**Supplementary Information for**

# Resolving origin of the multimode Jahn-Teller effect in metallophthalocyanines

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**Table S1** EDA analysis for MnPc in HS and LS point groups using different density functional approximations; energies are given in $cm^{-1}$.

| | LDA | | OPBE | | OPBE/LDA* | |
|---|---|---|---|---|---|---|
| | $D_{4h}$ | $D_{2h}$ | $D_{4h}$ | $D_{2h}$ | $D_{4h}$ | $D_{2h}$ |
| $E_{prep}$ ($Mn^{2+}$) | 35369 | 35369 | 38820 | 38820 | 38820 | 38820 |
| $E_{prep}$ ($Pc^{2-}$) | 3830 | 4005 | 3846 | 3950 | 5043 | 5224 |
| $E_{int}$ | -286926 | -287239 | -263128 | -263410 | -264268 | -264618 |
| $E_{Pauli}$ | 91115 | 91270 | 89844 | 89883 | 97513 | 97657 |
| $E_{elstat}$ | -218983 | -219139 | -203610 | -203670 | -207748 | -207892 |
| Total steric | -127869 | -127870 | -113765 | -113787 | -110234 | -110234 |
| $A_g$ | -74362 | -74493 | -71795 | -71994 | -73470 | -73632 |
| $B_{1g}$ | -11498 | -11554 | -9726 | -9758 | -10423 | -10470 |
| $B_{2g}$ | -6249 | -6361 | -3752 | -3975 | -4463 | -4599 |
| $B_{3g}$ | -18470 | -18400 | -16516 | -16243 | -17185 | -17094 |
| $A_u$ | -4027 | -4023 | -3978 | -3981 | -4011 | -4009 |
| $B_{1u}$ | -19911 | -19956 | -19165 | -19190 | -19778 | -19828 |
| $B_{2u}$ | -12623 | -12649 | -12482 | -12514 | -12628 | -12652 |
| $B_{3u}$ | -11915 | -11931 | -11948 | -11968 | -12075 | -12099 |
| $\Delta E_{orbint}$ | -159057 | -159368 | -149363 | -149623 | -154033 | -154384 |

*OPBE single point on LDA geometries

**Table S2** EDA analysis for MgPc in HS and LS point groups using different density functional approximations; energies are given in $cm^{-1}$.

| | LDA | | OPBE | | OPBE/LDA* | |
|---|---|---|---|---|---|---|
| | $D_{4h}$ | $D_{2h}$ | $D_{4h}$ | $D_{2h}$ | $D_{4h}$ | $D_{2h}$ |
| $E_{prep}$ ($Pc^{3-}$) | 2408 | 2112 | 2251 | 1969 | 2307 | 2007 |
| $E_{int}$ | -278703 | -278807 | -268217 | -268357 | -268730 | -268839 |
| $E_{Pauli}$ | 36502 | 36576 | 35057 | 35049 | 37866 | 37945 |
| $E_{elstat}$ | -227656 | -227839 | -218998 | -219163 | -221235 | -221425 |
| Total steric | -191154 | -191263 | -183941 | -184114 | -183368 | -183480 |
| $A_g$ | -19733 | -19778 | -19065 | -19104 | -19062 | -19108 |
| $B_{1g}$ | -4751 | -4765 | -4706 | -4718 | -4830 | -4845 |
| $B_{2g}$ | -11931 | -11931 | -11292 | -11281 | -11541 | -11536 |
| $B_{3g}$ | -10135 | -9952 | -9787 | -9607 | -10042 | -9861 |
| $A_u$ | -3738 | -3751 | -3714 | -3723 | -3726 | -3738 |
| $B_{1u}$ | -15335 | -15388 | -14521 | -14572 | -14875 | -14930 |
| $B_{2u}$ | -10897 | -10914 | -10522 | -10530 | -10568 | -10580 |
| $B_{3u}$ | -11029 | -11064 | -10670 | -10708 | -10718 | -10759 |
| $\Delta E_{orbint}$ | -87549 | -87544 | -84277 | -84243 | -85363 | -85358 |

*OPBE single point on LDA geometries

**Cartesian coordinates and electronic occupations for all spin states of MnPc obtained by all performed DFAs.**

level of theory bp86
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.40279915 | 2.40279915 | 0.00000000 |
| N | -2.40279915 | 2.40279915 | 0.00000000 |
| N | -2.40279915 | -2.40279915 | 0.00000000 |
| N | 2.40279915 | -2.40279915 | 0.00000000 |
| N | 0.00000000 | 2.02952598 | 0.00000000 |
| C | 1.13176726 | 2.81196693 | 0.00000000 |
| C | 0.70834608 | 4.21068983 | 0.00000000 |
| C | -0.70834608 | 4.21068983 | 0.00000000 |
| C | -1.13176726 | 2.81196693 | 0.00000000 |
| N | -2.02952598 | 0.00000000 | 0.00000000 |
| C | -2.81196693 | 1.13176726 | 0.00000000 |
| C | -4.21068983 | 0.70834608 | 0.00000000 |
| C | -4.21068983 | -0.70834608 | 0.00000000 |
| C | -2.81196693 | -1.13176726 | 0.00000000 |
| N | 0.00000000 | -2.02952598 | 0.00000000 |
| C | -1.13176726 | -2.81196693 | 0.00000000 |
| C | -0.70834608 | -4.21068983 | 0.00000000 |
| C | 0.70834608 | -4.21068983 | 0.00000000 |
| C | 1.13176726 | -2.81196693 | 0.00000000 |
| N | 2.02952598 | 0.00000000 | 0.00000000 |
| C | 2.81196693 | -1.13176726 | 0.00000000 |
| C | 4.21068983 | -0.70834608 | 0.00000000 |
| C | 4.21068983 | 0.70834608 | 0.00000000 |
| C | 2.81196693 | 1.13176726 | 0.00000000 |
| C | -5.40686430 | -1.42505052 | 0.00000000 |
| C | -6.60197884 | -0.70362423 | 0.00000000 |
| C | -6.60197884 | 0.70362423 | 0.00000000 |
| C | -5.40686430 | 1.42505052 | 0.00000000 |
| C | -1.42505052 | 5.40686430 | 0.00000000 |
| C | -0.70362423 | 6.60197884 | 0.00000000 |
| C | 0.70362423 | 6.60197884 | 0.00000000 |
| C | 1.42505052 | 5.40686430 | 0.00000000 |
| C | 5.40686430 | 1.42505052 | 0.00000000 |
| C | 6.60197884 | 0.70362423 | 0.00000000 |
| C | 6.60197884 | -0.70362423 | 0.00000000 |
| C | 5.40686430 | -1.42505052 | 0.00000000 |
| C | 1.42505052 | -5.40686430 | 0.00000000 |
| C | 0.70362423 | -6.60197884 | 0.00000000 |
| C | -0.70362423 | -6.60197884 | 0.00000000 |
| C | -1.42505052 | -5.40686430 | 0.00000000 |
| H | -5.39810748 | -2.51324161 | 0.00000000 |
| H | -7.55227746 | -1.23589823 | 0.00000000 |
| H | -7.55227746 | 1.23589823 | 0.00000000 |
| H | -5.39810748 | 2.51324161 | 0.00000000 |
| H | -2.51324161 | 5.39810748 | 0.00000000 |
| H | -1.23589823 | 7.55227746 | 0.00000000 |
| H | 1.23589823 | 7.55227746 | 0.00000000 |
| H | 2.51324161 | 5.39810748 | 0.00000000 |
| H | 5.39810748 | 2.51324161 | 0.00000000 |
| H | 7.55227746 | 1.23589823 | 0.00000000 |
| H | 7.55227746 | -1.23589823 | 0.00000000 |
| H | 5.39810748 | -2.51324161 | 0.00000000 |
| H | 2.51324161 | -5.39810748 | 0.00000000 |
| H | 1.23589823 | -7.55227746 | 0.00000000 |
| H | -1.23589823 | -7.55227746 | 0.00000000 |
| H | -2.51324161 | -5.39810748 | 0.00000000 |

