9880 | 1.25 |
| C7 | 0.23 ± 0.02 | 0.9550 | 0.30 ± 0.02 | 0.23 ± 0.03 | 0.9821 | 1.30 |
| C8 | -0.31 ± 0.04 | 0.9256 | -0.52 ± 0.01 | -0.24 ± 0.02 | 0.9945 | 2.17 |
| C8a | -1.66 ±0.16 | 0.9664 | -2.01 ± 0.13 | -1.91 ± 0.19 | 0.9826 | 1.05 |
| ***meta*-substituted series** | | | | | | |
| C1 | -1.26 ± 0.16 | 0.9465 | -1.23 ± 0.08 | -0.38 ±0.17 | 0.9625 | 3.24 |
| N2 | -1.97 ± 0.24 | 0.9531 | -1.63 ± 0.15 | -0.81 ± 0.32 | 0.9555 | 2.01 |
| C3 | -0.47± 0.09 | 0.9029 | -0.42 ± 0.05 | -0.08 ±0.11 | 0.9165 | 5.25 |
| C4 | -0.35 ± 0.03 | 0.9734 | -0.34 ±0.01 | -0.11 ±0.03 | 0.9854 | 3.09 |
| C4a | 0.29 ± 0.07 | 0.8581 | 0.23 ± 0.01 | 0.31 ±0.03 | 0.9891 | 0.73 |
| C5 | 0.52 ± 0.07 | 0.9456 | 0.44 ± 0.02 | 0.36 ± 0.04 | 0.9900 | 1.22 |
| C6 | 0.71 ± 0.06 | 0.9741 | 0.64 ± 0.01 | 0.38 ± 0.03 | 0.9969 | 1.68 |
| C7 | 0.41 ± 0.04 | 0.9648 | 0.36 ± 0.01 | 0.25 ± 0.02 | 0.9970 | 1.44 |
| C8 | -0.51 ± 0.04 | 0.9837 | -0.45 ± 0.02 | -0.22 ±0.04 | 0.9895 | 2.05 |
| C8a | -2.47± 0.16 | 0.9858 | -2.34 ± 0.05 | -0.99 ±0.10 | 0.9966 | 2.36 |

[a] *s*, standard deviation; *r*, correlation coefficient; $\sigma_F$ and $\sigma_R$ values are from ref 22a except those for Br which are from ref. 21.

**TABLE S7. Correlation parameters ρ from eq 1 and $\rho_F$ and $\rho_R$ and from the DSP eq 2 (calculated with substituent parameters given by Reynolds et al.[23]) for the NMR shift data of 1-(*para*- or *meta*-substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines.[a]**

| | ρ ± *s* | *r* | $\rho_F \pm s$ | $\rho_R \pm s$ | *r* | $\rho_F/\rho_R$ |
|---|---|---|---|---|---|---|
| ***para*-substituted series** | | | | | | |
| C1 | -0.70 ± 0.25 | 0.7008 | -2.22 ± 0.09 | 0.29 ± 0.14 | 0.9800 | -7.66 |
| N2 | 10.7 ± 0.5 | 0.9897 | 9.4 ± 0.3 | 16.7 ± 0.4 | 0.9983 | 0.56 |
| C3 | 0.33 ± 0.03 | 0.9773 | 0.27 ± 0.02 | 0.55 ± 0.03 | 0.9943 | 0.49 |
| C4 | -0.26 ± 0.01 | 0.9888 | -0.27 ± 0.03 | -0.35 ± 0.04 | 0.9735 | 0.77 |
| C4a | -0.19 ± 0.04 | 0.8602 | -0.006 ± 0.045 | -0.42 ± 0.07 | 0.8898 | 0.014 |
| C5 | 0.24 ± 0.03 | 0.9557 | 0.34 ± 0.02 | 0.27 ± 0.03 | 0.9874 | 1.26 |
| C6 | 0.61 ± 0.04 | 0.9834 | 0.71 ± 0.04 | 0.77 ± 0.05 | 0.9914 | 0.92 |
| C7 | 0.31 ± 0.02 | 0.9904 | 0.37 ± 0.01 | 0.41 ± 0.02 | 0.9974 | 0.90 |
| C8 | -0.76 ± 0.07 | 0.9638 | -1.15±0.02 | -0.76±0.03 | 0.9979 | 1.51 |
| C8a | -0.82 ± 0.09 | 0.9542 | -1.21±0.05 | -0.84±0.07 | 0.9918 | 1.44 |
| ***meta*-substituted series** | | | | | | |
| C1 | -2.90 ± 0.20 | 0.9830 | -2.82 ± 0.10 | -0.98 ± 0.21 | 0.9899 | 2.88 |
| N2 | 10.2 ± 1.1 | 0.9617 | 8.5 ± 0.5 | 6.1 ± 1.1 | 0.9773 | 1.39 |
| C3 | 0.24 ± 0.04 | 0.9276 | 0.18 ± 0.02 | 0.19 ± 0.03 | 0.9706 | 0.95 |
| C4 | -0.24 ± 0.02 | 0.9751 | -0.25 ± 0.01 | -0.08 ± 0.02 | 0.9870 | 3.13 |
| C4a | 0.18 ± 0.06 | 0.7646 | 0.12 ± 0.02 | 0.21 ± 0.05 | 0.8364 | 0.57 |
| C5 | 0.48 ± 0.07 | 0.9254 | 0.40 ± 0.02 | 0.37 ± 0.05 | 0.9826 | 1.08 |
| C6 | 0.83 ± 0.08 | 0.9657 | 0.75 ± 0.03 | 0.47 ± 0.06 | 0.9895 | 1.60 |
| C7 | 0.45 ± 0.05 | 0.9637 | 0.39 ± 0.01 | 0.29 ± 0.03 | 0.9937 | 1.34 |
| C8 | -1.30 ± 0.10 | 0.9784 | -1.19 ± 0.02 | -0.69 ± 0.05 | 0.9971 | 1.72 |
| C8a | -1.52 ± 0.11 | 0.9835 | -1.42 ± 0.02 | -0.74 ± 0.04 | 0.9984 | 1.92 |

[a] *s*, standard deviation; *r*, correlation coefficient; $\sigma_F$, $\sigma_R^o$ from ref 23.

**TABLE S8. Correlation parameters ρ from eq 1 and $\rho_F$ and $\rho_R$ and from the DSP eq 2 (calculated with substituent parameters given by Reynolds et al.[23]) for the NMR shift data of 1-(para- or meta-substituted phenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines[a]**

| | ρ ± s | *r* | $\rho_F$ ± s | $\rho_R$ ± s | *r* | $\rho_F/\rho_R$ |
|---|---|---|---|---|---|---|
| **para-substituted series** | | | | | | |
| C1 | -0.10 ± 0.16 | 0.2147 | -1.19 ± 0.10 | 0.78±0.15 | 0.8829 | -1.53 |
| N2 | -1.88 ± 0.23 | 0.9453 | -1.68 ± 0.22 | -2.98 ± 0.33 | 0.9691 | 0.56 |
| C3 | -0.20 ± 0.07 | 0.7026 | -0.31 ± 0.08 | -0.24 ± 0.13 | 0.7293 | 1.29 |
| C4 | -0.21 ± 0.02 | 0.9546 | -0.31 ± 0.01 | -0.22 ± 0.02 | 0.9900 | 1.41 |
| C4a | 0.10 ± 0.02 | 0.8466 | 0.11 ± 0.02 | 0.14 ± 0.04 | 0.8773 | 0.79 |
| C5 | 0.25 ± 0.03 | 0.9508 | 0.34 ± 0.02 | 0.28 ± 0.03 | 0.9819 | 1.21 |
| C6 | 0.41 ± 0.04 | 0.9677 | 0.56 ± 0.02 | 0.46 ± 0.03 | 0.9946 | 1.22 |
| C7 | 0.23 ± 0.02 | 0.9550 | 0.31 ± 0.02 | 0.26 ± 0.03 | 0.9872 | 1.19 |
| C8 | -0.31 ± 0.04 | 0.9256 | -0.53 ± 0.01 | -0.25 ± 0.02 | 0.9953 | 2.12 |
| C8a | -1.66 ±0.16 | 0.9664 | -2.10 ± 0.11 | -2.07 ± 0.18 | 0.9887 | 1.01 |
| **meta-substituted series** | | | | | | |
| C1 | -1.26 ± 0.16 | 0.9465 | -1.25 ± 0.08 | -0.38 ± 0.17 | 0.9663 | 3.29 |
| N2 | -1.97 ± 0.24 | 0.9531 | -1.67 ± 0.16 | -0.86 ± 0.34 | 0.9478 | 1.94 |
| C3 | -0.47± 0.09 | 0.9029 | -0.43 ± 0.05 | -0.09 ± 0.11 | 0.9054 | 4.78 |
| C4 | -0.35 ± 0.03 | 0.9734 | -0.34 ± 0.02 | -0.11 ± 0.03 | 0.9834 | 3.09 |
| C4a | 0.29 ± 0.07 | 0.8581 | 0.24 ± 0.02 | 0.31 ± 0.03 | 0.9819 | 0.77 |
| C5 | 0.52 ± 0.07 | 0.9456 | 0.45 ±0.02 | 0.36 ± 0.04 | 0.9870 | 1.25 |
| C6 | 0.71 ± 0.06 | 0.9741 | 0.66 ± 0.02 | 0.38 ± 0.04 | 0.9953 | 1.74 |
| C7 | 0.41 ± 0.04 | 0.9648 | 0.37 ± 0.01 | 0.25 ± 0.02 | 0.9967 | 1.48 |
| C8 | -0.51 ± 0.04 | 0.9837 | -0.46 ± 0.02 | -0.22 ± 0.04 | 0.9875 | 2.09 |
| C8a | -2.47± 0.16 | 0.9858 | -2.38 ± 0.05 | -1.03 ± 0.10 | 0.9968 | 2.31 |

[a] s, standard deviation; *r*, correlation coefficient; $\sigma_F$, $\sigma_R^o$ from ref 23.

**TABLE S9. Analytical data of 1-(substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines**

| X | Mp °C | Solvent | Lit mp °C | Formula | M.w. | Anal. Calcd/Found | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | C | H | N |
| *p*-$NO_2$ | 151-153 | ethyl acetate | 150-152[24c] | $C_{17}H_{16}N_2O_4$ | 312.33 | 65.38/65.50 | 5.16/5.36 | 8.97/8.85 |
| *m*-$NO_2$ | 114-115 | ethyl acetate | | $C_{17}H_{16}N_2O_4$ | 312.22 | 65.38/65.44 | 5.16/5.41 | 8.97/9.04 |
| *p*-CN | 146-147 | ethyl acetate | | $C_{18}H_{16}N_2O_2$ | 292.34 | 73.96/73.81 | 5.52/5.71 | 9.58/9.44 |
| *m*-CN | 156-158 | diisopropyl ether | | $C_{18}H_{16}N_2O_2$ | 292.34 | 73.96/74.04 | 5.52/5.57 | 9.58/9.41 |
| *p*-$CF_3$ | 134-136 | ethyl acetate | | $C_{18}H_{16}F_3NO_2$ | 335.33 | 64.47/64.39 | 4.81/4.94 | 4.18/4.31 |
| *m*-$CF_3$ | oil | | 163-165[a, 24b] | $C_{18}H_{17}ClF_3NO_2$ | 371.79 | 58.15/58.21 | 4.61/4.77 | 3.77/3.69 |
| *p*-F | 125-126 | diisopropyl ether | | $C_{17}H_{16}FNO_2$ | 285.32 | 71.56/71.60 | 5.65/5.54 | 4.91/5.02 |
| *m*-F | 128-130 | diisopropyl ether | | $C_{17}H_{16}FNO_2$ | 285.32 | 71.56/71.47 | 5.65/5.73 | 4.91/4.83 |
| *p*-Cl | 125-126 | ethyl acetate | 120-122[24c] | $C_{17}H_{16}ClNO_2$ | 301.78 | 67.66/67.50 | 5.34/5.56 | 4.64/4.66 |
| *m*-Cl | 113-114 | ethyl acetate | 107[25a] | $C_{17}H_{16}ClNO_2$ | 301.78 | 67.66/67.64 | 5.34/5.49 | 4.64/4.54 |
| *p*-Br | 147-149 | ethyl acetate | 138-140[24c] | $C_{17}H_{16}BrNO_2$ | 346.23 | 58.97/59.08 | 4.66/4.78 | 4.05/4.14 |
| *m*-Br | 102-104 | ethyl acetate | 150-152[a, 25b] | $C_{17}H_{16}BrNO_2$ | 346.23 | 58.97/58.85 | 4.66/4.70 | 4.05/4.11 |
| H | 120-121 | diisopropyl ether | 112-113[24c] | $C_{17}H_{17}NO_2$ | 267.33 | 76.38/76.61 | 6.41/6.62 | 5.24/5.18 |
| *p*-Me | 129-130 | diisopropyl ether | 123-124[24c] | $C_{18}H_{19}NO_2$ | 281.36 | 76.84/76.80 | 6.81/6.96 | 4.98/5.04 |
| *m*-Me | 90-92 | diisopropyl ether | | $C_{18}H_{19}NO_2$ | 281.36 | 76.84/76.76 | 6.81/6.99 | 4.98/4.83 |
| *p*-MeO | 122-124 | diisopropyl ether | 118-119[24c] | $C_{18}H_{19}NO_3$ | 297.36 | 72.71/72.81 | 6.44/6.49 | 4.71/4.64 |
| *m*-MeO | oil | | 98-99[25c] | $C_{18}H_{20}ClNO_3$ | 333.82 | 64.77/64.67 | 6.04/6.16 | 4.20/4.19 |
| *p*-$N(Me)_2$ | 150-151 | ethyl acetate | | $C_{19}H_{22}N2O_2$ | 310.40 | 73.52/73.40 | 7.14/7.20 | 9.02/8.87 |

[a]Mp of HCl salt.

**TABLE S10. Analytical data of 1-(substituted phenyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines**

| X | Mp °C | Solvent | Lit mp °C | Formula | M.w. | Anal. Calcd/Found | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | C | H | N |
| *p*-$NO_2$ | 142-145 | ethanol | 139-140[26a] | $C_{17}H_{18}N_2O_4$ | 314.35 | 64.96/65.00 | 5.77/5.90 | 8.91/8.71 |
| *m*-$NO_2$ | 106-110 | ethanol | 108-110[26a] | $C_{17}H_{18}N_2O_4$ | 314.35 | 64.96/64.77 | 5.77/5.87 | 8.91/8.91 |
| *p*-CN | 125-127 | ethyl acetate | | $C_{18}H_{18}N_2O_2$ | 294.36 | 73.45/73.39 | 6.16/6.26 | 9.52/9.47 |
| *m*-CN | 141-142 | ethyl acetate | | $C_{18}H_{18}N_2O_2$ | 294.36 | 73.45/73.40 | 6.16/6.23 | 9.52/9.61 |
| *p*-$CF_3$ | 150-151 | ethyl acetate | | $C_{18}H_{18}F_3NO_2$ | 337.35 | 64.09/64.10 | 5.38/5.44 | 4.15/4.24 |
| *m*-$CF_3$ | oil | | 163-165[a, 24b] | $C_{18}H_{19}ClF_3NO_2$ | 373.81 | 57.84/59.91 | 5.12/530 | 3.75/3.64 |
| *p*-F | 94-96 | ethyl acetate | | $C_{17}H_{18}FNO_2$ | 287.34 | 71.06/71.13 | 6.31/6.40 | 4.87/4.46 |
| *m*-F | 124-125 | ethyl acetate | | $C_{17}H_{18}FNO_2$ | 287.34 | 71.06/71.14 | 6.31/6.45 | 4.87/4.96 |
| *p*-Cl | 116-118 | ethyl acetate | 114-115[26a] | $C_{17}H_{18}ClNO_2$ | 303.79 | 67.21/67.12 | 5.97/6.04 | 4.61/4.60 |
| *m*-Cl | 118-120 | ethyl acetate | 115-116[26a] | $C_{17}H_{18}ClNO_2$ | 303.79 | 67.21/67.19 | 5.97/5.99 | 4.61/4.73 |
| *p*-Br | 132-134 | ethyl acetate | 130-132[26a] | $C_{17}H_{18}BrNO_2$ | 348.25 | 58.63/58.63 | 5.21/5.39 | 4.02/3.96 |
| *m*-Br | 102-103 | ethyl acetate | 110-111[26a] | $C_{17}H_{18}BrNO_2$ | 348.25 | 58.63/58.79 | 5.21/5.33 | 4.02/3.97 |
| H | 114-118 | ethyl acetate | 112-114[26b] | $C_{17}H_{19}NO_2$ | 269.35 | 75.81/75.60 | 7.11/7.20 | 5.20/5.30 |
| *p*-Me | 115-117 | diisopropyl ether | 109-110[26a] | $C_{18}H_{21}NO_2$ | 283.38 | 76.30/76.44 | 7.47/7.57 | 4.94/4.97 |
| *m*-Me | 108-110 | diisopropyl ether | | $C_{18}H_{21}NO_2$ | 283.38 | 76.30/76.50 | 7.47/7.48 | 4.94/5.04 |
| *p*-MeO | 96-97 | ethyl acetate | 145[a, 26c] | $C_{18}H_{21}NO_3$ | 299.37 | 72.22/72.30 | 7.07/7.20 | 4.68/4.40 |
| *m*-MeO | 96-98 | ethyl acetate | 95-96[24d] | $C_{18}H_{21}NO_3$ | 299.37 | 72.22/72.24 | 7.07/7.14 | 4.68/4.68 |
| *p*-$N(Me)_2$ | 97-99 | ethyl acetate | | $C_{19}H_{24}N_2O_2$ | 312.42 | 73.05/73.11 | 7.74/7.84 | 8.97/9.02 |

[a]Mp of HCl salt.

**TABLE S11. Atomic charges of 1-(substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines for the minimum energy structures**

| X | C–1 | N–2 | C–3 | C–4 | C–4a | C–5 | C-6 | C–7 | C–8 | C–8a | O–6 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *p*-$NO_2$ | 0.292755 | -0.513079 | -0.148710 | -0.354578 | 0.030507 | -0.279801 | 0.383194 | 0.354496 | -0.245376 | -0.063033 | -0.668826 |
| *m*-$NO_2$ | 0.304144 | -0.522354 | -0.147507 | -0.354024 | 0.030808 | -0.279651 | 0.383269 | 0.356299 | -0.243751 | -0.063325 | -0.669697 |
| *p*-CN | 0.293131 | -0.515518 | -0.147807 | -0.354288 | 0.030471 | -0.280005 | 0.382696 | 0.354088 | -0.245925 | -0.063576 | -0.668944 |
| *m*-CN | 0.299913 | -0.520539 | -0.147209 | -0.353949 | 0.030605 | -0.279837 | 0.382866 | 0.355525 | -0.246322 | -0.064284 | -0.669457 |
| *p*-$CF_3$ | 0.294993 | -0.517222 | -0.146720 | -0.353852 | 0.030275 | -0.280308 | 0.382002 | 0.353323 | -0.245384 | -0.064322 | -0.669187 |
| *m*-$CF_3$ | 0.300195 | -0.521315 | -0.146225 | -0.353628 | 0.030425 | -0.280239 | 0.382148 | 0.354246 | -0.245973 | -0.064550 | -0.669596 |
| *p*-F | 0.303387 | -0.524328 | -0.144718 | -0.353081 | 0.030129 | -0.280610 | 0.380913 | 0.352900 | -0.246546 | -0.066467 | -0.669457 |
| *m*-F | 0.295896 | -0.517168 | -0.145838 | -0.353680 | 0.030128 | -0.280653 | 0.381300 | 0.352335 | -0.244080 | -0.064567 | -0.669360 |
| *p*-Cl | 0.299329 | -0.520764 | -0.145699 | -0.353484 | 0.030275 | -0.280475 | 0.381457 | 0.353072 | -0.246182 | -0.065497 | -0.669339 |
| *m*-Cl | 0.296483 | -0.518070 | -0.146154 | -0.353835 | 0.030409 | -0.280472 | 0.381527 | 0.352749 | -0.245126 | -0.065109 | -0.669216 |
| *p*-Br | 0.298772 | -0.520136 | -0.145860 | -0.353537 | 0.030253 | -0.280458 | 0.381508 | 0.353110 | -0.246025 | -0.065325 | -0.669316 |
| *m*-Br | 0.297334 | -0.517914 | -0.146220 | -0.353834 | 0.030371 | -0.280461 | 0.381537 | 0.352804 | -0.245230 | -0.064888 | -0.669207 |
| H | 0.296958 | -0.521109 | -0.144151 | -0.352934 | 0.029969 | -0.280883 | 0.380322 | 0.351759 | -0.244856 | -0.066032 | -0.669733 |
| *p*-Me | 0.300501 | -0.523877 | -0.143506 | -0.352666 | 0.029777 | -0.281050 | 0.380016 | 0.351598 | -0.245107 | -0.066021 | -0.669823 |
| *m*-Me | 0.296404 | -0.521300 | -0.143845 | -0.352867 | 0.029863 | -0.281022 | 0.380150 | 0.351489 | -0.244271 | -0.065788 | -0.669860 |
| *p*-MeO | 0.301554 | -0.524730 | -0.143841 | -0.352626 | 0.029927 | -0.281078 | 0.380506 | 0.351892 | -0.245795 | -0.066553 | -0.669665 |
| *m*-MeO | 0.294785 | -0.524132 | -0.143905 | -0.352898 | 0.029639 | -0.281339 | 0.380854 | 0.351254 | -0.243139 | -0.065017 | -0.669818 |
| *p*-$N(Me)_2$ | 0.305264 | -0.528149 | -0.142625 | -0.352265 | 0.029554 | -0.281318 | 0.379667 | 0.351344 | -0.245658 | -0.066191 | -0.669856 |
| *m*-$N(Me)_2$ | 0.292889 | -0.517881 | -0.144288 | -0.352890 | 0.029682 | -0.280842 | 0.379936 | 0.351495 | -0.243987 | -0.066585 | -0.669648 |

**TABLE S12. Atomic charges of 1-(*meta*-substituted phenyl)-6,7-dimethoxy-3,4-dihydroisoquinolines in different conformations**[a]

| X | C–1 | N–2 | C–8 |
|---|---|---|---|
| ***m*-$NO_2$_1** | 0.304144 | -0.522354 | -0.243751 |
| *m*-$NO_2$_2 | 0.300875 | -0.516372 | -0.247057 |
| ***m*-CN_1** | 0.299913 | -0.520539 | -0.246322 |
| *m*-CN_2 | 0.298465 | -0.518022 | -0.246753 |
| ***m*-$CF_3$_1** | 0.300195 | -0.521315 | -0.245973 |
| *m*-$CF_3$_2 | 0.298769 | -0.519475 | -0.246076 |
| ***m*-F_1** | 0.295896 | -0.517168 | -0.244080 |
| *m*-F_2 | 0.295911 | -0.516882 | -0.243543 |
| *m*-Cl_1 | 0.296499 | -0.518643 | -0.244731 |
| ***m*-Cl_2** | 0.296483 | -0.518070 | -0.245126 |
| *m*-Br_1 | 0.297821 | -0.519158 | -0.244643 |
| ***m*-Br_2** | 0.297334 | -0.517914 | -0.245230 |
| H | 0.296958 | -0.521109 | -0.244856 |
| *m*-Me_1 | 0.295036 | -0.520160 | -0.244030 |
| ***m*-Me_2** | 0.296404 | -0.521300 | -0.244271 |
| *m*-MeO_1 | 0.290787 | -0.515541 | -0.245342 |
| ***m*-MeO_2** | 0.294785 | -0.524132 | -0.243139 |
| ***m*-$N(Me)_2$_1** | 0.292889 | -0.517881 | -0.243987 |
| *m*-$N(Me)_2$_2 | 0.293434 | -0.522962 | -0.242841 |

[a]In each case the minimum energy conformation in bold face. 1 refers to the X-*in* conformation and 2 to the X-*out* conformation (see Pictures S1 and S2).

**Table S13**. Calculated Energies (HF/6-31G*) for the *para* and *meta* DHIQ derivatives.[a]

| Phenyl substituent X | Energy in Hartrees |
|---|---|
| *p*-$NO_2$ | -1061,2772 |
| *p*-CN | -949,54084 |
| *p*-$CF_3$ | -1193,4276 |
| *p*-F | -956,65693 |
| *p*-Cl | -1316,7055 |
| *p*-Br | -3427,1125 |
| H | -857,80522 |
| *p*-Me | -896,84259 |
| *p*-MeO | -971,68348 |
| *p*-$NMe_2$ | -990,88385 |
| *m*-$NO_2$_1 | -1061,2773 |
| *m*-$NO_2$_2 | -1061,277 |
| *m*-CN_1 | -949,54078 |
| *m*-CN_2 | -949,54076 |
| *m*-$CF_3$_1 | -1193,4276 |
| *m*- $CF_3$_2 | -1193,4276 |
| *m*-F_1 | -956,65644 |
| *m*-F_2 | -956,65629 |
| *m*-Cl_1 | -1316,705 |
| *m*-Cl_2 | -1316,7052 |
| *m*-Br_1 | -3427,1121 |
| *m*-Br_2 | -3427,1122 |
| *m*-Me_1 | -896,84216 |
| *m*-Me_2 | -896,84225 |
| *m*-MeO_1 | -971,68489 |
| *m*-MeO_2 | -971,68561 |
| *m*-$NMe_2$_1 | -990,88252 |
| *m*-$NMe_2$_2 | -990,88216 |

[a] *m*-X_1 refers to the X-*in* conformation and *m*-X_2 refers to the X- *out* conformation (see Pictures S1 and S2).

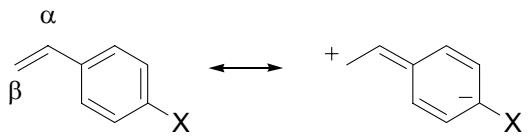
**On the DSP analysis of atomic charges**

A distinct difference in the $\rho_F/\rho_R$ ratio is observed when compared the correlation coefficients obtained for the atomic charges (Tables S1) with those obtained for the NMR chemical shift analysis (Tables 1 and 2). This obviously at least partly reflects the fact that due to the different intervening medium for the theoretical calculations (gas phase) and for the NMR measurements in solvent ($CDCl_3$), the through-space effects are experienced differently at some atoms. So, for instance for *para* C-1 for which the $\delta_C$ vs $q_C$(C-1) correlation is poor but $q_C$(C-1) shows a satisfactory DSP correlation, the $\rho_F/\rho_R$ ratio has a value of 0.24 (Table S1) while the corresponding value for the $\delta_C$(C-1) correlation has a value of -15.7 (Table 1). The latter $\rho_F/\rho_R$ value is exceptionally high and negative because of the small positive $\rho_R$ value, which is due to two contradicting resonance effects. At C-3, C-4a, C-5 and C-7 the $\rho_F/\rho_R$ ratio shows that the substituent effects observed with NMR shifts give smaller relative contribution of the inductive effect than the Mulliken atomic charges do. However, for other atoms (*para*) the situation is just opposite: The computational charge data show the contribution of the resonance effect higher than the NMR shift data do. Further, for C-8a the direction of the substituent effects on the atomic charges is normal while NMR chemical shift behavior shows a reverse trend. For C-8 the extents of $\rho_F$ and $\rho_R$ for the atomic charge correlations are closely similar but their signs are opposite. Both the NMR behavior and the Mulliken atomic charges show the general trends in the substituent sensitive polarization of the isoquinoline moiety but they give different significance of the resonance contributors possessing partial charges at the probe atoms.

**Examples of the use of the resonance polarization concept**

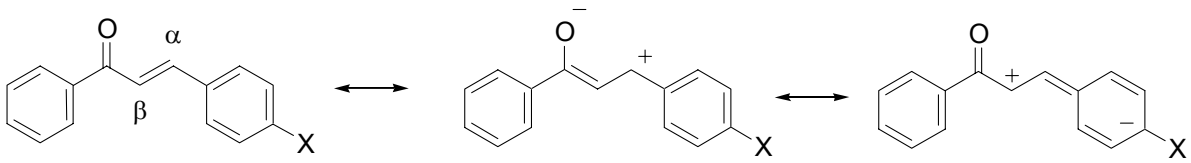
The resonance polarization concept was recently used by us in explaining the effect of various groups Y in X-$C_6H_4$-CH=N-Y on the sensitivity of the shielding of the C=N carbon towards substituent X. It was shown that groups Y capable to increase the contribution of the resonance structures possessing negative charge at the C=N carbon (X-$C_6H_4$-$CH^-$-N=$Y^+$ ) increase the substituent sensitivity of the $^{13}$C NMR chemical shift of the carbon in question to substitution X, both $\rho_F(X)$ and $\rho_R(X)$ being negative (cf. Scheme 1; **5**).[4d] There are in literature several other examples of substituent effects on NMR chemical shifts which can be explained by the resonance polarization model. For styrenes **1** an unbalance between the $\rho_F$ values for C($\alpha$) and C($\beta$) is observed (Scheme 10). This is thought to be a consequence of the extended polarization which increases the effect at C($\beta$).[1,2] On the other hand, for examples for chalcones[1] **28** and for barbiturates[17] **29** closely similar $\rho_F$ values are observed at C($\alpha$) and C($\beta$). The groups attached at the C=C system increase the contribution of the resonance structures possessing positive charge at C($\alpha$) and thereby increase the partial positive charge at the carbon in question, an enhanced substituent sensitivity to X as compared to **1** (a reverse effect; cf. Scheme 1; **4**) as a consequence.

**SCHEME 10.**



**1**

C-α: $\rho_I = -2.39$ $\rho_R = -0.36$
C-β: $\rho_I = 4.96$ $\rho_R = 8.9$

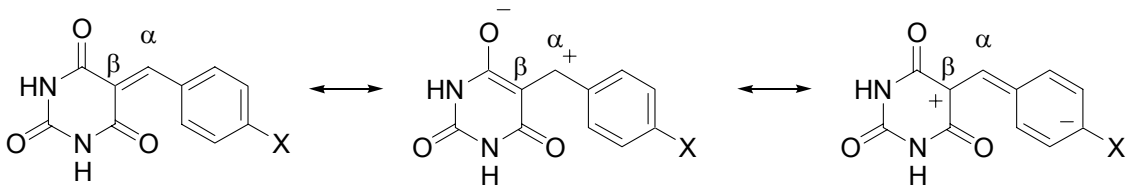


**28**

stabilized by EDG,
i.e., EDG causes deshielding
reverse effect at C(α)

stabilized by EWG,
i.e., EWG causes deshielding
normal effect at C(β)

C-α: $\rho_I = -4.0$ $\rho_R = -1.8$
C-β: $\rho_I = 4.5$ $\rho_R = 6.0$



**29**

C-α: $\rho_I = -4.32$ $\rho_R = -1.12$
C-β: $\rho_I = 4.43$ $\rho_R = 5.21$

**Cartesian coordinates for the optimized structures of the *para* and *meta* DHIQ derivatives**
The calculations were carried out at the Hartree-Fock level by means of 6-31G* split-valence basis set.