level of theory bp86
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39266329 | 2.39266329 | 0.00000000 |
| N | -2.39266329 | 2.39266329 | 0.00000000 |
| N | -2.39266329 | -2.39266329 | 0.00000000 |
| N | 2.39266329 | -2.39266329 | 0.00000000 |
| N | 0.00000000 | 1.94821420 | 0.00000000 |
| C | 1.12597065 | 2.76852572 | 0.00000000 |
| C | 0.70440636 | 4.15443193 | 0.00000000 |
| C | -0.70440636 | 4.15443193 | 0.00000000 |
| C | -1.12597065 | 2.76852572 | 0.00000000 |
| N | -1.94821420 | 0.00000000 | 0.00000000 |
| C | -2.76852572 | 1.12597065 | 0.00000000 |
| C | -4.15443193 | 0.70440636 | 0.00000000 |
| C | -4.15443193 | -0.70440636 | 0.00000000 |
| C | -2.76852572 | -1.12597065 | 0.00000000 |
| N | 0.00000000 | -1.94821420 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -1.12597065 | -2.76852572 | 0.00000000 |
| C | -0.70440636 | -4.15443193 | 0.00000000 |
| C | 0.70440636 | -4.15443193 | 0.00000000 |
| C | 1.12597065 | -2.76852572 | 0.00000000 |
| N | 1.94821420 | 0.00000000 | 0.00000000 |
| C | 2.76852572 | -1.12597065 | 0.00000000 |
| C | 4.15443193 | -0.70440636 | 0.00000000 |
| C | 4.15443193 | 0.70440636 | 0.00000000 |
| C | 2.76852572 | 1.12597065 | 0.00000000 |
| C | -5.34993224 | -1.42667297 | 0.00000000 |
| C | -6.54263637 | -0.70500009 | 0.00000000 |
| C | -6.54263637 | 0.70500009 | 0.00000000 |
| C | -5.34993224 | 1.42667297 | 0.00000000 |
| C | -1.42667297 | 5.34993224 | 0.00000000 |
| C | -0.70500009 | 6.54263637 | 0.00000000 |
| C | 0.70500009 | 6.54263637 | 0.00000000 |
| C | 1.42667297 | 5.34993224 | 0.00000000 |
| C | 5.34993224 | 1.42667297 | 0.00000000 |
| C | 6.54263637 | 0.70500009 | 0.00000000 |
| C | 6.54263637 | -0.70500009 | 0.00000000 |
| C | 5.34993224 | -1.42667297 | 0.00000000 |
| C | 1.42667297 | -5.34993224 | 0.00000000 |
| C | 0.70500009 | -6.54263637 | 0.00000000 |
| C | -0.70500009 | -6.54263637 | 0.00000000 |
| C | -1.42667297 | -5.34993224 | 0.00000000 |
| H | -5.33956777 | -2.51464076 | 0.00000000 |
| H | -7.49332023 | -1.23638189 | 0.00000000 |
| H | -7.49332023 | 1.23638189 | 0.00000000 |
| H | -5.33956777 | 2.51464076 | 0.00000000 |
| H | -2.51464076 | 5.33956777 | 0.00000000 |
| H | -1.23638189 | 7.49332023 | 0.00000000 |
| H | 1.23638189 | 7.49332023 | 0.00000000 |
| H | 2.51464076 | 5.33956777 | 0.00000000 |
| H | 5.33956777 | 2.51464076 | 0.00000000 |
| H | 7.49332023 | 1.23638189 | 0.00000000 |
| H | 7.49332023 | -1.23638189 | 0.00000000 |
| H | 5.33956777 | -2.51464076 | 0.00000000 |
| H | 2.51464076 | -5.33956777 | 0.00000000 |
| H | 1.23638189 | -7.49332023 | 0.00000000 |
| H | -1.23638189 | -7.49332023 | 0.00000000 |
| H | -2.51464076 | -5.33956777 | 0.00000000 |

level of theory bp86
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39149539 | 2.39149539 | 0.00000000 |
| N | -2.39149539 | 2.39149539 | 0.00000000 |
| N | -2.39149539 | -2.39149539 | 0.00000000 |
| N | 2.39149539 | -2.39149539 | 0.00000000 |
| N | 0.00000000 | 1.95674982 | 0.00000000 |
| C | 1.12113079 | 2.76956290 | 0.00000000 |
| C | 0.70486674 | 4.16135992 | 0.00000000 |
| C | -0.70486674 | 4.16135992 | 0.00000000 |
| C | -1.12113079 | 2.76956290 | 0.00000000 |
| N | -1.95674982 | 0.00000000 | 0.00000000 |
| C | -2.76956290 | 1.12113079 | 0.00000000 |
| C | -4.16135992 | 0.70486674 | 0.00000000 |
| C | -4.16135992 | -0.70486674 | 0.00000000 |
| C | -2.76956290 | -1.12113079 | 0.00000000 |
| N | 0.00000000 | -1.95674982 | 0.00000000 |
| C | -1.12113079 | -2.76956290 | 0.00000000 |
| C | -0.70486674 | -4.16135992 | 0.00000000 |
| C | 0.70486674 | -4.16135992 | 0.00000000 |
| C | 1.12113079 | -2.76956290 | 0.00000000 |
| N | 1.95674982 | 0.00000000 | 0.00000000 |
| C | 2.76956290 | -1.12113079 | 0.00000000 |
| C | 4.16135992 | -0.70486674 | 0.00000000 |
| C | 4.16135992 | 0.70486674 | 0.00000000 |
| C | 2.76956290 | 1.12113079 | 0.00000000 |
| C | -5.35608075 | -1.42638775 | 0.00000000 |
| C | -6.54946964 | -0.70452013 | 0.00000000 |
| C | -6.54946964 | 0.70452013 | 0.00000000 |
| C | -5.35608075 | 1.42638775 | 0.00000000 |
| C | -1.42638775 | 5.35608075 | 0.00000000 |
| C | -0.70452013 | 6.54946964 | 0.00000000 |
| C | 0.70452013 | 6.54946964 | 0.00000000 |
| C | 1.42638775 | 5.35608075 | 0.00000000 |
| C | 5.35608075 | 1.42638775 | 0.00000000 |
| C | 6.54946964 | 0.70452013 | 0.00000000 |
| C | 6.54946964 | -0.70452013 | 0.00000000 |
| C | 5.35608075 | -1.42638775 | 0.00000000 |
| C | 1.42638775 | -5.35608075 | 0.00000000 |
| C | 0.70452013 | -6.54946964 | 0.00000000 |
| C | -0.70452013 | -6.54946964 | 0.00000000 |
| C | -1.42638775 | -5.35608075 | 0.00000000 |
| H | -5.34404567 | -2.51443385 | 0.00000000 |
| H | -7.50048318 | -1.23539498 | 0.00000000 |
| H | -7.50048318 | 1.23539498 | 0.00000000 |
| H | -5.34404567 | 2.51443385 | 0.00000000 |
| H | -2.51443385 | 5.34404567 | 0.00000000 |
| H | -1.23539498 | 7.50048318 | 0.00000000 |
| H | 1.23539498 | 7.50048318 | 0.00000000 |
| H | 2.51443385 | 5.34404567 | 0.00000000 |
| H | 5.34404567 | 2.51443385 | 0.00000000 |
| H | 7.50048318 | 1.23539498 | 0.00000000 |
| H | 7.50048318 | -1.23539498 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | 5.34404567 | -2.51443385 | 0.00000000 |
| H | 2.51443385 | -5.34404567 | 0.00000000 |
| H | 1.23539498 | -7.50048318 | 0.00000000 |
| H | -1.23539498 | -7.50048318 | 0.00000000 |
| H | -2.51443385 | -5.34404567 | 0.00000000 |