Iso_H

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.278581 | -0.174886 | -0.766848 |
| 2 | 6 | 0 | 0.199595 | -0.143384 | 0.621535 |
| 3 | 6 | 0 | 1.373395 | -0.066812 | 1.370795 |
| 4 | 6 | 0 | 2.593267 | 0.024111 | 0.722889 |
| 5 | 6 | 0 | 2.665507 | 0.013530 | -0.659541 |
| 6 | 6 | 0 | 1.499501 | -0.101345 | -1.409361 |
| 7 | 1 | 0 | -0.604191 | -0.259042 | -1.370953 |
| 8 | 6 | 0 | -1.092557 | -0.254859 | 1.368089 |
| 9 | 6 | 0 | 1.240228 | -0.097927 | 2.872707 |
| 10 | 1 | 0 | 3.510384 | 0.086872 | 1.280782 |
| 11 | 8 | 0 | 3.878394 | 0.067093 | -1.266177 |
| 12 | 8 | 0 | 1.549174 | -0.109304 | -2.769302 |
| 13 | 6 | 0 | 4.221773 | 1.309944 | -1.839773 |
| 14 | 6 | 0 | 1.889648 | -1.345536 | -3.355493 |
| 15 | 6 | 0 | 0.077768 | -1.010715 | 3.244165 |
| 16 | 7 | 0 | -1.153469 | -0.655684 | 2.561123 |
| 17 | 6 | 0 | -2.383137 | 0.103453 | 0.696797 |
| 18 | 6 | 0 | -2.504396 | 1.244079 | -0.089577 |
| 19 | 6 | 0 | -3.723037 | 1.584702 | -0.655063 |
| 20 | 6 | 0 | -4.831929 | 0.781604 | -0.450876 |
| 21 | 6 | 0 | -4.720024 | -0.357868 | 0.331374 |
| 22 | 6 | 0 | -3.506756 | -0.690131 | 0.906737 |
| 23 | 1 | 0 | 1.043930 | 0.904718 | 3.248520 |
| 24 | 1 | 0 | 2.159368 | -0.441463 | 3.335127 |
| 25 | 1 | 0 | 4.256949 | 2.083464 | -1.079706 |
| 26 | 1 | 0 | 3.516794 | 1.589883 | -2.610875 |
| 27 | 1 | 0 | 5.204480 | 1.187539 | -2.271454 |
| 28 | 1 | 0 | 1.883847 | -1.192543 | -4.425121 |
| 29 | 1 | 0 | 1.159531 | -2.105564 | -3.097428 |
| 30 | 1 | 0 | 2.873701 | -1.667310 | -3.039531 |
| 31 | 1 | 0 | -0.111837 | -0.971478 | 4.309613 |
| 32 | 1 | 0 | 0.325394 | -2.043370 | 3.001964 |
| 33 | 1 | 0 | -1.651566 | 1.877826 | -0.251417 |
| 34 | 1 | 0 | -3.803295 | 2.475636 | -1.251953 |
| 35 | 1 | 0 | -5.776270 | 1.041467 | -0.895189 |
| 36 | 1 | 0 | -5.578241 | -0.984871 | 0.495601 |
| 37 | 1 | 0 | -3.419797 | -1.562048 | 1.526644 |

Iso_mBr_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.041568 | -0.068799 | 0.005327 |
| 2 | 6 | 0 | -0.021305 | -0.074391 | 1.394979 |
| 3 | 6 | 0 | 1.161656 | -0.054278 | 2.133457 |
| 4 | 6 | 0 | 2.376518 | 0.019478 | 1.474470 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 2.433902 | 0.046777 | 0.091449 |
| 6 | 6 | 0 | 1.257260 | -0.013276 | -0.648683 |
| 7 | 1 | 0 | -0.848566 | -0.110440 | -0.592580 |
| 8 | 6 | 0 | -1.305753 | -0.169006 | 2.154358 |
| 9 | 6 | 0 | 1.043552 | -0.123442 | 3.635507 |
| 10 | 1 | 0 | 3.300948 | 0.039848 | 2.023233 |
| 11 | 8 | 0 | 3.640886 | 0.083029 | -0.526293 |
| 12 | 8 | 0 | 1.292010 | 0.015561 | -2.007874 |
| 13 | 6 | 0 | 4.012837 | 1.330695 | -1.072939 |
| 14 | 6 | 0 | 1.594917 | -1.211373 | -2.633744 |
| 15 | 6 | 0 | -0.142044 | -1.010291 | 3.996523 |
| 16 | 7 | 0 | -1.368885 | -0.600510 | 3.335741 |
| 17 | 6 | 0 | -2.595762 | 0.247968 | 1.514183 |
| 18 | 6 | 0 | -2.684082 | 1.414039 | 0.762740 |
| 19 | 6 | 0 | -3.903329 | 1.798765 | 0.236302 |
| 20 | 6 | 0 | -5.042314 | 1.042310 | 0.428828 |
| 21 | 6 | 0 | -4.950676 | -0.120422 | 1.177684 |
| 22 | 6 | 0 | -3.741713 | -0.512368 | 1.722109 |
| 23 | 1 | 0 | 0.883229 | 0.873829 | 4.041192 |
| 24 | 1 | 0 | 1.956260 | -0.508278 | 4.077368 |
| 25 | 1 | 0 | 4.076674 | 2.083266 | -0.294116 |
| 26 | 1 | 0 | 3.308169 | 1.648632 | -1.829262 |
| 27 | 1 | 0 | 4.987416 | 1.191795 | -1.517541 |
| 28 | 1 | 0 | 1.579588 | -1.026871 | -3.698134 |
| 29 | 1 | 0 | 0.849311 | -1.960393 | -2.388158 |
| 30 | 1 | 0 | 2.574482 | -1.565806 | -2.339790 |
| 31 | 1 | 0 | -0.320279 | -0.993241 | 5.064321 |
| 32 | 1 | 0 | 0.069913 | -2.043188 | 3.724203 |
| 33 | 1 | 0 | -1.819057 | 2.026407 | 0.598245 |
| 34 | 35 | 0 | -4.010526 | 3.404980 | -0.774194 |
| 35 | 1 | 0 | -5.978150 | 1.353957 | 0.006280 |
| 36 | 1 | 0 | -5.829888 | -0.718102 | 1.336911 |
| 37 | 1 | 0 | -3.675206 | -1.403259 | 2.316079 |

Iso_mBr_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.061598 | -0.072917 | -0.013121 |
| 2 | 6 | 0 | -0.014069 | -0.078728 | 1.375819 |
| 3 | 6 | 0 | 1.161907 | -0.053948 | 2.125117 |
| 4 | 6 | 0 | 2.382548 | 0.024013 | 1.477126 |
| 5 | 6 | 0 | 2.452547 | 0.051416 | 0.094708 |
| 6 | 6 | 0 | 1.282894 | -0.012230 | -0.656066 |
| 7 | 1 | 0 | -0.823195 | -0.119110 | -0.618541 |
| 8 | 6 | 0 | -1.305374 | -0.178432 | 2.123066 |
| 9 | 6 | 0 | 1.030247 | -0.123367 | 3.626091 |
| 10 | 1 | 0 | 3.301852 | 0.047094 | 2.034347 |
| 11 | 8 | 0 | 3.665105 | 0.091048 | -0.512152 |
| 12 | 8 | 0 | 1.329652 | 0.017639 | -2.015175 |
| 13 | 6 | 0 | 4.040073 | 1.339843 | -1.053159 |
| 14 | 6 | 0 | 1.641700 | -1.208581 | -2.638589 |
| 15 | 6 | 0 | -0.155721 | -1.013969 | 3.976854 |
| 16 | 7 | 0 | -1.377531 | -0.609203 | 3.304004 |
| 17 | 6 | 0 | -2.589464 | 0.233241 | 1.467937 |
| 18 | 6 | 0 | -3.728052 | -0.539971 | 1.672031 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 6 | 0 | -4.926387 | -0.151317 | 1.110035 |
| 20 | 6 | 0 | -5.031084 | 1.004012 | 0.355925 |
| 21 | 6 | 0 | -3.900786 | 1.778409 | 0.165761 |
| 22 | 6 | 0 | -2.686207 | 1.394702 | 0.711203 |
| 23 | 1 | 0 | 0.862982 | 0.873553 | 4.029977 |
| 24 | 1 | 0 | 1.940189 | -0.504955 | 4.076360 |
| 25 | 1 | 0 | 4.095341 | 2.091525 | -0.272741 |
| 26 | 1 | 0 | 3.342161 | 1.657822 | -1.815832 |
| 27 | 1 | 0 | 5.019052 | 1.203473 | -1.488807 |
| 28 | 1 | 0 | 1.636434 | -1.023816 | -3.703068 |
| 29 | 1 | 0 | 0.895625 | -1.959418 | -2.400420 |
| 30 | 1 | 0 | 2.619223 | -1.560488 | -2.335113 |
| 31 | 1 | 0 | -0.344144 | -0.996422 | 5.042827 |
| 32 | 1 | 0 | 0.062003 | -2.046410 | 3.707635 |
| 33 | 1 | 0 | -3.667320 | -1.427538 | 2.269012 |
| 34 | 35 | 0 | -6.470937 | -1.225973 | 1.378344 |
| 35 | 1 | 0 | -5.973679 | 1.289968 | -0.069716 |
| 36 | 1 | 0 | -3.967742 | 2.684103 | -0.409302 |
| 37 | 1 | 0 | -1.818978 | 2.009485 | 0.556964 |

Iso_mCF3_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.953325 | -0.756995 | -0.516941 |
| 2 | 6 | 0 | 0.911709 | -0.801369 | 0.872902 |
| 3 | 6 | 0 | 2.105777 | -0.797009 | 1.593522 |
| 4 | 6 | 0 | 3.310013 | -0.699092 | 0.918340 |
| 5 | 6 | 0 | 3.346128 | -0.632456 | -0.464063 |
| 6 | 6 | 0 | 2.158503 | -0.677503 | -1.187683 |
| 7 | 1 | 0 | 0.054634 | -0.787330 | -1.102724 |
| 8 | 6 | 0 | -0.360187 | -0.921905 | 1.649245 |
| 9 | 6 | 0 | 2.011187 | -0.910413 | 3.094582 |
| 10 | 1 | 0 | 4.242671 | -0.689945 | 1.453300 |
| 11 | 8 | 0 | 4.543222 | -0.573024 | -1.098620 |
| 12 | 8 | 0 | 2.171907 | -0.610616 | -2.545703 |
| 13 | 6 | 0 | 4.901055 | 0.690982 | -1.616824 |
| 14 | 6 | 0 | 2.472584 | -1.817345 | -3.210860 |
| 15 | 6 | 0 | 0.835098 | -1.813169 | 3.447247 |
| 16 | 7 | 0 | -0.403347 | -1.388236 | 2.818360 |
| 17 | 6 | 0 | -1.661084 | -0.488928 | 1.043529 |
| 18 | 6 | 0 | -1.770279 | 0.688926 | 0.319069 |
| 19 | 6 | 0 | -3.000632 | 1.098921 | -0.175251 |
| 20 | 6 | 0 | -4.131499 | 0.331694 | 0.038359 |
| 21 | 6 | 0 | -4.028322 | -0.846264 | 0.761899 |
| 22 | 6 | 0 | -2.806725 | -1.248972 | 1.265770 |
| 23 | 1 | 0 | 1.852830 | 0.073768 | 3.531811 |
| 24 | 1 | 0 | 2.932225 | -1.303715 | 3.510897 |
| 25 | 1 | 0 | 4.975243 | 1.421938 | -0.818597 |
| 26 | 1 | 0 | 4.182452 | 1.026651 | -2.352048 |
| 27 | 1 | 0 | 5.868447 | 0.568477 | -2.081439 |
| 28 | 1 | 0 | 2.440729 | -1.602403 | -4.269121 |
| 29 | 1 | 0 | 1.734742 | -2.577498 | -2.976234 |
| 30 | 1 | 0 | 3.458242 | -2.174202 | -2.941265 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 1 | 0 | 0.673565 | -1.829247 | 4.517692 |
| 32 | 1 | 0 | 1.046823 | -2.836369 | 3.140284 |
| 33 | 1 | 0 | -0.904274 | 1.301465 | 0.153598 |
| 34 | 6 | 0 | -3.079580 | 2.362773 | -0.984233 |
| 35 | 1 | 0 | -5.081828 | 0.649310 | -0.346390 |
| 36 | 1 | 0 | -4.904082 | -1.444370 | 0.936130 |
| 37 | 1 | 0 | -2.727303 | -2.150340 | 1.842484 |
| 38 | 9 | 0 | -2.283681 | 3.306313 | -0.504083 |
| 39 | 9 | 0 | -4.306165 | 2.859155 | -1.014020 |
| 40 | 9 | 0 | -2.714888 | 2.164756 | -2.244113 |

Iso_mCH3_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.001293 | -0.045297 | 0.034490 |
| 2 | 6 | 0 | -0.050761 | -0.071584 | 1.424196 |
| 3 | 6 | 0 | 1.138330 | -0.050341 | 2.152643 |
| 4 | 6 | 0 | 2.347409 | 0.043529 | 1.485205 |
| 5 | 6 | 0 | 2.393238 | 0.090305 | 0.102401 |
| 6 | 6 | 0 | 1.211115 | 0.031141 | -0.628341 |
| 7 | 1 | 0 | -0.894615 | -0.085492 | -0.554526 |
| 8 | 6 | 0 | -1.330922 | -0.189608 | 2.190377 |
| 9 | 6 | 0 | 1.032799 | -0.141643 | 3.654262 |
| 10 | 1 | 0 | 3.276019 | 0.064127 | 2.027019 |
| 11 | 8 | 0 | 3.595322 | 0.145371 | -0.525482 |
| 12 | 8 | 0 | 1.234919 | 0.080595 | -1.988235 |
| 13 | 6 | 0 | 3.953952 | 1.404783 | -1.051488 |
| 14 | 6 | 0 | 1.538008 | -1.136188 | -2.632784 |
| 15 | 6 | 0 | -0.141324 | -1.045470 | 4.010619 |
| 16 | 7 | 0 | -1.377636 | -0.639089 | 3.366544 |
| 17 | 6 | 0 | -2.626922 | 0.220398 | 1.559600 |
| 18 | 6 | 0 | -2.738748 | 1.400281 | 0.835364 |
| 19 | 6 | 0 | -3.952784 | 1.810177 | 0.293805 |
| 20 | 6 | 0 | -5.063263 | 0.999157 | 0.476686 |
| 21 | 6 | 0 | -4.965456 | -0.182137 | 1.196840 |
| 22 | 6 | 0 | -3.757514 | -0.569346 | 1.743663 |
| 23 | 1 | 0 | 0.864764 | 0.848212 | 4.075002 |
| 24 | 1 | 0 | 1.953062 | -0.522688 | 4.083950 |
| 25 | 1 | 0 | 4.021210 | 2.143244 | -0.259373 |
| 26 | 1 | 0 | 3.239833 | 1.732978 | -1.794664 |
| 27 | 1 | 0 | 4.924868 | 1.281160 | -1.508765 |
| 28 | 1 | 0 | 1.515956 | -0.937515 | -3.694678 |
| 29 | 1 | 0 | 0.796590 | -1.891296 | -2.393184 |
| 30 | 1 | 0 | 2.520547 | -1.491435 | -2.349715 |
| 31 | 1 | 0 | -0.310193 | -1.046024 | 5.080296 |
| 32 | 1 | 0 | 0.080415 | -2.072125 | 3.722249 |
| 33 | 1 | 0 | -1.871265 | 2.021794 | 0.698619 |
| 34 | 6 | 0 | -4.054214 | 3.120230 | -0.453709 |
| 35 | 1 | 0 | -6.010771 | 1.289648 | 0.056820 |
| 36 | 1 | 0 | -5.835882 | -0.799704 | 1.330721 |
| 37 | 1 | 0 | -3.678730 | -1.474783 | 2.314389 |
| 38 | 1 | 0 | -3.185257 | 3.284445 | -1.082054 |
| 39 | 1 | 0 | -4.122046 | 3.957772 | 0.235346 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | -4.933624 | 3.144486 | -1.087160 |

Iso_mCH3_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.120002 | -0.091804 | -0.068652 |
| 2 | 6 | 0 | 0.008747 | -0.125175 | 1.317429 |
| 3 | 6 | 0 | 1.164744 | -0.081032 | 2.096469 |
| 4 | 6 | 0 | 2.399016 | 0.042322 | 1.482145 |
| 5 | 6 | 0 | 2.503262 | 0.096118 | 0.102769 |
| 6 | 6 | 0 | 1.355311 | 0.013891 | -0.678421 |
| 7 | 1 | 0 | -0.748433 | -0.148691 | -0.696139 |
| 8 | 6 | 0 | -1.300212 | -0.274481 | 2.027616 |
| 9 | 6 | 0 | 0.997069 | -0.181420 | 3.591799 |
| 10 | 1 | 0 | 3.302753 | 0.081015 | 2.063568 |
| 11 | 8 | 0 | 3.729758 | 0.180469 | -0.472488 |
| 12 | 8 | 0 | 1.436514 | 0.069258 | -2.035842 |
| 13 | 6 | 0 | 4.082295 | 1.449929 | -0.978306 |
| 14 | 6 | 0 | 1.794433 | -1.137799 | -2.670442 |
| 15 | 6 | 0 | -0.170813 | -1.112561 | 3.894059 |
| 16 | 7 | 0 | -1.387054 | -0.730344 | 3.199119 |
| 17 | 6 | 0 | -2.575702 | 0.112453 | 1.342839 |
| 18 | 6 | 0 | -3.699721 | -0.695898 | 1.489370 |
| 19 | 6 | 0 | -4.913966 | -0.360461 | 0.911904 |
| 20 | 6 | 0 | -4.998134 | 0.824198 | 0.185290 |
| 21 | 6 | 0 | -3.893935 | 1.642563 | 0.041045 |
| 22 | 6 | 0 | -2.681176 | 1.287853 | 0.611526 |
| 23 | 1 | 0 | 0.789197 | 0.802508 | 4.008560 |
| 24 | 1 | 0 | 1.906321 | -0.544099 | 4.059186 |
| 25 | 1 | 0 | 4.098090 | 2.186341 | -0.181621 |
| 26 | 1 | 0 | 3.393971 | 1.764993 | -1.750894 |
| 27 | 1 | 0 | 5.074801 | 1.350157 | -1.393080 |
| 28 | 1 | 0 | 1.812765 | -0.935596 | -3.731737 |
| 29 | 1 | 0 | 1.061033 | -1.910517 | -2.464670 |
| 30 | 1 | 0 | 2.771988 | -1.471659 | -2.346992 |
| 31 | 1 | 0 | -0.385287 | -1.121800 | 4.955511 |
| 32 | 1 | 0 | 0.085888 | -2.132732 | 3.611704 |
| 33 | 1 | 0 | -3.612490 | -1.593522 | 2.072566 |
| 34 | 6 | 0 | -6.118423 | -1.262839 | 1.052782 |
| 35 | 1 | 0 | -5.933944 | 1.107147 | -0.265746 |
| 36 | 1 | 0 | -3.974646 | 2.560687 | -0.513345 |
| 37 | 1 | 0 | -1.830363 | 1.934596 | 0.499163 |
| 38 | 1 | 0 | -5.981045 | -1.979677 | 1.853785 |
| 39 | 1 | 0 | -6.297916 | -1.820287 | 0.137306 |
| 40 | 1 | 0 | -7.015182 | -0.690534 | 1.266598 |

Iso_mCN_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.043708 | -0.133241 | -0.023352 |
| 2 | 6 | 0 | -0.023477 | -0.062911 | 1.364478 |
| 3 | 6 | 0 | 1.156726 | 0.001222 | 2.104672 |
| 4 | 6 | 0 | 2.373213 | 0.044842 | 1.445951 |
| 5 | 6 | 0 | 2.434987 | -0.001526 | 0.063600 |
| 6 | 6 | 0 | 1.260906 | -0.107821 | -0.676087 |
| 7 | 1 | 0 | -0.843646 | -0.213800 | -0.621645 |
| 8 | 6 | 0 | -1.308688 | -0.118879 | 2.124749 |
| 9 | 6 | 0 | 1.034111 | 0.010973 | 3.608086 |
| 10 | 1 | 0 | 3.295853 | 0.098977 | 1.995367 |
| 11 | 8 | 0 | 3.643236 | 0.007969 | -0.551164 |
| 12 | 8 | 0 | 1.298573 | -0.152639 | -2.034089 |
| 13 | 6 | 0 | 4.010378 | 1.225897 | -1.165563 |
| 14 | 6 | 0 | 1.619717 | -1.407179 | -2.593532 |
| 15 | 6 | 0 | -0.150037 | -0.859138 | 4.012290 |
| 16 | 7 | 0 | -1.375818 | -0.486810 | 3.327042 |
| 17 | 6 | 0 | -2.598271 | 0.265203 | 1.463414 |
| 18 | 6 | 0 | -2.691684 | 1.380209 | 0.643604 |
| 19 | 6 | 0 | -3.917076 | 1.746317 | 0.097156 |
| 20 | 6 | 0 | -5.057517 | 0.996879 | 0.353948 |
| 21 | 6 | 0 | -4.965279 | -0.115635 | 1.171206 |
| 22 | 6 | 0 | -3.749320 | -0.472778 | 1.726342 |
| 23 | 1 | 0 | 0.870344 | 1.027682 | 3.960573 |
| 24 | 1 | 0 | 1.946332 | -0.347878 | 4.072048 |
| 25 | 1 | 0 | 4.068001 | 2.020561 | -0.429364 |
| 26 | 1 | 0 | 3.306251 | 1.497429 | -1.940164 |
| 27 | 1 | 0 | 4.986862 | 1.067310 | -1.598987 |
| 28 | 1 | 0 | 1.603056 | -1.279421 | -3.666074 |
| 29 | 1 | 0 | 0.884156 | -2.152261 | -2.308781 |
| 30 | 1 | 0 | 2.603648 | -1.731539 | -2.280459 |
| 31 | 1 | 0 | -0.331743 | -0.786689 | 5.077068 |
| 32 | 1 | 0 | 0.064658 | -1.904230 | 3.794459 |
| 33 | 1 | 0 | -1.824938 | 1.978108 | 0.434701 |
| 34 | 6 | 0 | -4.001576 | 2.918009 | -0.744416 |
| 35 | 1 | 0 | -5.997264 | 1.285137 | -0.078850 |
| 36 | 1 | 0 | -5.842064 | -0.701213 | 1.378313 |
| 37 | 1 | 0 | -3.679963 | -1.324842 | 2.374729 |
| 38 | 7 | 0 | -4.069828 | 3.838627 | -1.407274 |

Iso_mCN_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.052511 | -0.107915 | -0.023232 |
| 2 | 6 | 0 | -0.014487 | -0.065070 | 1.365608 |
| 3 | 6 | 0 | 1.165869 | -0.017538 | 2.106811 |
| 4 | 6 | 0 | 2.382475 | 0.035579 | 1.448805 |
| 5 | 6 | 0 | 2.444095 | 0.015826 | 0.065802 |
| 6 | 6 | 0 | 1.269693 | -0.071760 | -0.675598 |
| 7 | 1 | 0 | -0.835419 | -0.175754 | -0.622232 |
| 8 | 6 | 0 | -1.300153 | -0.134744 | 2.124324 |
| 9 | 6 | 0 | 1.043502 | -0.035637 | 3.610220 |
| 10 | 1 | 0 | 3.305315 | 0.075660 | 1.999109 |
| 11 | 8 | 0 | 3.652648 | 0.032249 | -0.548905 |
| 12 | 8 | 0 | 1.307073 | -0.088861 | -2.034736 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | 4.027263 | 1.260563 | -1.135965 |
| 14 | 6 | 0 | 1.620719 | -1.334536 | -2.618688 |
| 15 | 6 | 0 | -0.143102 | -0.909396 | 3.999429 |
| 16 | 7 | 0 | -1.367598 | -0.523380 | 3.319816 |
| 17 | 6 | 0 | -2.588806 | 0.257776 | 1.466441 |
| 18 | 6 | 0 | -3.730958 | -0.493744 | 1.712957 |
| 19 | 6 | 0 | -4.943888 | -0.123885 | 1.150860 |
| 20 | 6 | 0 | -5.038066 | 1.009652 | 0.349010 |
| 21 | 6 | 0 | -3.907044 | 1.765842 | 0.114935 |
| 22 | 6 | 0 | -2.690698 | 1.388828 | 0.664699 |
| 23 | 1 | 0 | 0.883068 | 0.975043 | 3.981301 |
| 24 | 1 | 0 | 1.954816 | -0.405565 | 4.067156 |
| 25 | 1 | 0 | 4.089337 | 2.038839 | -0.382664 |
| 26 | 1 | 0 | 3.325279 | 1.553278 | -1.904963 |
| 27 | 1 | 0 | 5.003028 | 1.106086 | -1.572540 |
| 28 | 1 | 0 | 1.607827 | -1.185404 | -3.688583 |
| 29 | 1 | 0 | 0.879247 | -2.079732 | -2.350495 |
| 30 | 1 | 0 | 2.601550 | -1.671835 | -2.309770 |
| 31 | 1 | 0 | -0.325231 | -0.854027 | 5.065050 |
| 32 | 1 | 0 | 0.068553 | -1.951311 | 3.764581 |
| 33 | 1 | 0 | -3.669049 | -1.357835 | 2.344994 |
| 34 | 6 | 0 | -6.122133 | -0.923233 | 1.400103 |
| 35 | 1 | 0 | -5.983603 | 1.287507 | -0.077908 |
| 36 | 1 | 0 | -3.968448 | 2.648908 | -0.494053 |
| 37 | 1 | 0 | -1.820348 | 1.989704 | 0.476185 |
| 38 | 7 | 0 | -7.051117 | -1.549528 | 1.590383 |

Iso_mCl_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.041770 | -0.068938 | 0.004788 |
| 2 | 6 | 0 | -0.021513 | -0.072866 | 1.394427 |
| 3 | 6 | 0 | 1.161215 | -0.052379 | 2.133247 |
| 4 | 6 | 0 | 2.376323 | 0.019814 | 1.474510 |
| 5 | 6 | 0 | 2.434147 | 0.045189 | 0.091459 |
| 6 | 6 | 0 | 1.257696 | -0.014908 | -0.648929 |
| 7 | 1 | 0 | -0.848289 | -0.110783 | -0.593237 |
| 8 | 6 | 0 | -1.306342 | -0.165640 | 2.153398 |
| 9 | 6 | 0 | 1.042509 | -0.119468 | 3.635347 |
| 10 | 1 | 0 | 3.300604 | 0.040386 | 2.023532 |
| 11 | 8 | 0 | 3.641352 | 0.079900 | -0.525976 |
| 12 | 8 | 0 | 1.292921 | 0.012206 | -2.008177 |
| 13 | 6 | 0 | 4.014300 | 1.326565 | -1.074183 |
| 14 | 6 | 0 | 1.595056 | -1.215751 | -2.632390 |
| 15 | 6 | 0 | -0.143759 | -1.005152 | 3.997054 |
| 16 | 7 | 0 | -1.370157 | -0.595475 | 3.335351 |
| 17 | 6 | 0 | -2.595748 | 0.251363 | 1.511845 |
| 18 | 6 | 0 | -2.682725 | 1.418403 | 0.762015 |
| 19 | 6 | 0 | -3.901060 | 1.804007 | 0.233389 |
| 20 | 6 | 0 | -5.039910 | 1.046108 | 0.422974 |
| 21 | 6 | 0 | -4.948916 | -0.117588 | 1.170172 |
| 22 | 6 | 0 | -3.741227 | -0.510293 | 1.716702 |
| 23 | 1 | 0 | 0.882555 | 0.878470 | 4.039607 |
| 24 | 1 | 0 | 1.954840 | -0.504166 | 4.078107 |
| 25 | 1 | 0 | 4.078995 | 2.080017 | -0.296275 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | 3.309775 | 1.644275 | -1.830745 |
| 27 | 1 | 0 | 4.988667 | 1.186287 | -1.518837 |
| 28 | 1 | 0 | 1.580851 | -1.032465 | -3.697016 |
| 29 | 1 | 0 | 0.848465 | -1.963725 | -2.386593 |
| 30 | 1 | 0 | 2.573998 | -1.570900 | -2.337189 |
| 31 | 1 | 0 | -0.322335 | -0.986659 | 5.064772 |
| 32 | 1 | 0 | 0.067692 | -2.038531 | 3.726098 |
| 33 | 1 | 0 | -1.818093 | 2.032537 | 0.599717 |
| 34 | 17 | 0 | -3.997752 | 3.281191 | -0.691786 |
| 35 | 1 | 0 | -5.974621 | 1.359484 | -0.001623 |
| 36 | 1 | 0 | -5.828213 | -0.715822 | 1.326696 |
| 37 | 1 | 0 | -3.675667 | -1.402032 | 2.309464 |

Iso_mCl_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.059552 | -0.073850 | -0.012475 |
| 2 | 6 | 0 | -0.015333 | -0.078594 | 1.376517 |
| 3 | 6 | 0 | 1.161120 | -0.053799 | 2.125091 |
| 4 | 6 | 0 | 2.381424 | 0.023111 | 1.476350 |
| 5 | 6 | 0 | 2.450624 | 0.049396 | 0.093873 |
| 6 | 6 | 0 | 1.280518 | -0.014204 | -0.656150 |
| 7 | 1 | 0 | -0.825630 | -0.119849 | -0.617310 |
| 8 | 6 | 0 | -1.306240 | -0.177363 | 2.124604 |
| 9 | 6 | 0 | 1.030359 | -0.122036 | 3.626185 |
| 10 | 1 | 0 | 3.301060 | 0.046174 | 2.033022 |
| 11 | 8 | 0 | 3.662826 | 0.088002 | -0.513778 |
| 12 | 8 | 0 | 1.326557 | 0.014786 | -2.015311 |
| 13 | 6 | 0 | 4.037901 | 1.336243 | -1.055983 |
| 14 | 6 | 0 | 1.637759 | -1.211989 | -2.638023 |
| 15 | 6 | 0 | -0.155658 | -1.012012 | 3.978300 |
| 16 | 7 | 0 | -1.377751 | -0.607448 | 3.305851 |
| 17 | 6 | 0 | -2.590693 | 0.234620 | 1.470129 |
| 18 | 6 | 0 | -3.729020 | -0.537977 | 1.676008 |
| 19 | 6 | 0 | -4.928384 | -0.149732 | 1.115162 |
| 20 | 6 | 0 | -5.032560 | 1.005469 | 0.360274 |
| 21 | 6 | 0 | -3.902064 | 1.779012 | 0.168626 |
| 22 | 6 | 0 | -2.686895 | 1.395677 | 0.712731 |
| 23 | 1 | 0 | 0.863644 | 0.875224 | 4.029446 |
| 24 | 1 | 0 | 1.940453 | -0.503578 | 4.076186 |
| 25 | 1 | 0 | 4.093808 | 2.088547 | -0.276212 |
| 26 | 1 | 0 | 3.339674 | 1.653804 | -1.818548 |
| 27 | 1 | 0 | 5.016604 | 1.199215 | -1.492041 |
| 28 | 1 | 0 | 1.631895 | -1.027991 | -3.702630 |
| 29 | 1 | 0 | 0.891564 | -1.962390 | -2.398847 |
| 30 | 1 | 0 | 2.615348 | -1.564034 | -2.334910 |
| 31 | 1 | 0 | -0.343448 | -0.993580 | 5.044373 |
| 32 | 1 | 0 | 0.061624 | -2.044728 | 3.709775 |
| 33 | 1 | 0 | -3.669381 | -1.425388 | 2.273899 |
| 34 | 17 | 0 | -6.346714 | -1.136039 | 1.364734 |
| 35 | 1 | 0 | -5.976448 | 1.290350 | -0.064052 |
| 36 | 1 | 0 | -3.969364 | 2.684309 | -0.406967 |

| | | | | | |
|---|---|---|---|---|---|
| 37 | 1 | 0 | -1.819689 | 2.010107 | 0.557288 |

Iso_mF_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.040210 | -0.096439 | -0.013849 |
| 2 | 6 | 0 | -0.020598 | -0.050282 | 1.375089 |
| 3 | 6 | 0 | 1.163637 | -0.012423 | 2.110636 |
| 4 | 6 | 0 | 2.378202 | 0.026156 | 1.447788 |
| 5 | 6 | 0 | 2.433587 | 0.001361 | 0.064750 |
| 6 | 6 | 0 | 1.255211 | -0.075113 | -0.670975 |
| 7 | 1 | 0 | -0.851844 | -0.151914 | -0.607564 |
| 8 | 6 | 0 | -1.305134 | -0.107296 | 2.138599 |
| 9 | 6 | 0 | 1.047397 | -0.023779 | 3.614381 |
| 10 | 1 | 0 | 3.303608 | 0.058547 | 1.994374 |
| 11 | 8 | 0 | 3.639998 | 0.003450 | -0.555870 |
| 12 | 8 | 0 | 1.287938 | -0.095912 | -2.030813 |
| 13 | 6 | 0 | 4.024137 | 1.227126 | -1.145435 |
| 14 | 6 | 0 | 1.578045 | -1.348104 | -2.611310 |
| 15 | 6 | 0 | -0.144877 | -0.886363 | 4.010494 |
| 16 | 7 | 0 | -1.369316 | -0.493817 | 3.335273 |
| 17 | 6 | 0 | -2.591776 | 0.294944 | 1.482027 |
| 18 | 6 | 0 | -3.734603 | -0.459839 | 1.721176 |
| 19 | 6 | 0 | -4.925066 | -0.067571 | 1.154831 |
| 20 | 6 | 0 | -5.035441 | 1.057073 | 0.364889 |
| 21 | 6 | 0 | -3.897096 | 1.811225 | 0.140504 |
| 22 | 6 | 0 | -2.680947 | 1.433199 | 0.687344 |
| 23 | 1 | 0 | 0.895846 | 0.989520 | 3.982070 |
| 24 | 1 | 0 | 1.957698 | -0.398926 | 4.069413 |
| 25 | 1 | 0 | 4.096713 | 2.005802 | -0.393401 |
| 26 | 1 | 0 | 3.322046 | 1.526073 | -1.911983 |
| 27 | 1 | 0 | 4.996748 | 1.063074 | -1.585840 |
| 28 | 1 | 0 | 1.562449 | -1.203161 | -3.681866 |
| 29 | 1 | 0 | 0.826021 | -2.080442 | -2.336866 |
| 30 | 1 | 0 | 2.554835 | -1.700583 | -2.306051 |
| 31 | 1 | 0 | -0.321699 | -0.826359 | 5.076984 |
| 32 | 1 | 0 | 0.058555 | -1.930739 | 3.778591 |
| 33 | 1 | 0 | -3.697518 | -1.330911 | 2.345091 |
| 34 | 9 | 0 | -6.012682 | -0.801931 | 1.377602 |
| 35 | 1 | 0 | -5.987593 | 1.324397 | -0.053369 |
| 36 | 1 | 0 | -3.958076 | 2.698397 | -0.463359 |
| 37 | 1 | 0 | -1.808905 | 2.033306 | 0.506327 |