level of theory bp86
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39077889 | 2.39077889 | 0.00000000 |
| N | -2.39077889 | 2.39077889 | 0.00000000 |
| N | -2.39077889 | -2.39077889 | 0.00000000 |
| N | 2.39077889 | -2.39077889 | 0.00000000 |
| N | 0.00000000 | 1.95515965 | 0.00000000 |
| C | 1.12185100 | 2.76711175 | 0.00000000 |
| C | 0.70414547 | 4.15823301 | 0.00000000 |
| C | -0.70414547 | 4.15823301 | 0.00000000 |
| C | -1.12185100 | 2.76711175 | 0.00000000 |
| N | -1.95515965 | 0.00000000 | 0.00000000 |
| C | -2.76711175 | 1.12185100 | 0.00000000 |
| C | -4.15823301 | 0.70414547 | 0.00000000 |
| C | -4.15823301 | -0.70414547 | 0.00000000 |
| C | -2.76711175 | -1.12185100 | 0.00000000 |
| N | 0.00000000 | -1.95515965 | 0.00000000 |
| C | -1.12185100 | -2.76711175 | 0.00000000 |
| C | -0.70414547 | -4.15823301 | 0.00000000 |
| C | 0.70414547 | -4.15823301 | 0.00000000 |
| C | 1.12185100 | -2.76711175 | 0.00000000 |
| N | 1.95515965 | 0.00000000 | 0.00000000 |
| C | 2.76711175 | -1.12185100 | 0.00000000 |
| C | 4.15823301 | -0.70414547 | 0.00000000 |
| C | 4.15823301 | 0.70414547 | 0.00000000 |
| C | 2.76711175 | 1.12185100 | 0.00000000 |
| C | -5.35215108 | -1.42662641 | 0.00000000 |
| C | -6.54546165 | -0.70448044 | 0.00000000 |
| C | -6.54546165 | 0.70448044 | 0.00000000 |
| C | -5.35215108 | 1.42662641 | 0.00000000 |
| C | -1.42662641 | 5.35215108 | 0.00000000 |
| C | -0.70448044 | 6.54546165 | 0.00000000 |
| C | 0.70448044 | 6.54546165 | 0.00000000 |
| C | 1.42662641 | 5.35215108 | 0.00000000 |
| C | 5.35215108 | 1.42662641 | 0.00000000 |
| C | 6.54546165 | 0.70448044 | 0.00000000 |
| C | 6.54546165 | -0.70448044 | 0.00000000 |
| C | 5.35215108 | -1.42662641 | 0.00000000 |
| C | 1.42662641 | -5.35215108 | 0.00000000 |
| C | 0.70448044 | -6.54546165 | 0.00000000 |
| C | -0.70448044 | -6.54546165 | 0.00000000 |
| C | -1.42662641 | -5.35215108 | 0.00000000 |
| H | -5.34176703 | -2.51455927 | 0.00000000 |
| H | -7.49619737 | -1.23577440 | 0.00000000 |
| H | -7.49619737 | 1.23577440 | 0.00000000 |
| H | -5.34176703 | 2.51455927 | 0.00000000 |
| H | -2.51455927 | 5.34176703 | 0.00000000 |
| H | -1.23577440 | 7.49619737 | 0.00000000 |
| H | 1.23577440 | 7.49619737 | 0.00000000 |
| H | 2.51455927 | 5.34176703 | 0.00000000 |
| H | 5.34176703 | 2.51455927 | 0.00000000 |
| H | 7.49619737 | 1.23577440 | 0.00000000 |
| H | 7.49619737 | -1.23577440 | 0.00000000 |
| H | 5.34176703 | -2.51455927 | 0.00000000 |
| H | 2.51455927 | -5.34176703 | 0.00000000 |
| H | 1.23577440 | -7.49619737 | 0.00000000 |
| H | -1.23577440 | -7.49619737 | 0.00000000 |
| H | -2.51455927 | -5.34176703 | 0.00000000 |

level of theory bp86
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 20.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38936387 | 2.38936387 | 0.00000000 |
| N | -2.38936387 | 2.38936387 | 0.00000000 |
| N | -2.38936387 | -2.38936387 | 0.00000000 |
| N | 2.38936387 | -2.38936387 | 0.00000000 |
| N | 0.00000000 | 1.94217046 | 0.00000000 |
| C | 1.12377721 | 2.76540780 | 0.00000000 |
| C | 0.70389623 | 4.15217975 | 0.00000000 |
| C | -0.70389623 | 4.15217975 | 0.00000000 |
| C | -1.12377721 | 2.76540780 | 0.00000000 |
| N | -1.94217046 | 0.00000000 | 0.00000000 |
| C | -2.76540780 | 1.12377721 | 0.00000000 |
| C | -4.15217975 | 0.70389623 | 0.00000000 |
| C | -4.15217975 | -0.70389623 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -2.76540780 | -1.12377721 | 0.00000000 |
| N | 0.00000000 | -1.94217046 | 0.00000000 |
| C | -1.12377721 | -2.76540780 | 0.00000000 |
| C | -0.70389623 | -4.15217975 | 0.00000000 |
| C | 0.70389623 | -4.15217975 | 0.00000000 |
| C | 1.12377721 | -2.76540780 | 0.00000000 |
| N | 1.94217046 | 0.00000000 | 0.00000000 |
| C | 2.76540780 | -1.12377721 | 0.00000000 |
| C | 4.15217975 | -0.70389623 | 0.00000000 |
| C | 4.15217975 | 0.70389623 | 0.00000000 |
| C | 2.76540780 | 1.12377721 | 0.00000000 |
| C | -5.34702335 | -1.42637558 | 0.00000000 |
| C | -6.54012860 | -0.70467571 | 0.00000000 |
| C | -6.54012860 | 0.70467571 | 0.00000000 |
| C | -5.34702335 | 1.42637558 | 0.00000000 |
| C | -1.42637558 | 5.34702335 | 0.00000000 |
| C | -0.70467571 | 6.54012860 | 0.00000000 |
| C | 0.70467571 | 6.54012860 | 0.00000000 |
| C | 1.42637558 | 5.34702335 | 0.00000000 |
| C | 5.34702335 | 1.42637558 | 0.00000000 |
| C | 6.54012860 | 0.70467571 | 0.00000000 |
| C | 6.54012860 | -0.70467571 | 0.00000000 |
| C | 5.34702335 | -1.42637558 | 0.00000000 |
| C | 1.42637558 | -5.34702335 | 0.00000000 |
| C | 0.70467571 | -6.54012860 | 0.00000000 |
| C | -0.70467571 | -6.54012860 | 0.00000000 |
| C | -1.42637558 | -5.34702335 | 0.00000000 |
| H | -5.33566033 | -2.51431584 | 0.00000000 |
| H | -7.49068334 | -1.23627130 | 0.00000000 |
| H | -7.49068334 | 1.23627130 | 0.00000000 |
| H | -5.33566033 | 2.51431584 | 0.00000000 |
| H | -2.51431584 | 5.33566033 | 0.00000000 |
| H | -1.23627130 | 7.49068334 | 0.00000000 |
| H | 1.23627130 | 7.49068334 | 0.00000000 |
| H | 2.51431584 | 5.33566033 | 0.00000000 |
| H | 5.33566033 | 2.51431584 | 0.00000000 |
| H | 7.49068334 | 1.23627130 | 0.00000000 |
| H | 7.49068334 | -1.23627130 | 0.00000000 |
| H | 5.33566033 | -2.51431584 | 0.00000000 |
| H | 2.51431584 | -5.33566033 | 0.00000000 |
| H | 1.23627130 | -7.49068334 | 0.00000000 |
| H | -1.23627130 | -7.49068334 | 0.00000000 |
| H | -2.51431584 | -5.33566033 | 0.00000000 |