Iso_mF_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.035801 | -0.112600 | -0.009331 |
| 2 | 6 | 0 | -0.022702 | -0.053945 | 1.379247 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 1.162568 | -0.004002 | 2.112402 |
| 4 | 6 | 0 | 2.375768 | 0.034108 | 1.447164 |
| 5 | 6 | 0 | 2.428865 | -0.003220 | 0.064277 |
| 6 | 6 | 0 | 1.249615 | -0.092263 | -0.668723 |
| 7 | 1 | 0 | -0.856796 | -0.177446 | -0.601351 |
| 8 | 6 | 0 | -1.305681 | -0.108061 | 2.145342 |
| 9 | 6 | 0 | 1.048670 | -0.001725 | 3.616360 |
| 10 | 1 | 0 | 3.301969 | 0.076310 | 1.991744 |
| 11 | 8 | 0 | 3.634106 | -0.000660 | -0.558334 |
| 12 | 8 | 0 | 1.280273 | -0.126114 | -2.028137 |
| 13 | 6 | 0 | 4.009728 | 1.219117 | -1.161915 |
| 14 | 6 | 0 | 1.576443 | -1.381858 | -2.597350 |
| 15 | 6 | 0 | -0.139754 | -0.865037 | 4.022280 |
| 16 | 7 | 0 | -1.367019 | -0.482769 | 3.345988 |
| 17 | 6 | 0 | -2.594846 | 0.283492 | 1.487524 |
| 18 | 6 | 0 | -2.679426 | 1.420956 | 0.692581 |
| 19 | 6 | 0 | -3.898115 | 1.773710 | 0.155086 |
| 20 | 6 | 0 | -5.039714 | 1.033343 | 0.362746 |
| 21 | 6 | 0 | -4.947308 | -0.100913 | 1.154029 |
| 22 | 6 | 0 | -3.739777 | -0.472430 | 1.718269 |
| 23 | 1 | 0 | 0.893918 | 1.014383 | 3.974812 |
| 24 | 1 | 0 | 1.961030 | -0.369293 | 4.073485 |
| 25 | 1 | 0 | 4.079559 | 2.006000 | -0.418255 |
| 26 | 1 | 0 | 3.304014 | 1.505851 | -1.929721 |
| 27 | 1 | 0 | 4.982211 | 1.055877 | -1.602908 |
| 28 | 1 | 0 | 1.557937 | -1.246978 | -3.669157 |
| 29 | 1 | 0 | 0.829116 | -2.115954 | -2.314667 |
| 30 | 1 | 0 | 2.555808 | -1.726016 | -2.290728 |
| 31 | 1 | 0 | -0.314708 | -0.796312 | 5.088597 |
| 32 | 1 | 0 | 0.067255 | -1.910675 | 3.799132 |
| 33 | 1 | 0 | -1.824875 | 2.040601 | 0.498018 |
| 34 | 9 | 0 | -3.969601 | 2.872462 | -0.593411 |
| 35 | 1 | 0 | -5.966091 | 1.343917 | -0.082649 |
| 36 | 1 | 0 | -5.825329 | -0.694992 | 1.332179 |
| 37 | 1 | 0 | -3.675234 | -1.340851 | 2.344560 |

Iso_mNMe2_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.143011 | -0.106604 | 0.035894 |
| 2 | 6 | 0 | -0.148707 | -0.173880 | 1.425220 |
| 3 | 6 | 0 | 1.061405 | -0.122283 | 2.116434 |
| 4 | 6 | 0 | 2.243337 | 0.040707 | 1.414428 |
| 5 | 6 | 0 | 2.242267 | 0.127443 | 0.032819 |
| 6 | 6 | 0 | 1.040435 | 0.039140 | -0.661974 |
| 7 | 1 | 0 | -1.055473 | -0.167165 | -0.525346 |
| 8 | 6 | 0 | -1.397962 | -0.367072 | 2.226645 |
| 9 | 6 | 0 | 1.008252 | -0.258123 | 3.617444 |
| 10 | 1 | 0 | 3.187398 | 0.085443 | 1.927322 |
| 11 | 8 | 0 | 3.420063 | 0.250094 | -0.630652 |
| 12 | 8 | 0 | 1.017954 | 0.127570 | -2.020007 |
| 13 | 6 | 0 | 3.710417 | 1.537667 | -1.129477 |
| 14 | 6 | 0 | 1.350475 | -1.056672 | -2.709010 |
| 15 | 6 | 0 | -0.116220 | -1.218786 | 3.985128 |
| 16 | 7 | 0 | -1.388358 | -0.848551 | 3.390793 |
| 17 | 6 | 0 | -2.729427 | 0.001524 | 1.644694 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 6 | 0 | -2.906133 | 1.209048 | 0.970046 |
| 19 | 6 | 0 | -4.150200 | 1.584005 | 0.478622 |
| 20 | 6 | 0 | -5.224091 | 0.712994 | 0.661118 |
| 21 | 6 | 0 | -5.048945 | -0.491596 | 1.311204 |
| 22 | 6 | 0 | -3.807918 | -0.850790 | 1.814247 |
| 23 | 1 | 0 | 0.814222 | 0.712474 | 4.070661 |
| 24 | 1 | 0 | 1.956568 | -0.612156 | 4.007408 |
| 25 | 1 | 0 | 3.772280 | 2.255579 | -0.318241 |
| 26 | 1 | 0 | 2.960620 | 1.856886 | -1.840799 |
| 27 | 1 | 0 | 4.670784 | 1.467725 | -1.619251 |
| 28 | 1 | 0 | 1.285475 | -0.829656 | -3.763457 |
| 29 | 1 | 0 | 0.649594 | -1.849241 | -2.468360 |
| 30 | 1 | 0 | 2.355740 | -1.377336 | -2.467531 |
| 31 | 1 | 0 | -0.250675 | -1.253906 | 5.059081 |
| 32 | 1 | 0 | 0.137845 | -2.227582 | 3.662466 |
| 33 | 1 | 0 | -2.063885 | 1.861207 | 0.844473 |
| 34 | 7 | 0 | -4.380574 | 2.817711 | -0.180310 |
| 35 | 1 | 0 | -6.197989 | 0.999883 | 0.308571 |
| 36 | 1 | 0 | -5.889987 | -1.148474 | 1.445972 |
| 37 | 1 | 0 | -3.675792 | -1.774018 | 2.344831 |
| 38 | 6 | 0 | -4.733231 | 2.705217 | -1.584477 |
| 39 | 6 | 0 | -3.426726 | 3.877232 | 0.058374 |
| 40 | 1 | 0 | -5.109195 | 3.659227 | -1.936052 |
| 41 | 1 | 0 | -5.511295 | 1.968312 | -1.723789 |
| 42 | 1 | 0 | -3.881433 | 2.422189 | -2.206798 |
| 43 | 1 | 0 | -3.243704 | 3.979522 | 1.120173 |
| 44 | 1 | 0 | -3.846025 | 4.809966 | -0.300966 |
| 45 | 1 | 0 | -2.469890 | 3.727820 | -0.446682 |

Iso_mNMe2_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.341544 | -0.052794 | -0.244546 |
| 2 | 6 | 0 | 0.100741 | -0.208347 | 1.116603 |
| 3 | 6 | 0 | 1.170047 | -0.151653 | 2.010104 |
| 4 | 6 | 0 | 2.445196 | 0.103305 | 1.535573 |
| 5 | 6 | 0 | 2.677088 | 0.276894 | 0.181932 |
| 6 | 6 | 0 | 1.618542 | 0.184138 | -0.715658 |
| 7 | 1 | 0 | -0.456833 | -0.112828 | -0.958696 |
| 8 | 6 | 0 | -1.255633 | -0.503671 | 1.676337 |
| 9 | 6 | 0 | 0.867271 | -0.384575 | 3.468917 |
| 10 | 1 | 0 | 3.283463 | 0.153978 | 2.207182 |
| 11 | 8 | 0 | 3.943714 | 0.488771 | -0.257803 |
| 12 | 8 | 0 | 1.826207 | 0.357059 | -2.049664 |
| 13 | 6 | 0 | 4.248337 | 1.815439 | -0.629733 |
| 14 | 6 | 0 | 2.324803 | -0.769267 | -2.735080 |
| 15 | 6 | 0 | -0.250759 | -1.413997 | 3.579938 |
| 16 | 7 | 0 | -1.419884 | -1.059589 | 2.795162 |
| 17 | 6 | 0 | -2.483996 | -0.146026 | 0.893847 |
| 18 | 6 | 0 | -3.542178 | -1.048131 | 0.864308 |
| 19 | 6 | 0 | -4.727153 | -0.762973 | 0.187719 |
| 20 | 6 | 0 | -4.826468 | 0.482424 | -0.445857 |
| 21 | 6 | 0 | -3.782589 | 1.382648 | -0.400316 |

| | | | | | |
|---|---|---|---|---|---|
| 22 | 6 | 0 | -2.601479 | 1.080128 | 0.257940 |
| 23 | 1 | 0 | 0.546374 | 0.545858 | 3.934089 |
| 24 | 1 | 0 | 1.751940 | -0.721703 | 3.998514 |
| 25 | 1 | 0 | 4.132710 | 2.484458 | 0.216663 |
| 26 | 1 | 0 | 3.616323 | 2.145783 | -1.442973 |
| 27 | 1 | 0 | 5.280910 | 1.815691 | -0.947457 |
| 28 | 1 | 0 | 2.432002 | -0.479023 | -3.770407 |
| 29 | 1 | 0 | 1.629262 | -1.599124 | -2.665044 |
| 30 | 1 | 0 | 3.287005 | -1.069719 | -2.340336 |
| 31 | 1 | 0 | -0.565082 | -1.524988 | 4.610366 |
| 32 | 1 | 0 | 0.108493 | -2.387793 | 3.249508 |
| 33 | 1 | 0 | -3.418890 | -1.966312 | 1.398366 |
| 34 | 7 | 0 | -5.777854 | -1.689115 | 0.110875 |
| 35 | 1 | 0 | -5.712595 | 0.749430 | -0.986782 |
| 36 | 1 | 0 | -3.890663 | 2.333976 | -0.890837 |
| 37 | 1 | 0 | -1.799900 | 1.794388 | 0.286526 |
| 38 | 6 | 0 | -7.129526 | -1.162361 | 0.127882 |
| 39 | 6 | 0 | -5.623923 | -2.939610 | 0.821215 |
| 40 | 1 | 0 | -7.826601 | -1.987425 | 0.072313 |
| 41 | 1 | 0 | -7.317950 | -0.532992 | -0.730424 |
| 42 | 1 | 0 | -7.347537 | -0.588818 | 1.029148 |
| 43 | 1 | 0 | -4.719486 | -3.442804 | 0.506015 |
| 44 | 1 | 0 | -6.456192 | -3.585061 | 0.573849 |
| 45 | 1 | 0 | -5.592844 | -2.822149 | 1.905404 |

Iso_mNO2_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.802887 | -0.580363 | -0.572625 |
| 2 | 6 | 0 | 0.732989 | -0.581085 | 0.816759 |
| 3 | 6 | 0 | 1.909897 | -0.512190 | 1.561777 |
| 4 | 6 | 0 | 3.124071 | -0.392485 | 0.908473 |
| 5 | 6 | 0 | 3.187790 | -0.367985 | -0.474434 |
| 6 | 6 | 0 | 2.018575 | -0.480223 | -1.220927 |
| 7 | 1 | 0 | -0.080478 | -0.662379 | -1.176565 |
| 8 | 6 | 0 | -0.548826 | -0.719924 | 1.571107 |
| 9 | 6 | 0 | 1.786616 | -0.581774 | 3.063550 |
| 10 | 1 | 0 | 4.044078 | -0.332414 | 1.461623 |
| 11 | 8 | 0 | 4.395079 | -0.284117 | -1.085108 |
| 12 | 8 | 0 | 2.057969 | -0.458684 | -2.579347 |
| 13 | 6 | 0 | 4.716724 | 0.974802 | -1.640109 |
| 14 | 6 | 0 | 2.427709 | -1.671501 | -3.197554 |
| 15 | 6 | 0 | 0.634029 | -1.512338 | 3.421767 |
| 16 | 7 | 0 | -0.603969 | -1.149710 | 2.753258 |
| 17 | 6 | 0 | -1.851629 | -0.348336 | 0.928945 |
| 18 | 6 | 0 | -1.981326 | 0.800273 | 0.162476 |
| 19 | 6 | 0 | -3.222786 | 1.131457 | -0.350997 |
| 20 | 6 | 0 | -4.343940 | 0.352889 | -0.138647 |
| 21 | 6 | 0 | -4.208638 | -0.791969 | 0.626898 |
| 22 | 6 | 0 | -2.978582 | -1.133464 | 1.160636 |
| 23 | 1 | 0 | 1.587113 | 0.409697 | 3.465934 |
| 24 | 1 | 0 | 2.710765 | -0.931055 | 3.510840 |
| 25 | 1 | 0 | 4.747294 | 1.734243 | -0.866153 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | 4.001454 | 1.257992 | -2.400085 |
| 27 | 1 | 0 | 5.697304 | 0.872586 | -2.081164 |
| 28 | 1 | 0 | 2.409364 | -1.492339 | -4.262689 |
| 29 | 1 | 0 | 1.719804 | -2.456594 | -2.952871 |
| 30 | 1 | 0 | 3.422183 | -1.973852 | -2.896072 |
| 31 | 1 | 0 | 0.449300 | -1.499241 | 4.488362 |
| 32 | 1 | 0 | 0.885421 | -2.537117 | 3.152723 |
| 33 | 1 | 0 | -1.145577 | 1.441674 | -0.028187 |
| 34 | 7 | 0 | -3.350412 | 2.348693 | -1.144284 |
| 35 | 1 | 0 | -5.286183 | 0.639670 | -0.559009 |
| 36 | 1 | 0 | -5.064884 | -1.414377 | 0.809509 |
| 37 | 1 | 0 | -2.878768 | -2.011626 | 1.768891 |
| 38 | 8 | 0 | -4.426577 | 2.608178 | -1.591845 |
| 39 | 8 | 0 | -2.372831 | 3.015567 | -1.301260 |