level of theory opbe
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38860000 | 2.38860000 | 0.00000000 |
| N | -2.38860000 | 2.38860000 | 0.00000000 |
| N | -2.38860000 | -2.38860000 | 0.00000000 |
| N | 2.38860000 | -2.38860000 | 0.00000000 |
| N | 0.00000000 | 2.02570000 | 0.00000000 |
| C | 1.12340000 | 2.79840000 | 0.00000000 |
| C | 0.70480000 | 4.19490000 | 0.00000000 |
| C | -0.70480000 | 4.19490000 | 0.00000000 |
| C | -1.12340000 | 2.79840000 | 0.00000000 |
| N | -2.02570000 | 0.00000000 | 0.00000000 |
| C | -2.79840000 | 1.12340000 | 0.00000000 |
| C | -4.19490000 | 0.70480000 | 0.00000000 |
| C | -4.19490000 | -0.70480000 | 0.00000000 |
| C | -2.79840000 | -1.12340000 | 0.00000000 |
| N | 0.00000000 | -2.02570000 | 0.00000000 |
| C | -1.12340000 | -2.79840000 | 0.00000000 |
| C | -0.70480000 | -4.19490000 | 0.00000000 |
| C | 0.70480000 | -4.19490000 | 0.00000000 |
| C | 1.12340000 | -2.79840000 | 0.00000000 |
| N | 2.02570000 | 0.00000000 | 0.00000000 |
| C | 2.79840000 | -1.12340000 | 0.00000000 |
| C | 4.19490000 | -0.70480000 | 0.00000000 |
| C | 4.19490000 | 0.70480000 | 0.00000000 |
| C | 2.79840000 | 1.12340000 | 0.00000000 |
| C | -5.38930000 | -1.41840000 | 0.00000000 |
| C | -6.57910000 | -0.70030000 | 0.00000000 |
| C | -6.57910000 | 0.70030000 | 0.00000000 |
| C | -5.38930000 | 1.41840000 | 0.00000000 |
| C | -1.41840000 | 5.38930000 | 0.00000000 |
| C | -0.70030000 | 6.57910000 | 0.00000000 |
| C | 0.70030000 | 6.57910000 | 0.00000000 |
| C | 1.41840000 | 5.38930000 | 0.00000000 |
| C | 5.38930000 | 1.41840000 | 0.00000000 |
| C | 6.57910000 | 0.70030000 | 0.00000000 |
| C | 6.57910000 | -0.70030000 | 0.00000000 |
| C | 5.38930000 | -1.41840000 | 0.00000000 |
| C | 1.41840000 | -5.38930000 | 0.00000000 |
| C | 0.70030000 | -6.57910000 | 0.00000000 |
| C | -0.70030000 | -6.57910000 | 0.00000000 |
| C | -1.41840000 | -5.38930000 | 0.00000000 |
| H | -5.38570000 | -2.50540000 | 0.00000000 |
| H | -7.52870000 | -1.23230000 | 0.00000000 |
| H | -7.52870000 | 1.23230000 | 0.00000000 |
| H | -5.38570000 | 2.50540000 | 0.00000000 |
| H | -2.50540000 | 5.38570000 | 0.00000000 |
| H | -1.23230000 | 7.52870000 | 0.00000000 |
| H | 1.23230000 | 7.52870000 | 0.00000000 |
| H | 2.50540000 | 5.38570000 | 0.00000000 |
| H | 5.38570000 | 2.50540000 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | 7.52870000 | 1.23230000 | 0.00000000 |
| H | 7.52870000 | -1.23230000 | 0.00000000 |
| H | 5.38570000 | -2.50540000 | 0.00000000 |
| H | 2.50540000 | -5.38570000 | 0.00000000 |
| H | 1.23230000 | -7.52870000 | 0.00000000 |
| H | -1.23230000 | -7.52870000 | 0.00000000 |
| H | -2.50540000 | -5.38570000 | 0.00000000 |

level of theory opbe
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37830000 | 2.37830000 | 0.00000000 |
| N | -2.37830000 | 2.37830000 | 0.00000000 |
| N | -2.37830000 | -2.37830000 | 0.00000000 |
| N | 2.37830000 | -2.37830000 | 0.00000000 |
| N | 0.00000000 | 1.94090000 | 0.00000000 |
| C | 1.11700000 | 2.75220000 | 0.00000000 |
| C | 0.70080000 | 4.13490000 | 0.00000000 |
| C | -0.70080000 | 4.13490000 | 0.00000000 |
| C | -1.11700000 | 2.75220000 | 0.00000000 |
| N | -1.94090000 | 0.00000000 | 0.00000000 |
| C | -2.75220000 | 1.11700000 | 0.00000000 |
| C | -4.13490000 | 0.70080000 | 0.00000000 |
| C | -4.13490000 | -0.70080000 | 0.00000000 |
| C | -2.75220000 | -1.11700000 | 0.00000000 |
| N | 0.00000000 | -1.94090000 | 0.00000000 |
| C | -1.11700000 | -2.75220000 | 0.00000000 |
| C | -0.70080000 | -4.13490000 | 0.00000000 |
| C | 0.70080000 | -4.13490000 | 0.00000000 |
| C | 1.11700000 | -2.75220000 | 0.00000000 |
| N | 1.94090000 | 0.00000000 | 0.00000000 |
| C | 2.75220000 | -1.11700000 | 0.00000000 |
| C | 4.13490000 | -0.70080000 | 0.00000000 |
| C | 4.13490000 | 0.70080000 | 0.00000000 |
| C | 2.75220000 | 1.11700000 | 0.00000000 |
| C | -5.32850000 | -1.42040000 | 0.00000000 |
| C | -6.51550000 | -0.70180000 | 0.00000000 |
| C | -6.51550000 | 0.70180000 | 0.00000000 |
| C | -5.32850000 | 1.42040000 | 0.00000000 |
| C | -1.42040000 | 5.32850000 | 0.00000000 |
| C | -0.70180000 | 6.51550000 | 0.00000000 |
| C | 0.70180000 | 6.51550000 | 0.00000000 |
| C | 1.42040000 | 5.32850000 | 0.00000000 |
| C | 5.32850000 | 1.42040000 | 0.00000000 |
| C | 6.51550000 | 0.70180000 | 0.00000000 |
| C | 6.51550000 | -0.70180000 | 0.00000000 |
| C | 5.32850000 | -1.42040000 | 0.00000000 |
| C | 1.42040000 | -5.32850000 | 0.00000000 |
| C | 0.70180000 | -6.51550000 | 0.00000000 |
| C | -0.70180000 | -6.51550000 | 0.00000000 |
| C | -1.42040000 | -5.32850000 | 0.00000000 |
| H | -5.32390000 | -2.50700000 | 0.00000000 |
| H | -7.46550000 | -1.23290000 | 0.00000000 |
| H | -7.46550000 | 1.23290000 | 0.00000000 |
| H | -5.32390000 | 2.50700000 | 0.00000000 |
| H | -2.50700000 | 5.32390000 | 0.00000000 |
| H | -1.23290000 | 7.46550000 | 0.00000000 |
| H | 1.23290000 | 7.46550000 | 0.00000000 |
| H | 2.50700000 | 5.32390000 | 0.00000000 |
| H | 5.32390000 | 2.50700000 | 0.00000000 |
| H | 7.46550000 | 1.23290000 | 0.00000000 |
| H | 7.46550000 | -1.23290000 | 0.00000000 |
| H | 5.32390000 | -2.50700000 | 0.00000000 |
| H | 2.50700000 | -5.32390000 | 0.00000000 |
| H | 1.23290000 | -7.46550000 | 0.00000000 |
| H | -1.23290000 | -7.46550000 | 0.00000000 |
| H | -2.50700000 | -5.32390000 | 0.00000000 |

level of theory opbe
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37671336 | 2.37671336 | 0.00000000 |
| N | -2.37671336 | 2.37671336 | 0.00000000 |
| N | -2.37671336 | -2.37671336 | 0.00000000 |
| N | 2.37671336 | -2.37671336 | 0.00000000 |
| N | 0.00000000 | 1.94787870 | 0.00000000 |
| C | 1.11119285 | 2.75231913 | 0.00000000 |
| C | 0.70116250 | 4.14226932 | 0.00000000 |
| C | -0.70116250 | 4.14226932 | 0.00000000 |
| C | -1.11119285 | 2.75231913 | 0.00000000 |
| N | -1.94787870 | 0.00000000 | 0.00000000 |
| C | -2.75231913 | 1.11119285 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -4.14226932 | 0.70116250 | 0.00000000 |
| C | -4.14226932 | -0.70116250 | 0.00000000 |
| C | -2.75231913 | -1.11119285 | 0.00000000 |
| N | 0.00000000 | -1.94787870 | 0.00000000 |
| C | -1.11119285 | -2.75231913 | 0.00000000 |
| C | -0.70116250 | -4.14226932 | 0.00000000 |
| C | 0.70116250 | -4.14226932 | 0.00000000 |
| C | 1.11119285 | -2.75231913 | 0.00000000 |
| N | 1.94787870 | 0.00000000 | 0.00000000 |
| C | 2.75231913 | -1.11119285 | 0.00000000 |
| C | 4.14226932 | -0.70116250 | 0.00000000 |
| C | 4.14226932 | 0.70116250 | 0.00000000 |
| C | 2.75231913 | 1.11119285 | 0.00000000 |
| C | -5.33486762 | -1.42002915 | 0.00000000 |
| C | -6.52279117 | -0.70125405 | 0.00000000 |
| C | -6.52279117 | 0.70125405 | 0.00000000 |
| C | -5.33486762 | 1.42002915 | 0.00000000 |
| C | -1.42002915 | 5.33486762 | 0.00000000 |
| C | -0.70125405 | 6.52279117 | 0.00000000 |
| C | 0.70125405 | 6.52279117 | 0.00000000 |
| C | 1.42002915 | 5.33486762 | 0.00000000 |
| C | 5.33486762 | 1.42002915 | 0.00000000 |
| C | 6.52279117 | 0.70125405 | 0.00000000 |
| C | 6.52279117 | -0.70125405 | 0.00000000 |
| C | 5.33486762 | -1.42002915 | 0.00000000 |
| C | 1.42002915 | -5.33486762 | 0.00000000 |
| C | 0.70125405 | -6.52279117 | 0.00000000 |
| C | -0.70125405 | -6.52279117 | 0.00000000 |
| C | -1.42002915 | -5.33486762 | 0.00000000 |
| H | -5.33037702 | -2.50674861 | 0.00000000 |
| H | -7.47304481 | -1.23201036 | 0.00000000 |
| H | -7.47304481 | 1.23201036 | 0.00000000 |
| H | -5.33037702 | 2.50674861 | 0.00000000 |
| H | -2.50674861 | 5.33037702 | 0.00000000 |
| H | -1.23201036 | 7.47304481 | 0.00000000 |
| H | 1.23201036 | 7.47304481 | 0.00000000 |
| H | 2.50674861 | 5.33037702 | 0.00000000 |
| H | 5.33037702 | 2.50674861 | 0.00000000 |
| H | 7.47304481 | 1.23201036 | 0.00000000 |
| H | 7.47304481 | -1.23201036 | 0.00000000 |
| H | 5.33037702 | -2.50674861 | 0.00000000 |
| H | 2.50674861 | -5.33037702 | 0.00000000 |
| H | 1.23201036 | -7.47304481 | 0.00000000 |
| H | -1.23201036 | -7.47304481 | 0.00000000 |
| H | -2.50674861 | -5.33037702 | 0.00000000 |

level of theory opbe
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37615296 | 2.37615296 | 0.00000000 |
| N | -2.37615296 | 2.37615296 | 0.00000000 |
| N | -2.37615296 | -2.37615296 | 0.00000000 |
| N | 2.37615296 | -2.37615296 | 0.00000000 |
| N | 0.00000000 | 1.94998006 | 0.00000000 |
| C | 1.11249885 | 2.75195136 | 0.00000000 |
| C | 0.70057300 | 4.14115382 | 0.00000000 |
| C | -0.70057300 | 4.14115382 | 0.00000000 |
| C | -1.11249885 | 2.75195136 | 0.00000000 |
| N | -1.94998006 | 0.00000000 | 0.00000000 |
| C | -2.75195136 | 1.11249885 | 0.00000000 |
| C | -4.14115382 | 0.70057300 | 0.00000000 |
| C | -4.14115382 | -0.70057300 | 0.00000000 |
| C | -2.75195136 | -1.11249885 | 0.00000000 |
| N | 0.00000000 | -1.94998006 | 0.00000000 |
| C | -1.11249885 | -2.75195136 | 0.00000000 |
| C | -0.70057300 | -4.14115382 | 0.00000000 |
| C | 0.70057300 | -4.14115382 | 0.00000000 |
| C | 1.11249885 | -2.75195136 | 0.00000000 |
| N | 1.94998006 | 0.00000000 | 0.00000000 |
| C | 2.75195136 | -1.11249885 | 0.00000000 |
| C | 4.14115382 | -0.70057300 | 0.00000000 |
| C | 4.14115382 | 0.70057300 | 0.00000000 |
| C | 2.75195136 | 1.11249885 | 0.00000000 |
| C | -5.33293983 | -1.42022918 | 0.00000000 |
| C | -6.52079987 | -0.70114133 | 0.00000000 |
| C | -6.52079987 | 0.70114133 | 0.00000000 |
| C | -5.33293983 | 1.42022918 | 0.00000000 |
| C | -1.42022918 | 5.33293983 | 0.00000000 |
| C | -0.70114133 | 6.52079987 | 0.00000000 |
| C | 0.70114133 | 6.52079987 | 0.00000000 |
| C | 1.42022918 | 5.33293983 | 0.00000000 |
| C | 5.33293983 | 1.42022918 | 0.00000000 |
| C | 6.52079987 | 0.70114133 | 0.00000000 |
| C | 6.52079987 | -0.70114133 | 0.00000000 |
| C | 5.33293983 | -1.42022918 | 0.00000000 |
| C | 1.42022918 | -5.33293983 | 0.00000000 |
| C | 0.70114133 | -6.52079987 | 0.00000000 |
| C | -0.70114133 | -6.52079987 | 0.00000000 |
| C | -1.42022918 | -5.33293983 | 0.00000000 |
| H | -5.32833281 | -2.50690260 | 0.00000000 |
| H | -7.47086618 | -1.23209397 | 0.00000000 |
| H | -7.47086618 | 1.23209397 | 0.00000000 |
| H | -5.32833281 | 2.50690260 | 0.00000000 |
| H | -2.50690260 | 5.32833281 | 0.00000000 |
| H | -1.23209397 | 7.47086618 | 0.00000000 |
| H | 1.23209397 | 7.47086618 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | 2.50690260 | 5.32833281 | 0.00000000 |
| H | 5.32833281 | 2.50690260 | 0.00000000 |
| H | 7.47086618 | 1.23209397 | 0.00000000 |
| H | 7.47086618 | -1.23209397 | 0.00000000 |
| H | 5.32833281 | -2.50690260 | 0.00000000 |
| H | 2.50690260 | -5.32833281 | 0.00000000 |
| H | 1.23209397 | -7.47086618 | 0.00000000 |
| H | -1.23209397 | -7.47086618 | 0.00000000 |
| H | -2.50690260 | -5.32833281 | 0.00000000 |