Iso_mNO2_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.151268 | 0.080388 | -0.804800 |
| 2 | 6 | 0 | 1.007236 | 0.022314 | 0.577638 |
| 3 | 6 | 0 | 2.142162 | 0.065467 | 1.386876 |
| 4 | 6 | 0 | 3.389086 | 0.214303 | 0.804612 |
| 5 | 6 | 0 | 3.526467 | 0.294878 | -0.570691 |
| 6 | 6 | 0 | 2.399131 | 0.212207 | -1.382536 |
| 7 | 1 | 0 | 0.301322 | 0.017881 | -1.457203 |
| 8 | 6 | 0 | -0.312964 | -0.152352 | 1.255234 |
| 9 | 6 | 0 | 1.939395 | -0.062791 | 2.876235 |
| 10 | 1 | 0 | 4.278015 | 0.252826 | 1.408247 |
| 11 | 8 | 0 | 4.764436 | 0.403935 | -1.112912 |
| 12 | 8 | 0 | 2.510666 | 0.293025 | -2.735105 |
| 13 | 6 | 0 | 5.115960 | 1.685551 | -1.590157 |
| 14 | 6 | 0 | 2.913313 | -0.893500 | -3.384413 |
| 15 | 6 | 0 | 0.772042 | -1.007122 | 3.138149 |
| 16 | 7 | 0 | -0.429012 | -0.624048 | 2.416208 |
| 17 | 6 | 0 | -1.580350 | 0.231547 | 0.552358 |
| 18 | 6 | 0 | -2.697217 | -0.585401 | 0.681211 |
| 19 | 6 | 0 | -3.877868 | -0.209572 | 0.074252 |
| 20 | 6 | 0 | -4.001439 | 0.965359 | -0.648080 |
| 21 | 6 | 0 | -2.892704 | 1.779999 | -0.762026 |
| 22 | 6 | 0 | -1.691891 | 1.412581 | -0.172048 |
| 23 | 1 | 0 | 1.716539 | 0.912581 | 3.305094 |
| 24 | 1 | 0 | 2.839676 | -0.428073 | 3.358051 |
| 25 | 1 | 0 | 5.103243 | 2.409059 | -0.781840 |
| 26 | 1 | 0 | 4.444167 | 2.004931 | -2.375379 |
| 27 | 1 | 0 | 6.119584 | 1.602132 | -1.980416 |
| 28 | 1 | 0 | 2.950006 | -0.669538 | -4.440590 |
| 29 | 1 | 0 | 2.194648 | -1.687229 | -3.209774 |
| 30 | 1 | 0 | 3.891195 | -1.208865 | -3.044678 |
| 31 | 1 | 0 | 0.529528 | -1.031886 | 4.192746 |
| 32 | 1 | 0 | 1.040117 | -2.021456 | 2.847353 |
| 33 | 1 | 0 | -2.642054 | -1.490618 | 1.248638 |
| 34 | 7 | 0 | -5.041053 | -1.081719 | 0.198498 |
| 35 | 1 | 0 | -4.937196 | 1.223338 | -1.100207 |
| 36 | 1 | 0 | -2.961001 | 2.701735 | -1.309330 |
| 37 | 1 | 0 | -0.840580 | 2.060663 | -0.268494 |

| | | | | | |
|---|---|---|---|---|---|
| 38 | 8 | 0 | -6.062174 | -0.716592 | -0.302436 |
| 39 | 8 | 0 | -4.906243 | -2.109149 | 0.789699 |

Iso_mOMe_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.738335 | -0.471204 | -0.586336 |
| 2 | 6 | 0 | 0.655671 | -0.427209 | 0.801398 |
| 3 | 6 | 0 | 1.825679 | -0.317880 | 1.552651 |
| 4 | 6 | 0 | 3.044982 | -0.208673 | 0.906789 |
| 5 | 6 | 0 | 3.120760 | -0.233417 | -0.475301 |
| 6 | 6 | 0 | 1.959349 | -0.380306 | -1.226469 |
| 7 | 1 | 0 | -0.141328 | -0.576411 | -1.191417 |
| 8 | 6 | 0 | -0.634606 | -0.560017 | 1.546902 |
| 9 | 6 | 0 | 1.689335 | -0.332853 | 3.054484 |
| 10 | 1 | 0 | 3.959143 | -0.120034 | 1.466031 |
| 11 | 8 | 0 | 4.333757 | -0.161044 | -1.079846 |
| 12 | 8 | 0 | 2.013502 | -0.402604 | -2.586102 |
| 13 | 6 | 0 | 4.651297 | 1.082363 | -1.667108 |
| 14 | 6 | 0 | 2.377967 | -1.638866 | -3.156801 |
| 15 | 6 | 0 | 0.546130 | -1.265653 | 3.435499 |
| 16 | 7 | 0 | -0.690725 | -0.949148 | 2.743606 |
| 17 | 6 | 0 | -1.934378 | -0.238270 | 0.872046 |
| 18 | 6 | 0 | -2.072726 | 0.894732 | 0.092234 |
| 19 | 6 | 0 | -3.299611 | 1.215482 | -0.485218 |
| 20 | 6 | 0 | -4.389855 | 0.385934 | -0.292029 |
| 21 | 6 | 0 | -4.242747 | -0.754458 | 0.492019 |
| 22 | 6 | 0 | -3.037115 | -1.069280 | 1.077244 |
| 23 | 1 | 0 | 1.470538 | 0.670138 | 3.416668 |
| 24 | 1 | 0 | 2.614444 | -0.650426 | 3.523558 |
| 25 | 1 | 0 | 4.669440 | 1.864870 | -0.915696 |
| 26 | 1 | 0 | 3.941144 | 1.338762 | -2.441603 |
| 27 | 1 | 0 | 5.636766 | 0.975896 | -2.096808 |
| 28 | 1 | 0 | 2.373644 | -1.498217 | -4.228169 |
| 29 | 1 | 0 | 1.660511 | -2.408972 | -2.892885 |
| 30 | 1 | 0 | 3.366387 | -1.939759 | -2.833716 |
| 31 | 1 | 0 | 0.351959 | -1.215572 | 4.499675 |
| 32 | 1 | 0 | 0.816755 | -2.296001 | 3.208652 |
| 33 | 1 | 0 | -1.248466 | 1.561810 | -0.076009 |
| 34 | 8 | 0 | -3.318630 | 2.352150 | -1.213730 |
| 35 | 1 | 0 | -5.343383 | 0.605365 | -0.731545 |
| 36 | 1 | 0 | -5.092657 | -1.396413 | 0.641736 |
| 37 | 1 | 0 | -2.934417 | -1.940020 | 1.695099 |
| 38 | 6 | 0 | -4.509034 | 2.766860 | -1.818380 |
| 39 | 1 | 0 | -4.282830 | 3.691229 | -2.328543 |
| 40 | 1 | 0 | -5.286173 | 2.946953 | -1.082808 |
| 41 | 1 | 0 | -4.862042 | 2.039100 | -2.541799 |

Iso_mOMe_1a

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

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.537778 | -0.523483 | -0.652513 |
| 2 | 6 | 0 | 0.540244 | -0.528732 | 0.738545 |
| 3 | 6 | 0 | 1.757096 | -0.542112 | 1.419602 |
| 4 | 6 | 0 | 2.941425 | -0.504352 | 0.703789 |
| 5 | 6 | 0 | 2.934028 | -0.478791 | -0.680294 |
| 6 | 6 | 0 | 1.722305 | -0.501958 | -1.363320 |
| 7 | 1 | 0 | -0.381900 | -0.537826 | -1.205092 |
| 8 | 6 | 0 | -0.712241 | -0.586203 | 1.555622 |
| 9 | 6 | 0 | 1.707803 | -0.605946 | 2.925603 |
| 10 | 1 | 0 | 3.890946 | -0.511877 | 1.208412 |
| 11 | 8 | 0 | 4.111415 | -0.479628 | -1.355370 |
| 12 | 8 | 0 | 1.693891 | -0.470452 | -2.723559 |
| 13 | 6 | 0 | 4.498114 | 0.756732 | -1.914811 |
| 14 | 6 | 0 | 1.922216 | -1.706477 | -3.362837 |
| 15 | 6 | 0 | 0.514090 | -1.456072 | 3.343826 |
| 16 | 7 | 0 | -0.730256 | -1.012482 | 2.740671 |
| 17 | 6 | 0 | -2.015829 | -0.139112 | 0.964832 |
| 18 | 6 | 0 | -2.095830 | 1.054180 | 0.243902 |
| 19 | 6 | 0 | -3.313746 | 1.483238 | -0.256216 |
| 20 | 6 | 0 | -4.456123 | 0.714479 | -0.051811 |
| 21 | 6 | 0 | -4.369654 | -0.462926 | 0.658621 |
| 22 | 6 | 0 | -3.155302 | -0.894859 | 1.175873 |
| 23 | 1 | 0 | 1.596187 | 0.396419 | 3.335411 |
| 24 | 1 | 0 | 2.628634 | -1.016825 | 3.325446 |
| 25 | 1 | 0 | 4.624149 | 1.503658 | -1.137903 |
| 26 | 1 | 0 | 3.769455 | 1.101653 | -2.636014 |
| 27 | 1 | 0 | 5.445354 | 0.588380 | -2.406123 |
| 28 | 1 | 0 | 1.865398 | -1.520004 | -4.425611 |
| 29 | 1 | 0 | 1.161566 | -2.427973 | -3.083517 |
| 30 | 1 | 0 | 2.900457 | -2.097336 | -3.113929 |
| 31 | 1 | 0 | 0.387537 | -1.431958 | 4.418977 |
| 32 | 1 | 0 | 0.683442 | -2.495382 | 3.065723 |
| 33 | 1 | 0 | -1.208853 | 1.637694 | 0.096652 |
| 34 | 8 | 0 | -3.491214 | 2.626245 | -0.952377 |
| 35 | 1 | 0 | -5.389437 | 1.061196 | -0.454837 |
| 36 | 1 | 0 | -5.255544 | -1.052302 | 0.815124 |
| 37 | 1 | 0 | -3.091502 | -1.802969 | 1.743341 |
| 38 | 6 | 0 | -2.398103 | 3.458269 | -1.214843 |
| 39 | 1 | 0 | -2.783580 | 4.292766 | -1.781361 |
| 40 | 1 | 0 | -1.642097 | 2.947992 | -1.802532 |
| 41 | 1 | 0 | -1.950776 | 3.827499 | -0.297847 |

Iso_mOMe_1b

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.617099 | -0.539490 | -0.712881 |
| 2 | 6 | 0 | 0.617331 | -0.543457 | 0.678172 |
| 3 | 6 | 0 | 1.833004 | -0.558841 | 1.361598 |
| 4 | 6 | 0 | 3.018578 | -0.524294 | 0.648130 |
| 5 | 6 | 0 | 3.013606 | -0.501091 | -0.736076 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 1.803188 | -0.523045 | -1.421334 |
| 7 | 1 | 0 | -0.300943 | -0.550444 | -1.268223 |
| 8 | 6 | 0 | -0.635371 | -0.598766 | 1.493981 |
| 9 | 6 | 0 | 1.781487 | -0.620853 | 2.867609 |
| 10 | 1 | 0 | 3.967188 | -0.532735 | 1.154430 |
| 11 | 8 | 0 | 4.192247 | -0.505218 | -1.408542 |
| 12 | 8 | 0 | 1.778439 | -0.495960 | -2.781332 |
| 13 | 6 | 0 | 4.578305 | 0.728116 | -1.975939 |
| 14 | 6 | 0 | 1.999962 | -1.735184 | -3.415983 |
| 15 | 6 | 0 | 0.586490 | -1.469360 | 3.285020 |
| 16 | 7 | 0 | -0.656256 | -1.024717 | 2.679406 |
| 17 | 6 | 0 | -1.938671 | -0.149878 | 0.905336 |
| 18 | 6 | 0 | -2.031335 | 1.024422 | 0.167472 |
| 19 | 6 | 0 | -3.255933 | 1.446660 | -0.323468 |
| 20 | 6 | 0 | -4.396374 | 0.695190 | -0.101373 |
| 21 | 6 | 0 | -4.305309 | -0.476948 | 0.632178 |
| 22 | 6 | 0 | -3.089124 | -0.895127 | 1.141635 |
| 23 | 1 | 0 | 1.670361 | 0.382054 | 3.276243 |
| 24 | 1 | 0 | 2.701303 | -1.032290 | 3.269211 |
| 25 | 1 | 0 | 4.703514 | 1.479827 | -1.203569 |
| 26 | 1 | 0 | 3.849635 | 1.067962 | -2.699321 |
| 27 | 1 | 0 | 5.525896 | 0.557011 | -2.465656 |
| 28 | 1 | 0 | 1.946604 | -1.551683 | -4.479423 |
| 29 | 1 | 0 | 1.234024 | -2.450983 | -3.136234 |
| 30 | 1 | 0 | 2.975132 | -2.131884 | -3.163766 |
| 31 | 1 | 0 | 0.458215 | -1.444284 | 4.360000 |
| 32 | 1 | 0 | 0.755199 | -2.509087 | 3.008008 |
| 33 | 1 | 0 | -1.162441 | 1.623813 | -0.032261 |
| 34 | 8 | 0 | -3.327026 | 2.593784 | -1.056795 |
| 35 | 1 | 0 | -5.333977 | 1.026201 | -0.509676 |
| 36 | 1 | 0 | -5.187998 | -1.066137 | 0.805787 |
| 37 | 1 | 0 | -3.020580 | -1.794386 | 1.722891 |
| 38 | 6 | 0 | -3.590486 | 3.763871 | -0.324356 |
| 39 | 1 | 0 | -3.616703 | 4.578268 | -1.033979 |
| 40 | 1 | 0 | -2.812260 | 3.949809 | 0.408963 |
| 41 | 1 | 0 | -4.546335 | 3.699596 | 0.185751 |

Iso_mOMe_2

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.977602 | 0.014387 | -0.725757 |
| 2 | 6 | 0 | 0.819349 | -0.035874 | 0.655332 |
| 3 | 6 | 0 | 1.945304 | 0.027667 | 1.475382 |
| 4 | 6 | 0 | 3.197518 | 0.183438 | 0.905989 |
| 5 | 6 | 0 | 3.348657 | 0.251702 | -0.468251 |
| 6 | 6 | 0 | 2.230792 | 0.152698 | -1.290405 |
| 7 | 1 | 0 | 0.132525 | -0.053537 | -1.383419 |
| 8 | 6 | 0 | -0.509868 | -0.220599 | 1.316580 |
| 9 | 6 | 0 | 1.726604 | -0.084331 | 2.963393 |
| 10 | 1 | 0 | 4.079134 | 0.237216 | 1.519304 |
| 11 | 8 | 0 | 4.592394 | 0.367727 | -0.999483 |
| 12 | 8 | 0 | 2.358933 | 0.223315 | -2.643504 |
| 13 | 6 | 0 | 4.934994 | 1.649387 | -1.480457 |
| 14 | 6 | 0 | 2.763196 | -0.970098 | -3.276005 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 6 | 0 | 0.566753 | -1.038559 | 3.221552 |
| 16 | 7 | 0 | -0.631073 | -0.681196 | 2.482367 |
| 17 | 6 | 0 | -1.767204 | 0.136938 | 0.581983 |
| 18 | 6 | 0 | -2.849798 | -0.719356 | 0.643575 |
| 19 | 6 | 0 | -4.044271 | -0.400148 | 0.004842 |
| 20 | 6 | 0 | -4.158748 | 0.792756 | -0.690537 |
| 21 | 6 | 0 | -3.069905 | 1.654979 | -0.739994 |
| 22 | 6 | 0 | -1.879587 | 1.338100 | -0.121114 |
| 23 | 1 | 0 | 1.486138 | 0.893751 | 3.376487 |
| 24 | 1 | 0 | 2.625428 | -0.432187 | 3.461201 |
| 25 | 1 | 0 | 4.908175 | 2.377623 | -0.676558 |
| 26 | 1 | 0 | 4.266863 | 1.958223 | -2.273047 |
| 27 | 1 | 0 | 5.942935 | 1.574682 | -1.862015 |
| 28 | 1 | 0 | 2.814517 | -0.757272 | -4.334159 |
| 29 | 1 | 0 | 2.038972 | -1.759330 | -3.103110 |
| 30 | 1 | 0 | 3.735463 | -1.287471 | -2.921445 |
| 31 | 1 | 0 | 0.313485 | -1.053951 | 4.274259 |
| 32 | 1 | 0 | 0.852892 | -2.053021 | 2.947468 |
| 33 | 1 | 0 | -2.785892 | -1.638002 | 1.193136 |
| 34 | 8 | 0 | -5.029551 | -1.315411 | 0.119928 |
| 35 | 1 | 0 | -5.069097 | 1.063520 | -1.188988 |
| 36 | 1 | 0 | -3.163742 | 2.584900 | -1.272121 |
| 37 | 1 | 0 | -1.050874 | 2.019815 | -0.168086 |
| 38 | 6 | 0 | -6.274747 | -1.071666 | -0.466608 |
| 39 | 1 | 0 | -6.891240 | -1.926811 | -0.233093 |
| 40 | 1 | 0 | -6.194785 | -0.975173 | -1.544612 |
| 41 | 1 | 0 | -6.737437 | -0.178177 | -0.060293 |

Iso_mOMe_2a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.826940 | 0.001180 | -0.923129 |
| 2 | 6 | 0 | 0.820732 | 0.001142 | 0.467920 |
| 3 | 6 | 0 | 2.033593 | 0.024450 | 1.156141 |
| 4 | 6 | 0 | 3.220618 | 0.095848 | 0.447656 |
| 5 | 6 | 0 | 3.221003 | 0.117165 | -0.936491 |
| 6 | 6 | 0 | 2.014813 | 0.054559 | -1.626592 |
| 7 | 1 | 0 | -0.088038 | -0.040656 | -1.481703 |
| 8 | 6 | 0 | -0.433005 | -0.093584 | 1.279405 |
| 9 | 6 | 0 | 1.977738 | -0.041661 | 2.661687 |
| 10 | 1 | 0 | 4.166753 | 0.118126 | 0.958135 |
| 11 | 8 | 0 | 4.401985 | 0.150343 | -1.604251 |
| 12 | 8 | 0 | 1.994060 | 0.078513 | -2.987065 |
| 13 | 6 | 0 | 4.752052 | 1.396005 | -2.167862 |
| 14 | 6 | 0 | 2.265196 | -1.152440 | -3.618630 |
| 15 | 6 | 0 | 0.811939 | -0.934037 | 3.069884 |
| 16 | 7 | 0 | -0.442785 | -0.528002 | 2.462201 |
| 17 | 6 | 0 | -1.746788 | 0.326319 | 0.690809 |
| 18 | 6 | 0 | -2.878459 | -0.441586 | 0.969738 |
| 19 | 6 | 0 | -4.113927 | -0.059602 | 0.480805 |
| 20 | 6 | 0 | -4.231020 | 1.099886 | -0.284103 |
| 21 | 6 | 0 | -3.114260 | 1.859819 | -0.546641 |
| 22 | 6 | 0 | -1.865443 | 1.477915 | -0.068321 |
| 23 | 1 | 0 | 1.827603 | 0.955404 | 3.071916 |
| 24 | 1 | 0 | 2.909888 | -0.420444 | 3.066927 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 1 | 0 | 4.849782 | 2.150125 | -1.393913 |
| 26 | 1 | 0 | 4.016615 | 1.713996 | -2.894434 |
| 27 | 1 | 0 | 5.706889 | 1.255532 | -2.653225 |
| 28 | 1 | 0 | 2.209421 | -0.972921 | -4.682669 |
| 29 | 1 | 0 | 1.525780 | -1.896335 | -3.340735 |
| 30 | 1 | 0 | 3.253587 | -1.511437 | -3.361763 |
| 31 | 1 | 0 | 0.678958 | -0.919759 | 4.144517 |
| 32 | 1 | 0 | 1.018389 | -1.965561 | 2.787376 |
| 33 | 1 | 0 | -2.761660 | -1.315428 | 1.577051 |
| 34 | 8 | 0 | -5.259748 | -0.741382 | 0.688873 |
| 35 | 1 | 0 | -5.200534 | 1.379199 | -0.652539 |
| 36 | 1 | 0 | -3.209263 | 2.759692 | -1.127789 |
| 37 | 1 | 0 | -1.004848 | 2.085708 | -0.276176 |
| 38 | 6 | 0 | -5.245467 | -1.895269 | 1.479992 |
| 39 | 1 | 0 | -6.265428 | -2.247977 | 1.516501 |
| 40 | 1 | 0 | -4.904586 | -1.681299 | 2.487196 |
| 41 | 1 | 0 | -4.617708 | -2.666402 | 1.045854 |

Iso_pBr_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.052698 | -0.077493 | -0.073673 |
| 2 | 6 | 0 | -0.065026 | -0.204285 | 1.306679 |
| 3 | 6 | 0 | 1.085668 | -0.197165 | 2.094533 |
| 4 | 6 | 0 | 2.321077 | -0.015603 | 1.497122 |
| 5 | 6 | 0 | 2.431815 | 0.132621 | 0.125161 |
| 6 | 6 | 0 | 1.289220 | 0.086377 | -0.667536 |
| 7 | 1 | 0 | -0.810393 | -0.107602 | -0.710631 |
| 8 | 6 | 0 | -1.373392 | -0.417576 | 1.998765 |
| 9 | 6 | 0 | 0.911715 | -0.401337 | 3.578775 |
| 10 | 1 | 0 | 3.221184 | -0.003617 | 2.085191 |
| 11 | 8 | 0 | 3.659399 | 0.272418 | -0.434833 |
| 12 | 8 | 0 | 1.375820 | 0.233936 | -2.016898 |
| 13 | 6 | 0 | 3.996892 | 1.576979 | -0.855812 |
| 14 | 6 | 0 | 1.760118 | -0.920410 | -2.730474 |
| 15 | 6 | 0 | -0.244929 | -1.366168 | 3.810945 |
| 16 | 7 | 0 | -1.462387 | -0.952065 | 3.135826 |
| 17 | 6 | 0 | -2.652874 | -0.000504 | 1.340028 |
| 18 | 6 | 0 | -2.772120 | 1.213152 | 0.673416 |
| 19 | 6 | 0 | -3.979859 | 1.606987 | 0.120257 |
| 20 | 6 | 0 | -5.073416 | 0.770888 | 0.227285 |
| 21 | 6 | 0 | -4.981689 | -0.442115 | 0.886147 |
| 22 | 6 | 0 | -3.774099 | -0.817244 | 1.445010 |
| 23 | 1 | 0 | 0.689192 | 0.549118 | 4.060490 |
| 24 | 1 | 0 | 1.823197 | -0.783506 | 4.025465 |
| 25 | 1 | 0 | 3.997812 | 2.260396 | -0.013167 |
| 26 | 1 | 0 | 3.308581 | 1.931466 | -1.611058 |
| 27 | 1 | 0 | 4.992942 | 1.517283 | -1.269446 |
| 28 | 1 | 0 | 1.780025 | -0.645189 | -3.775030 |
| 29 | 1 | 0 | 1.040180 | -1.718576 | -2.582820 |
| 30 | 1 | 0 | 2.742009 | -1.257258 | -2.424028 |
| 31 | 1 | 0 | -0.465297 | -1.450470 | 4.867629 |
| 32 | 1 | 0 | 0.025287 | -2.361187 | 3.460333 |
| 33 | 1 | 0 | -1.925563 | 1.869518 | 0.591986 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 1 | 0 | -4.065831 | 2.550226 | -0.383991 |
| 35 | 35 | 0 | -6.729350 | 1.294718 | -0.540399 |
| 36 | 1 | 0 | -5.840344 | -1.081018 | 0.963691 |
| 37 | 1 | 0 | -3.695214 | -1.747970 | 1.973036 |

Iso_pCF3_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.421375 | -0.464077 | -0.632184 |
| 2 | 6 | 0 | 1.426079 | -0.457342 | 0.758905 |
| 3 | 6 | 0 | 2.643453 | -0.457597 | 1.439170 |
| 4 | 6 | 0 | 3.826243 | -0.416979 | 0.721322 |
| 5 | 6 | 0 | 3.816993 | -0.402126 | -0.663023 |
| 6 | 6 | 0 | 2.604604 | -0.440638 | -1.344852 |
| 7 | 1 | 0 | 0.502353 | -0.491029 | -1.185632 |
| 8 | 6 | 0 | 0.178317 | -0.516548 | 1.580004 |
| 9 | 6 | 0 | 2.596936 | -0.509755 | 2.945903 |
| 10 | 1 | 0 | 4.776485 | -0.413326 | 1.224466 |
| 11 | 8 | 0 | 4.992977 | -0.399072 | -1.338698 |
| 12 | 8 | 0 | 2.573339 | -0.421791 | -2.704327 |
| 13 | 6 | 0 | 5.368225 | 0.835039 | -1.912846 |
| 14 | 6 | 0 | 2.819187 | -1.659438 | -3.334928 |
| 15 | 6 | 0 | 1.410021 | -1.364299 | 3.374411 |
| 16 | 7 | 0 | 0.162164 | -0.934571 | 2.767644 |
| 17 | 6 | 0 | -1.131307 | -0.076042 | 0.997816 |
| 18 | 6 | 0 | -1.239417 | 1.084225 | 0.241745 |
| 19 | 6 | 0 | -2.469682 | 1.503321 | -0.237971 |
| 20 | 6 | 0 | -3.603213 | 0.755950 | 0.026606 |
| 21 | 6 | 0 | -3.507281 | -0.404794 | 0.781416 |
| 22 | 6 | 0 | -2.281251 | -0.812256 | 1.268083 |
| 23 | 1 | 0 | 2.480410 | 0.495073 | 3.347983 |
| 24 | 1 | 0 | 3.520731 | -0.912084 | 3.347169 |
| 25 | 1 | 0 | 5.488609 | 1.591189 | -1.144204 |
| 26 | 1 | 0 | 4.635489 | 1.165201 | -2.636633 |
| 27 | 1 | 0 | 6.316151 | 0.668898 | -2.403286 |
| 28 | 1 | 0 | 2.757286 | -1.481345 | -4.398699 |
| 29 | 1 | 0 | 2.069803 | -2.389908 | -3.048605 |
| 30 | 1 | 0 | 3.803598 | -2.033537 | -3.085065 |
| 31 | 1 | 0 | 1.283647 | -1.330780 | 4.449119 |
| 32 | 1 | 0 | 1.584493 | -2.404947 | 3.105232 |
| 33 | 1 | 0 | -0.367393 | 1.676547 | 0.035792 |
| 34 | 1 | 0 | -2.540065 | 2.410030 | -0.808066 |
| 35 | 6 | 0 | -4.934315 | 1.167781 | -0.535656 |
| 36 | 1 | 0 | -4.387250 | -0.982222 | 0.995413 |
| 37 | 1 | 0 | -2.205454 | -1.698106 | 1.868338 |
| 38 | 9 | 0 | -4.983493 | 2.463556 | -0.800969 |
| 39 | 9 | 0 | -5.926577 | 0.897671 | 0.298523 |
| 40 | 9 | 0 | -5.207085 | 0.533516 | -1.668238 |

Iso_pCH3_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.566711 | -0.253324 | -0.747129 |
| 2 | 6 | 0 | 0.567498 | -0.252376 | 0.643858 |
| 3 | 6 | 0 | 1.784274 | -0.252236 | 1.325532 |
| 4 | 6 | 0 | 2.968700 | -0.203912 | 0.610687 |
| 5 | 6 | 0 | 2.962279 | -0.182844 | -0.773459 |
| 6 | 6 | 0 | 1.751595 | -0.222674 | -1.457107 |
| 7 | 1 | 0 | -0.351780 | -0.280422 | -1.301025 |
| 8 | 6 | 0 | -0.684715 | -0.319582 | 1.461229 |
| 9 | 6 | 0 | 1.734923 | -0.317968 | 2.831367 |
| 10 | 1 | 0 | 3.917782 | -0.200155 | 1.116195 |
| 11 | 8 | 0 | 4.140241 | -0.172437 | -1.447767 |
| 12 | 8 | 0 | 1.723927 | -0.199291 | -2.817649 |
| 13 | 6 | 0 | 4.511793 | 1.066781 | -2.011295 |
| 14 | 6 | 0 | 1.969605 | -1.435496 | -3.449284 |
| 15 | 6 | 0 | 0.551996 | -1.184914 | 3.245603 |
| 16 | 7 | 0 | -0.696699 | -0.750405 | 2.645679 |
| 17 | 6 | 0 | -1.990253 | 0.121320 | 0.876374 |
| 18 | 6 | 0 | -2.102515 | 1.272648 | 0.110182 |
| 19 | 6 | 0 | -3.335996 | 1.689266 | -0.369590 |
| 20 | 6 | 0 | -4.487063 | 0.962590 | -0.108736 |
| 21 | 6 | 0 | -4.370601 | -0.192532 | 0.661701 |
| 22 | 6 | 0 | -3.147918 | -0.603041 | 1.152171 |
| 23 | 1 | 0 | 1.608846 | 0.681984 | 3.242784 |
| 24 | 1 | 0 | 2.660961 | -0.717077 | 3.231236 |
| 25 | 1 | 0 | 4.628047 | 1.817869 | -1.236923 |
| 26 | 1 | 0 | 3.779146 | 1.400209 | -2.733839 |
| 27 | 1 | 0 | 5.461318 | 0.908548 | -2.501663 |
| 28 | 1 | 0 | 1.910881 | -1.256232 | -4.513250 |
| 29 | 1 | 0 | 1.218852 | -2.165963 | -3.166201 |
| 30 | 1 | 0 | 2.952959 | -1.811632 | -3.197726 |
| 31 | 1 | 0 | 0.425907 | -1.168191 | 4.321066 |
| 32 | 1 | 0 | 0.734724 | -2.220603 | 2.961948 |
| 33 | 1 | 0 | -1.230792 | 1.863370 | -0.105491 |
| 34 | 1 | 0 | -3.394877 | 2.592507 | -0.951501 |
| 35 | 6 | 0 | -5.831422 | 1.396150 | -0.644379 |
| 36 | 1 | 0 | -5.249661 | -0.773690 | 0.882809 |
| 37 | 1 | 0 | -3.077376 | -1.485859 | 1.758763 |
| 38 | 1 | 0 | -5.774740 | 2.374030 | -1.108098 |
| 39 | 1 | 0 | -6.571659 | 1.444489 | 0.148062 |
| 40 | 1 | 0 | -6.198341 | 0.696340 | -1.389932 |

Iso_pCN_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.062316 | -0.094855 | -0.086277 |
| 2 | 6 | 0 | -0.063231 | -0.212389 | 1.294164 |
| 3 | 6 | 0 | 1.081240 | -0.186647 | 2.090606 |
| 4 | 6 | 0 | 2.318659 | 0.002809 | 1.500141 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 2.437563 | 0.141390 | 0.127675 |
| 6 | 6 | 0 | 1.301115 | 0.077224 | -0.672974 |
| 7 | 1 | 0 | -0.795429 | -0.138570 | -0.729834 |
| 8 | 6 | 0 | -1.372472 | -0.434182 | 1.979448 |
| 9 | 6 | 0 | 0.898593 | -0.376421 | 3.575865 |
| 10 | 1 | 0 | 3.214504 | 0.029462 | 2.094118 |
| 11 | 8 | 0 | 3.667221 | 0.289391 | -0.424039 |
| 12 | 8 | 0 | 1.394722 | 0.215790 | -2.022256 |
| 13 | 6 | 0 | 3.994760 | 1.593457 | -0.855917 |
| 14 | 6 | 0 | 1.801257 | -0.937787 | -2.725680 |
| 15 | 6 | 0 | -0.251478 | -1.347893 | 3.813204 |
| 16 | 7 | 0 | -1.467258 | -0.956541 | 3.120937 |
| 17 | 6 | 0 | -2.654587 | -0.037070 | 1.310473 |
| 18 | 6 | 0 | -2.782210 | 1.177611 | 0.644809 |
| 19 | 6 | 0 | -3.989736 | 1.550641 | 0.083290 |
| 20 | 6 | 0 | -5.082899 | 0.699453 | 0.173683 |
| 21 | 6 | 0 | -4.966795 | -0.517479 | 0.837170 |
| 22 | 6 | 0 | -3.761192 | -0.875924 | 1.405792 |
| 23 | 1 | 0 | 0.666242 | 0.577721 | 4.045427 |
| 24 | 1 | 0 | 1.809767 | -0.746635 | 4.032824 |
| 25 | 1 | 0 | 3.981729 | 2.285141 | -0.020231 |
| 26 | 1 | 0 | 3.309015 | 1.932802 | -1.620310 |
| 27 | 1 | 0 | 4.994657 | 1.539505 | -1.260678 |
| 28 | 1 | 0 | 1.823529 | -0.669040 | -3.771759 |
| 29 | 1 | 0 | 1.092392 | -1.745561 | -2.576991 |
| 30 | 1 | 0 | 2.786077 | -1.257410 | -2.410622 |
| 31 | 1 | 0 | -0.480598 | -1.418356 | 4.868855 |
| 32 | 1 | 0 | 0.028746 | -2.345677 | 3.479186 |
| 33 | 1 | 0 | -1.942895 | 1.843708 | 0.573718 |
| 34 | 1 | 0 | -4.085104 | 2.494299 | -0.420558 |
| 35 | 6 | 0 | -6.343180 | 1.079458 | -0.421970 |
| 36 | 1 | 0 | -5.815914 | -1.171493 | 0.906717 |
| 37 | 1 | 0 | -3.668621 | -1.804989 | 1.933698 |
| 38 | 7 | 0 | -7.333930 | 1.377928 | -0.891999 |