level of theory opbe
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 12.0 |
| $A_{1u}$ | 1.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38120000 | 2.38120000 | 0.00000000 |
| N | -2.38120000 | 2.38120000 | 0.00000000 |
| N | -2.38120000 | -2.38120000 | 0.00000000 |
| N | 2.38120000 | -2.38120000 | 0.00000000 |
| N | 0.00000000 | 1.93180000 | 0.00000000 |
| C | 1.11680000 | 2.74840000 | 0.00000000 |
| C | 0.69960000 | 4.13590000 | 0.00000000 |
| C | -0.69960000 | 4.13590000 | 0.00000000 |
| C | -1.11680000 | 2.74840000 | 0.00000000 |
| N | -1.93180000 | 0.00000000 | 0.00000000 |
| C | -2.74840000 | 1.11680000 | 0.00000000 |
| C | -4.13590000 | 0.69960000 | 0.00000000 |
| C | -4.13590000 | -0.69960000 | 0.00000000 |
| C | -2.74840000 | -1.11680000 | 0.00000000 |
| N | 0.00000000 | -1.93180000 | 0.00000000 |
| C | -1.11680000 | -2.74840000 | 0.00000000 |
| C | -0.69960000 | -4.13590000 | 0.00000000 |
| C | 0.69960000 | -4.13590000 | 0.00000000 |
| C | 1.11680000 | -2.74840000 | 0.00000000 |
| N | 1.93180000 | 0.00000000 | 0.00000000 |
| C | 2.74840000 | -1.11680000 | 0.00000000 |
| C | 4.13590000 | -0.69960000 | 0.00000000 |
| C | 4.13590000 | 0.69960000 | 0.00000000 |
| C | 2.74840000 | 1.11680000 | 0.00000000 |
| C | -5.32580000 | -1.41830000 | 0.00000000 |
| C | -6.51860000 | -0.69940000 | 0.00000000 |
| C | -6.51860000 | 0.69940000 | 0.00000000 |
| C | -5.32580000 | 1.41830000 | 0.00000000 |
| C | -1.41830000 | 5.32580000 | 0.00000000 |
| C | -0.69940000 | 6.51860000 | 0.00000000 |
| C | 0.69940000 | 6.51860000 | 0.00000000 |
| C | 1.41830000 | 5.32580000 | 0.00000000 |
| C | 5.32580000 | 1.41830000 | 0.00000000 |
| C | 6.51860000 | 0.69940000 | 0.00000000 |
| C | 6.51860000 | -0.69940000 | 0.00000000 |
| C | 5.32580000 | -1.41830000 | 0.00000000 |
| C | 1.41830000 | -5.32580000 | 0.00000000 |
| C | 0.69940000 | -6.51860000 | 0.00000000 |
| C | -0.69940000 | -6.51860000 | 0.00000000 |
| C | -1.41830000 | -5.32580000 | 0.00000000 |
| H | -5.32100000 | -2.50500000 | 0.00000000 |
| H | -7.46730000 | -1.23270000 | 0.00000000 |
| H | -7.46730000 | 1.23270000 | 0.00000000 |
| H | -5.32100000 | 2.50500000 | 0.00000000 |
| H | -2.50500000 | 5.32100000 | 0.00000000 |
| H | -1.23270000 | 7.46730000 | 0.00000000 |
| H | 1.23270000 | 7.46730000 | 0.00000000 |
| H | 2.50500000 | 5.32100000 | 0.00000000 |
| H | 5.32100000 | 2.50500000 | 0.00000000 |
| H | 7.46730000 | 1.23270000 | 0.00000000 |
| H | 7.46730000 | -1.23270000 | 0.00000000 |
| H | 5.32100000 | -2.50500000 | 0.00000000 |
| H | 2.50500000 | -5.32100000 | 0.00000000 |
| H | 1.23270000 | -7.46730000 | 0.00000000 |
| H | -1.23270000 | -7.46730000 | 0.00000000 |
| H | -2.50500000 | -5.32100000 | 0.00000000 |

level of theory s12g
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.40525665 | 2.40525665 | 0.00000000 |
| N | -2.40525665 | 2.40525665 | 0.00000000 |
| N | -2.40525665 | -2.40525665 | 0.00000000 |
| N | 2.40525665 | -2.40525665 | 0.00000000 |
| N | 0.00000000 | 2.02877984 | 0.00000000 |
| C | 1.13026386 | 2.80832619 | 0.00000000 |
| C | 0.70576105 | 4.20483448 | 0.00000000 |
| C | -0.70576105 | 4.20483448 | 0.00000000 |
| C | -1.13026386 | 2.80832619 | 0.00000000 |

| | | | |
|---|---|---|---|
| N | -2.02877984 | 0.00000000 | 0.00000000 |
| C | -2.80832619 | 1.13026386 | 0.00000000 |
| C | -4.20483448 | 0.70576105 | 0.00000000 |
| C | -4.20483448 | -0.70576105 | 0.00000000 |
| C | -2.80832619 | -1.13026386 | 0.00000000 |
| N | 0.00000000 | -2.02877984 | 0.00000000 |
| C | -1.13026386 | -2.80832619 | 0.00000000 |
| C | -0.70576105 | -4.20483448 | 0.00000000 |
| C | 0.70576105 | -4.20483448 | 0.00000000 |
| C | 1.13026386 | -2.80832619 | 0.00000000 |
| N | 2.02877984 | 0.00000000 | 0.00000000 |
| C | 2.80832619 | -1.13026386 | 0.00000000 |
| C | 4.20483448 | -0.70576105 | 0.00000000 |
| C | 4.20483448 | 0.70576105 | 0.00000000 |
| C | 2.80832619 | 1.13026386 | 0.00000000 |
| C | -5.39926056 | -1.41957089 | 0.00000000 |
| C | -6.59083542 | -0.70135406 | 0.00000000 |
| C | -6.59083542 | 0.70135406 | 0.00000000 |
| C | -5.39926056 | 1.41957089 | 0.00000000 |
| C | -1.41957089 | 5.39926056 | 0.00000000 |
| C | -0.70135406 | 6.59083542 | 0.00000000 |
| C | 0.70135406 | 6.59083542 | 0.00000000 |
| C | 1.41957089 | 5.39926056 | 0.00000000 |
| C | 5.39926056 | 1.41957089 | 0.00000000 |
| C | 6.59083542 | 0.70135406 | 0.00000000 |
| C | 6.59083542 | -0.70135406 | 0.00000000 |
| C | 5.39926056 | -1.41957089 | 0.00000000 |
| C | 1.41957089 | -5.39926056 | 0.00000000 |
| C | 0.70135406 | -6.59083542 | 0.00000000 |
| C | -0.70135406 | -6.59083542 | 0.00000000 |
| C | -1.41957089 | -5.39926056 | 0.00000000 |
| H | -5.39190711 | -2.50781649 | 0.00000000 |
| H | -7.54107742 | -1.23396832 | 0.00000000 |
| H | -7.54107742 | 1.23396832 | 0.00000000 |
| H | -5.39190711 | 2.50781649 | 0.00000000 |
| H | -2.50781649 | 5.39190711 | 0.00000000 |
| H | -1.23396832 | 7.54107742 | 0.00000000 |
| H | 1.23396832 | 7.54107742 | 0.00000000 |
| H | 2.50781649 | 5.39190711 | 0.00000000 |
| H | 5.39190711 | 2.50781649 | 0.00000000 |
| H | 7.54107742 | 1.23396832 | 0.00000000 |
| H | 7.54107742 | -1.23396832 | 0.00000000 |
| H | 5.39190711 | -2.50781649 | 0.00000000 |
| H | 2.50781649 | -5.39190711 | 0.00000000 |
| H | 1.23396832 | -7.54107742 | 0.00000000 |
| H | -1.23396832 | -7.54107742 | 0.00000000 |
| H | -2.50781649 | -5.39190711 | 0.00000000 |