Iso_pCl_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.873215 | -0.329227 | -0.712026 |
| 2 | 6 | 0 | 0.872405 | -0.329334 | 0.679064 |
| 3 | 6 | 0 | 2.087597 | -0.328656 | 1.363414 |
| 4 | 6 | 0 | 3.272862 | -0.278893 | 0.650181 |
| 5 | 6 | 0 | 3.268645 | -0.256374 | -0.734050 |
| 6 | 6 | 0 | 2.058970 | -0.296848 | -1.420261 |
| 7 | 1 | 0 | -0.043676 | -0.358330 | -1.268810 |
| 8 | 6 | 0 | -0.378885 | -0.397674 | 1.495212 |
| 9 | 6 | 0 | 2.036010 | -0.393019 | 2.869423 |
| 10 | 1 | 0 | 4.221218 | -0.274402 | 1.156899 |
| 11 | 8 | 0 | 4.447222 | -0.244372 | -1.405593 |
| 12 | 8 | 0 | 2.032554 | -0.271583 | -2.779972 |
| 13 | 6 | 0 | 4.818697 | 0.994637 | -1.971127 |
| 14 | 6 | 0 | 2.286023 | -1.505155 | -3.415135 |
| 15 | 6 | 0 | 0.851860 | -1.257652 | 3.285084 |
| 16 | 7 | 0 | -0.395625 | -0.825399 | 2.679861 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 6 | 0 | -1.686292 | 0.042991 | 0.911030 |
| 18 | 6 | 0 | -1.795791 | 1.198858 | 0.147191 |
| 19 | 6 | 0 | -3.023550 | 1.621185 | -0.335933 |
| 20 | 6 | 0 | -4.149844 | 0.871105 | -0.059996 |
| 21 | 6 | 0 | -4.068317 | -0.283226 | 0.698654 |
| 22 | 6 | 0 | -2.838853 | -0.686021 | 1.185457 |
| 23 | 1 | 0 | 1.911951 | 0.607661 | 3.279530 |
| 24 | 1 | 0 | 2.960640 | -0.793509 | 3.270740 |
| 25 | 1 | 0 | 4.933348 | 1.746812 | -1.197686 |
| 26 | 1 | 0 | 4.086744 | 1.325948 | -2.695223 |
| 27 | 1 | 0 | 5.768886 | 0.835788 | -2.459690 |
| 28 | 1 | 0 | 2.227596 | -1.322614 | -4.478395 |
| 29 | 1 | 0 | 1.538633 | -2.240128 | -3.135110 |
| 30 | 1 | 0 | 3.271007 | -1.876369 | -3.163141 |
| 31 | 1 | 0 | 0.722682 | -1.236337 | 4.359853 |
| 32 | 1 | 0 | 1.032795 | -2.294526 | 3.005416 |
| 33 | 1 | 0 | -0.923810 | 1.788936 | -0.066047 |
| 34 | 1 | 0 | -3.102013 | 2.520352 | -0.916682 |
| 35 | 17 | 0 | -5.697881 | 1.387088 | -0.675236 |
| 36 | 1 | 0 | -4.952929 | -0.854385 | 0.906778 |
| 37 | 1 | 0 | -2.766439 | -1.570145 | 1.788984 |

Iso_pF_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.051229 | -0.074792 | -0.073300 |
| 2 | 6 | 0 | -0.066223 | -0.203007 | 1.306887 |
| 3 | 6 | 0 | 1.085424 | -0.197670 | 2.093590 |
| 4 | 6 | 0 | 2.320489 | -0.015153 | 1.495747 |
| 5 | 6 | 0 | 2.430456 | 0.135240 | 0.123962 |
| 6 | 6 | 0 | 1.287438 | 0.089838 | -0.667809 |
| 7 | 1 | 0 | -0.812258 | -0.104848 | -0.709604 |
| 8 | 6 | 0 | -1.375235 | -0.416147 | 1.999472 |
| 9 | 6 | 0 | 0.912896 | -0.407631 | 3.577101 |
| 10 | 1 | 0 | 3.220971 | -0.004639 | 2.083313 |
| 11 | 8 | 0 | 3.657884 | 0.275929 | -0.436816 |
| 12 | 8 | 0 | 1.373215 | 0.238638 | -2.017386 |
| 13 | 6 | 0 | 3.994932 | 1.581295 | -0.854943 |
| 14 | 6 | 0 | 1.756695 | -0.915293 | -2.731705 |
| 15 | 6 | 0 | -0.242741 | -1.374726 | 3.804638 |
| 16 | 7 | 0 | -1.461193 | -0.955177 | 3.135174 |
| 17 | 6 | 0 | -2.653302 | 0.003901 | 1.342149 |
| 18 | 6 | 0 | -2.770303 | 1.214624 | 0.668257 |
| 19 | 6 | 0 | -3.977828 | 1.613554 | 0.118225 |
| 20 | 6 | 0 | -5.065415 | 0.779259 | 0.243277 |
| 21 | 6 | 0 | -4.989401 | -0.428527 | 0.904808 |
| 22 | 6 | 0 | -3.780424 | -0.805470 | 1.458579 |
| 23 | 1 | 0 | 0.689109 | 0.540420 | 4.063003 |
| 24 | 1 | 0 | 1.825258 | -0.790478 | 4.021546 |
| 25 | 1 | 0 | 3.996272 | 2.262941 | -0.010826 |
| 26 | 1 | 0 | 3.306125 | 1.937507 | -1.608980 |
| 27 | 1 | 0 | 4.990768 | 1.522857 | -1.269391 |
| 28 | 1 | 0 | 1.776056 | -0.639714 | -3.776235 |
| 29 | 1 | 0 | 1.036748 | -1.713481 | -2.583999 |
| 30 | 1 | 0 | 2.738723 | -1.252627 | -2.426145 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 1 | 0 | -0.460745 | -1.466253 | 4.861317 |
| 32 | 1 | 0 | 0.028452 | -2.367187 | 3.447274 |
| 33 | 1 | 0 | -1.919849 | 1.864861 | 0.579440 |
| 34 | 1 | 0 | -4.080175 | 2.550867 | -0.395374 |
| 35 | 9 | 0 | -6.226037 | 1.149045 | -0.289682 |
| 36 | 1 | 0 | -5.862547 | -1.048848 | 0.981399 |
| 37 | 1 | 0 | -3.701908 | -1.732687 | 1.992634 |

Iso_pNMe2_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.191504 | -0.052050 | -0.128463 |
| 2 | 6 | 0 | -0.019537 | -0.387861 | 1.204773 |
| 3 | 6 | 0 | 1.059549 | -0.380446 | 2.088583 |
| 4 | 6 | 0 | 2.309526 | 0.009158 | 1.639200 |
| 5 | 6 | 0 | 2.509317 | 0.365260 | 0.316462 |
| 6 | 6 | 0 | 1.444482 | 0.319462 | -0.577004 |
| 7 | 1 | 0 | -0.611159 | -0.077227 | -0.839860 |
| 8 | 6 | 0 | -1.348024 | -0.829402 | 1.736187 |
| 9 | 6 | 0 | 0.796536 | -0.821860 | 3.506368 |
| 10 | 1 | 0 | 3.154204 | 0.024586 | 2.304491 |
| 11 | 8 | 0 | 3.754028 | 0.707439 | -0.103659 |
| 12 | 8 | 0 | 1.619904 | 0.667567 | -1.881195 |
| 13 | 6 | 0 | 3.973187 | 2.086324 | -0.307328 |
| 14 | 6 | 0 | 2.178838 | -0.331552 | -2.703858 |
| 15 | 6 | 0 | -0.254054 | -1.925720 | 3.487009 |
| 16 | 7 | 0 | -1.457435 | -1.537137 | 2.774185 |
| 17 | 6 | 0 | -2.607807 | -0.446420 | 1.028566 |
| 18 | 6 | 0 | -2.808105 | 0.816076 | 0.496513 |
| 19 | 6 | 0 | -4.013271 | 1.169526 | -0.096697 |
| 20 | 6 | 0 | -5.053020 | 0.253535 | -0.194696 |
| 21 | 6 | 0 | -4.844384 | -1.027219 | 0.329872 |
| 22 | 6 | 0 | -3.658056 | -1.361193 | 0.940504 |
| 23 | 1 | 0 | 0.426078 | 0.016063 | 4.094349 |
| 24 | 1 | 0 | 1.709451 | -1.169171 | 3.978351 |
| 25 | 1 | 0 | 3.831089 | 2.635459 | 0.617666 |
| 26 | 1 | 0 | 3.309994 | 2.477022 | -1.067317 |
| 27 | 1 | 0 | 4.998800 | 2.189693 | -0.630733 |
| 28 | 1 | 0 | 2.250980 | 0.089513 | -3.696411 |
| 29 | 1 | 0 | 1.538999 | -1.207441 | -2.731001 |
| 30 | 1 | 0 | 3.164311 | -0.614331 | -2.356481 |
| 31 | 1 | 0 | -0.539777 | -2.196737 | 4.495919 |
| 32 | 1 | 0 | 0.157913 | -2.820107 | 3.021138 |
| 33 | 1 | 0 | -2.031203 | 1.556287 | 0.559180 |
| 34 | 1 | 0 | -4.126744 | 2.168324 | -0.471446 |
| 35 | 7 | 0 | -6.281629 | 0.546689 | -0.822650 |
| 36 | 1 | 0 | -5.616964 | -1.767702 | 0.235464 |
| 37 | 1 | 0 | -3.524879 | -2.345682 | 1.347140 |
| 38 | 6 | 0 | -6.336015 | 1.728304 | -1.652380 |
| 39 | 6 | 0 | -7.466765 | 0.403020 | 0.004761 |
| 40 | 1 | 0 | -7.250863 | 1.703256 | -2.232502 |
| 41 | 1 | 0 | -5.503267 | 1.737684 | -2.343391 |
| 42 | 1 | 0 | -6.327397 | 2.661074 | -1.084336 |
| 43 | 1 | 0 | -7.445526 | -0.528440 | 0.550107 |
| 44 | 1 | 0 | -8.345372 | 0.398124 | -0.629673 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 1 | 0 | -7.568913 | 1.216161 | 0.726041 |

Iso_pNO2_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.156738 | -0.325601 | -0.602061 |
| 2 | 6 | 0 | 1.065798 | -0.283663 | 0.785499 |
| 3 | 6 | 0 | 2.229808 | -0.176817 | 1.545858 |
| 4 | 6 | 0 | 3.453017 | -0.067150 | 0.907465 |
| 5 | 6 | 0 | 3.537971 | -0.087598 | -0.474314 |
| 6 | 6 | 0 | 2.381243 | -0.232834 | -1.234621 |
| 7 | 1 | 0 | 0.282809 | -0.434561 | -1.215473 |
| 8 | 6 | 0 | -0.226260 | -0.414025 | 1.523553 |
| 9 | 6 | 0 | 2.083388 | -0.191494 | 3.047173 |
| 10 | 1 | 0 | 4.363708 | 0.019714 | 1.472354 |
| 11 | 8 | 0 | 4.753931 | -0.014635 | -1.069146 |
| 12 | 8 | 0 | 2.441555 | -0.250055 | -2.592528 |
| 13 | 6 | 0 | 5.078521 | 1.228515 | -1.655788 |
| 14 | 6 | 0 | 2.824725 | -1.479459 | -3.169579 |
| 15 | 6 | 0 | 0.932855 | -1.116948 | 3.424764 |
| 16 | 7 | 0 | -0.297161 | -0.799159 | 2.719652 |
| 17 | 6 | 0 | -1.523465 | -0.085612 | 0.845280 |
| 18 | 6 | 0 | -1.661479 | 1.050934 | 0.054743 |
| 19 | 6 | 0 | -2.879469 | 1.370262 | -0.517488 |
| 20 | 6 | 0 | -3.954069 | 0.530417 | -0.299130 |
| 21 | 6 | 0 | -3.848004 | -0.606766 | 0.481824 |
| 22 | 6 | 0 | -2.628767 | -0.904967 | 1.056858 |
| 23 | 1 | 0 | 1.870580 | 0.813100 | 3.408166 |
| 24 | 1 | 0 | 3.003005 | -0.515759 | 3.521689 |
| 25 | 1 | 0 | 5.092044 | 2.011148 | -0.904654 |
| 26 | 1 | 0 | 4.375098 | 1.484701 | -2.436298 |
| 27 | 1 | 0 | 6.066994 | 1.119010 | -2.076948 |
| 28 | 1 | 0 | 2.822684 | -1.331418 | -4.239617 |
| 29 | 1 | 0 | 2.115437 | -2.259318 | -2.913080 |
| 30 | 1 | 0 | 3.815266 | -1.768985 | -2.843669 |
| 31 | 1 | 0 | 0.728918 | -1.060240 | 4.486307 |
| 32 | 1 | 0 | 1.197241 | -2.149867 | 3.204156 |
| 33 | 1 | 0 | -0.821981 | 1.700219 | -0.107317 |
| 34 | 1 | 0 | -2.996504 | 2.248831 | -1.118498 |
| 35 | 7 | 0 | -5.238473 | 0.853563 | -0.908557 |
| 36 | 1 | 0 | -4.701739 | -1.235361 | 0.633228 |
| 37 | 1 | 0 | -2.526190 | -1.771479 | 1.680148 |
| 38 | 8 | 0 | -5.304853 | 1.844695 | -1.571221 |
| 39 | 8 | 0 | -6.149787 | 0.108280 | -0.710652 |

Iso_pOMe_1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.963908 | -0.306922 | -0.700563 |
| 2 | 6 | 0 | 0.873099 | -0.257158 | 0.686635 |
| 3 | 6 | 0 | 2.037296 | -0.121003 | 1.442493 |
| 4 | 6 | 0 | 3.257095 | 0.011032 | 0.801578 |
| 5 | 6 | 0 | 3.340030 | -0.017113 | -0.580013 |
| 6 | 6 | 0 | 2.185447 | -0.192080 | -1.335869 |
| 7 | 1 | 0 | 0.090369 | -0.438877 | -1.309521 |
| 8 | 6 | 0 | -0.418928 | -0.410140 | 1.426294 |
| 9 | 6 | 0 | 1.894974 | -0.138043 | 2.943786 |
| 10 | 1 | 0 | 4.166680 | 0.119762 | 1.364707 |
| 11 | 8 | 0 | 4.554161 | 0.077688 | -1.178934 |
| 12 | 8 | 0 | 2.245626 | -0.218636 | -2.695010 |
| 13 | 6 | 0 | 4.849096 | 1.324002 | -1.771687 |
| 14 | 6 | 0 | 2.638515 | -1.449306 | -3.259933 |
| 15 | 6 | 0 | 0.769161 | -1.094286 | 3.318804 |
| 16 | 7 | 0 | -0.471081 | -0.796902 | 2.624769 |
| 17 | 6 | 0 | -1.717380 | -0.114015 | 0.742829 |
| 18 | 6 | 0 | -1.881232 | 0.997657 | -0.075896 |
| 19 | 6 | 0 | -3.108574 | 1.284153 | -0.650743 |
| 20 | 6 | 0 | -4.187070 | 0.448434 | -0.421136 |
| 21 | 6 | 0 | -4.039386 | -0.667799 | 0.388252 |
| 22 | 6 | 0 | -2.815645 | -0.938561 | 0.970197 |
| 23 | 1 | 0 | 1.653959 | 0.860092 | 3.305354 |
| 24 | 1 | 0 | 2.824462 | -0.436734 | 3.416551 |
| 25 | 1 | 0 | 4.846432 | 2.111056 | -1.024798 |
| 26 | 1 | 0 | 4.138502 | 1.560910 | -2.551966 |
| 27 | 1 | 0 | 5.839105 | 1.235754 | -2.194920 |
| 28 | 1 | 0 | 2.634910 | -1.312589 | -4.331738 |
| 29 | 1 | 0 | 1.936597 | -2.233292 | -2.995526 |
| 30 | 1 | 0 | 3.631943 | -1.727512 | -2.932082 |
| 31 | 1 | 0 | 0.571570 | -1.051254 | 4.382702 |
| 32 | 1 | 0 | 1.061393 | -2.118271 | 3.089757 |
| 33 | 1 | 0 | -1.052232 | 1.656064 | -0.260573 |
| 34 | 1 | 0 | -3.233870 | 2.143702 | -1.283570 |
| 35 | 8 | 0 | -5.383955 | 0.708712 | -1.016199 |
| 36 | 1 | 0 | -4.880531 | -1.318022 | 0.546883 |
| 37 | 1 | 0 | -2.700795 | -1.794031 | 1.608045 |
| 38 | 6 | 0 | -6.295663 | 1.449986 | -0.244322 |
| 39 | 1 | 0 | -5.892120 | 2.426241 | 0.004718 |
| 40 | 1 | 0 | -6.547682 | 0.928541 | 0.673308 |
| 41 | 1 | 0 | -7.186230 | 1.571643 | -0.843802 |