level of theory s12g
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39712954 | 2.39712954 | 0.00000000 |
| N | -2.39712954 | 2.39712954 | 0.00000000 |
| N | -2.39712954 | -2.39712954 | 0.00000000 |
| N | 2.39712954 | -2.39712954 | 0.00000000 |
| N | 0.00000000 | 1.95179990 | 0.00000000 |
| C | 1.12694063 | 2.76777164 | 0.00000000 |
| C | 0.70206263 | 4.15002547 | 0.00000000 |
| C | -0.70206263 | 4.15002547 | 0.00000000 |
| C | -1.12694063 | 2.76777164 | 0.00000000 |
| N | -1.95179990 | 0.00000000 | 0.00000000 |
| C | -2.76777164 | 1.12694063 | 0.00000000 |
| C | -4.15002547 | 0.70206263 | 0.00000000 |
| C | -4.15002547 | -0.70206263 | 0.00000000 |
| C | -2.76777164 | -1.12694063 | 0.00000000 |
| N | 0.00000000 | -1.95179990 | 0.00000000 |
| C | -1.12694063 | -2.76777164 | 0.00000000 |
| C | -0.70206263 | -4.15002547 | 0.00000000 |
| C | 0.70206263 | -4.15002547 | 0.00000000 |
| C | 1.12694063 | -2.76777164 | 0.00000000 |
| N | 1.95179990 | 0.00000000 | 0.00000000 |
| C | 2.76777164 | -1.12694063 | 0.00000000 |
| C | 4.15002547 | -0.70206263 | 0.00000000 |
| C | 4.15002547 | 0.70206263 | 0.00000000 |
| C | 2.76777164 | 1.12694063 | 0.00000000 |
| C | -5.34442403 | -1.42105629 | 0.00000000 |
| C | -6.53332127 | -0.70284264 | 0.00000000 |
| C | -6.53332127 | 0.70284264 | 0.00000000 |
| C | -5.34442403 | 1.42105629 | 0.00000000 |
| C | -1.42105629 | 5.34442403 | 0.00000000 |
| C | -0.70284264 | 6.53332127 | 0.00000000 |
| C | 0.70284264 | 6.53332127 | 0.00000000 |
| C | 1.42105629 | 5.34442403 | 0.00000000 |
| C | 5.34442403 | 1.42105629 | 0.00000000 |
| C | 6.53332127 | 0.70284264 | 0.00000000 |
| C | 6.53332127 | -0.70284264 | 0.00000000 |
| C | 5.34442403 | -1.42105629 | 0.00000000 |
| C | 1.42105629 | -5.34442403 | 0.00000000 |
| C | 0.70284264 | -6.53332127 | 0.00000000 |
| C | -0.70284264 | -6.53332127 | 0.00000000 |
| C | -1.42105629 | -5.34442403 | 0.00000000 |
| H | -5.33454482 | -2.50909075 | 0.00000000 |
| H | -7.48398026 | -1.23451284 | 0.00000000 |
| H | -7.48398026 | 1.23451284 | 0.00000000 |
| H | -5.33454482 | 2.50909075 | 0.00000000 |
| H | -2.50909075 | 5.33454482 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -1.23451284 | 7.48398026 | 0.00000000 |
| H | 1.23451284 | 7.48398026 | 0.00000000 |
| H | 2.50909075 | 5.33454482 | 0.00000000 |
| H | 5.33454482 | 2.50909075 | 0.00000000 |
| H | 7.48398026 | 1.23451284 | 0.00000000 |
| H | 7.48398026 | -1.23451284 | 0.00000000 |
| H | 5.33454482 | -2.50909075 | 0.00000000 |
| H | 2.50909075 | -5.33454482 | 0.00000000 |
| H | 1.23451284 | -7.48398026 | 0.00000000 |
| H | -1.23451284 | -7.48398026 | 0.00000000 |
| H | -2.50909075 | -5.33454482 | 0.00000000 |

level of theory s12g
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39453816 | 2.39453816 | 0.00000000 |
| N | -2.39453816 | 2.39453816 | 0.00000000 |
| N | -2.39453816 | -2.39453816 | 0.00000000 |
| N | 2.39453816 | -2.39453816 | 0.00000000 |
| N | 0.00000000 | 1.95774679 | 0.00000000 |
| C | 1.12011213 | 2.76632540 | 0.00000000 |
| C | 0.70235579 | 4.15610625 | 0.00000000 |
| C | -0.70235579 | 4.15610625 | 0.00000000 |
| C | -1.12011213 | 2.76632540 | 0.00000000 |
| N | -1.95774679 | 0.00000000 | 0.00000000 |
| C | -2.76632540 | 1.12011213 | 0.00000000 |
| C | -4.15610625 | 0.70235579 | 0.00000000 |
| C | -4.15610625 | -0.70235579 | 0.00000000 |
| C | -2.76632540 | -1.12011213 | 0.00000000 |
| N | 0.00000000 | -1.95774679 | 0.00000000 |
| C | -1.12011213 | -2.76632540 | 0.00000000 |
| C | -0.70235579 | -4.15610625 | 0.00000000 |
| C | 0.70235579 | -4.15610625 | 0.00000000 |
| C | 1.12011213 | -2.76632540 | 0.00000000 |
| N | 1.95774679 | 0.00000000 | 0.00000000 |
| C | 2.76632540 | -1.12011213 | 0.00000000 |
| C | 4.15610625 | -0.70235579 | 0.00000000 |
| C | 4.15610625 | 0.70235579 | 0.00000000 |
| C | 2.76632540 | 1.12011213 | 0.00000000 |
| C | -5.34919986 | -1.42093246 | 0.00000000 |
| C | -6.53895065 | -0.70233516 | 0.00000000 |
| C | -6.53895065 | 0.70233516 | 0.00000000 |
| C | -5.34919986 | 1.42093246 | 0.00000000 |
| C | -1.42093246 | 5.34919986 | 0.00000000 |
| C | -0.70233516 | 6.53895065 | 0.00000000 |
| C | 0.70233516 | 6.53895065 | 0.00000000 |
| C | 1.42093246 | 5.34919986 | 0.00000000 |
| C | 5.34919986 | 1.42093246 | 0.00000000 |
| C | 6.53895065 | 0.70233516 | 0.00000000 |
| C | 6.53895065 | -0.70233516 | 0.00000000 |
| C | 5.34919986 | -1.42093246 | 0.00000000 |
| C | 1.42093246 | -5.34919986 | 0.00000000 |
| C | 0.70233516 | -6.53895065 | 0.00000000 |
| C | -0.70233516 | -6.53895065 | 0.00000000 |
| C | -1.42093246 | -5.34919986 | 0.00000000 |
| H | -5.33905236 | -2.50904471 | 0.00000000 |
| H | -7.48980491 | -1.23373812 | 0.00000000 |
| H | -7.48980491 | 1.23373812 | 0.00000000 |
| H | -5.33905236 | 2.50904471 | 0.00000000 |
| H | -2.50904471 | 5.33905236 | 0.00000000 |
| H | -1.23373812 | 7.48980491 | 0.00000000 |
| H | 1.23373812 | 7.48980491 | 0.00000000 |
| H | 2.50904471 | 5.33905236 | 0.00000000 |
| H | 5.33905236 | 2.50904471 | 0.00000000 |
| H | 7.48980491 | 1.23373812 | 0.00000000 |
| H | 7.48980491 | -1.23373812 | 0.00000000 |
| H | 5.33905236 | -2.50904471 | 0.00000000 |
| H | 2.50904471 | -5.33905236 | 0.00000000 |
| H | 1.23373812 | -7.48980491 | 0.00000000 |
| H | -1.23373812 | -7.48980491 | 0.00000000 |
| H | -2.50904471 | -5.33905236 | 0.00000000 |

level of theory s12g
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39383065 | 2.39383065 | 0.00000000 |
| N | -2.39383065 | 2.39383065 | 0.00000000 |
| N | -2.39383065 | -2.39383065 | 0.00000000 |
| N | 2.39383065 | -2.39383065 | 0.00000000 |
| N | 0.00000000 | 1.95651434 | 0.00000000 |
| C | 1.12116572 | 2.76441295 | 0.00000000 |
| C | 0.70165252 | 4.15329314 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -0.70165252 | 4.15329314 | 0.00000000 |
| C | -1.12116572 | 2.76441295 | 0.00000000 |
| N | -1.95651434 | 0.00000000 | 0.00000000 |
| C | -2.76441295 | 1.12116572 | 0.00000000 |
| C | -4.15329314 | 0.70165252 | 0.00000000 |
| C | -4.15329314 | -0.70165252 | 0.00000000 |
| C | -2.76441295 | -1.12116572 | 0.00000000 |
| N | 0.00000000 | -1.95651434 | 0.00000000 |
| C | -1.12116572 | -2.76441295 | 0.00000000 |
| C | -0.70165252 | -4.15329314 | 0.00000000 |
| C | 0.70165252 | -4.15329314 | 0.00000000 |
| C | 1.12116572 | -2.76441295 | 0.00000000 |
| N | 1.95651434 | 0.00000000 | 0.00000000 |
| C | 2.76441295 | -1.12116572 | 0.00000000 |
| C | 4.15329314 | -0.70165252 | 0.00000000 |
| C | 4.15329314 | 0.70165252 | 0.00000000 |
| C | 2.76441295 | 1.12116572 | 0.00000000 |
| C | -5.34555224 | -1.42121028 | 0.00000000 |
| C | -6.53523054 | -0.70221345 | 0.00000000 |
| C | -6.53523054 | 0.70221345 | 0.00000000 |
| C | -5.34555224 | 1.42121028 | 0.00000000 |
| C | -1.42121028 | 5.34555224 | 0.00000000 |
| C | -0.70221345 | 6.53523054 | 0.00000000 |
| C | 0.70221345 | 6.53523054 | 0.00000000 |
| C | 1.42121028 | 5.34555224 | 0.00000000 |
| C | 5.34555224 | 1.42121028 | 0.00000000 |
| C | 6.53523054 | 0.70221345 | 0.00000000 |
| C | 6.53523054 | -0.70221345 | 0.00000000 |
| C | 5.34555224 | -1.42121028 | 0.00000000 |
| C | 1.42121028 | -5.34555224 | 0.00000000 |
| C | 0.70221345 | -6.53523054 | 0.00000000 |
| C | -0.70221345 | -6.53523054 | 0.00000000 |
| C | -1.42121028 | -5.34555224 | 0.00000000 |
| H | -5.33675837 | -2.50920346 | 0.00000000 |
| H | -7.48588688 | -1.23386566 | 0.00000000 |
| H | -7.48588688 | 1.23386566 | 0.00000000 |
| H | -5.33675837 | 2.50920346 | 0.00000000 |
| H | -2.50920346 | 5.33675837 | 0.00000000 |
| H | -1.23386566 | 7.48588688 | 0.00000000 |
| H | 1.23386566 | 7.48588688 | 0.00000000 |
| H | 2.50920346 | 5.33675837 | 0.00000000 |
| H | 5.33675837 | 2.50920346 | 0.00000000 |
| H | 7.48588688 | 1.23386566 | 0.00000000 |
| H | 7.48588688 | -1.23386566 | 0.00000000 |
| H | 5.33675837 | -2.50920346 | 0.00000000 |
| H | 2.50920346 | -5.33675837 | 0.00000000 |
| H | 1.23386566 | -7.48588688 | 0.00000000 |
| H | -1.23386566 | -7.48588688 | 0.00000000 |
| H | -2.50920346 | -5.33675837 | 0.00000000 |

level of theory s12g
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 12.0 |
| $A_{1u}$ | 1.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39990084 | 2.39990084 | 0.00000000 |
| N | -2.39990084 | 2.39990084 | 0.00000000 |
| N | -2.39990084 | -2.39990084 | 0.00000000 |
| N | 2.39990084 | -2.39990084 | 0.00000000 |
| N | 0.00000000 | 1.94279225 | 0.00000000 |
| C | 1.12673796 | 2.76405470 | 0.00000000 |
| C | 0.70084288 | 4.15092560 | 0.00000000 |
| C | -0.70084288 | 4.15092560 | 0.00000000 |
| C | -1.12673796 | 2.76405470 | 0.00000000 |
| N | -1.94279225 | 0.00000000 | 0.00000000 |
| C | -2.76405470 | 1.12673796 | 0.00000000 |
| C | -4.15092560 | 0.70084288 | 0.00000000 |
| C | -4.15092560 | -0.70084288 | 0.00000000 |
| C | -2.76405470 | -1.12673796 | 0.00000000 |
| N | 0.00000000 | -1.94279225 | 0.00000000 |
| C | -1.12673796 | -2.76405470 | 0.00000000 |
| C | -0.70084288 | -4.15092560 | 0.00000000 |
| C | 0.70084288 | -4.15092560 | 0.00000000 |
| C | 1.12673796 | -2.76405470 | 0.00000000 |
| N | 1.94279225 | 0.00000000 | 0.00000000 |
| C | 2.76405470 | -1.12673796 | 0.00000000 |
| C | 4.15092560 | -0.70084288 | 0.00000000 |
| C | 4.15092560 | 0.70084288 | 0.00000000 |
| C | 2.76405470 | 1.12673796 | 0.00000000 |
| C | -5.34136327 | -1.41897080 | 0.00000000 |
| C | -6.53645347 | -0.70023644 | 0.00000000 |
| C | -6.53645347 | 0.70023644 | 0.00000000 |
| C | -5.34136327 | 1.41897080 | 0.00000000 |
| C | -1.41897080 | 5.34136327 | 0.00000000 |
| C | -0.70023644 | 6.53645347 | 0.00000000 |
| C | 0.70023644 | 6.53645347 | 0.00000000 |
| C | 1.41897080 | 5.34136327 | 0.00000000 |
| C | 5.34136327 | 1.41897080 | 0.00000000 |
| C | 6.53645347 | 0.70023644 | 0.00000000 |
| C | 6.53645347 | -0.70023644 | 0.00000000 |
| C | 5.34136327 | -1.41897080 | 0.00000000 |
| C | 1.41897080 | -5.34136327 | 0.00000000 |
| C | 0.70023644 | -6.53645347 | 0.00000000 |
| C | -0.70023644 | -6.53645347 | 0.00000000 |
| C | -1.41897080 | -5.34136327 | 0.00000000 |
| H | -5.33125070 | -2.50709310 | 0.00000000 |
| H | -7.48566039 | -1.23432498 | 0.00000000 |
| H | -7.48566039 | 1.23432498 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -5.33125070 | 2.50709310 | 0.00000000 |
| H | -2.50709310 | 5.33125070 | 0.00000000 |
| H | -1.23432498 | 7.48566039 | 0.00000000 |
| H | 1.23432498 | 7.48566039 | 0.00000000 |
| H | 2.50709310 | 5.33125070 | 0.00000000 |
| H | 5.33125070 | 2.50709310 | 0.00000000 |
| H | 7.48566039 | 1.23432498 | 0.00000000 |
| H | 7.48566039 | -1.23432498 | 0.00000000 |
| H | 5.33125070 | -2.50709310 | 0.00000000 |
| H | 2.50709310 | -5.33125070 | 0.00000000 |
| H | 1.23432498 | -7.48566039 | 0.00000000 |
| H | -1.23432498 | -7.48566039 | 0.00000000 |
| H | -2.50709310 | -5.33125070 | 0.00000000 |

level of theory ssb-d
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.40640972 | 2.40640972 | 0.00000000 |
| N | -2.40640972 | 2.40640972 | 0.00000000 |
| N | -2.40640972 | -2.40640972 | 0.00000000 |
| N | 2.40640972 | -2.40640972 | 0.00000000 |
| N | 0.00000000 | 2.02121049 | 0.00000000 |
| C | 1.12800004 | 2.80138180 | 0.00000000 |
| C | 0.70471328 | 4.19439275 | 0.00000000 |
| C | -0.70471328 | 4.19439275 | 0.00000000 |
| C | -1.12800004 | 2.80138180 | 0.00000000 |
| N | -2.02121049 | 0.00000000 | 0.00000000 |
| C | -2.80138180 | 1.12800004 | 0.00000000 |
| C | -4.19439275 | 0.70471328 | 0.00000000 |
| C | -4.19439275 | -0.70471328 | 0.00000000 |
| C | -2.80138180 | -1.12800004 | 0.00000000 |
| N | 0.00000000 | -2.02121049 | 0.00000000 |
| C | -1.12800004 | -2.80138180 | 0.00000000 |
| C | -0.70471328 | -4.19439275 | 0.00000000 |
| C | 0.70471328 | -4.19439275 | 0.00000000 |
| C | 1.12800004 | -2.80138180 | 0.00000000 |
| N | 2.02121049 | 0.00000000 | 0.00000000 |
| C | 2.80138180 | -1.12800004 | 0.00000000 |
| C | 4.19439275 | -0.70471328 | 0.00000000 |
| C | 4.19439275 | 0.70471328 | 0.00000000 |
| C | 2.80138180 | 1.12800004 | 0.00000000 |
| C | -5.38663333 | -1.41929519 | 0.00000000 |
| C | -6.57619785 | -0.70085029 | 0.00000000 |
| C | -6.57619785 | 0.70085029 | 0.00000000 |
| C | -5.38663333 | 1.41929519 | 0.00000000 |
| C | -1.41929519 | 5.38663333 | 0.00000000 |
| C | -0.70085029 | 6.57619785 | 0.00000000 |
| C | 0.70085029 | 6.57619785 | 0.00000000 |
| C | 1.41929519 | 5.38663333 | 0.00000000 |
| C | 5.38663333 | 1.41929519 | 0.00000000 |
| C | 6.57619785 | 0.70085029 | 0.00000000 |
| C | 6.57619785 | -0.70085029 | 0.00000000 |
| C | 5.38663333 | -1.41929519 | 0.00000000 |
| C | 1.41929519 | -5.38663333 | 0.00000000 |
| C | 0.70085029 | -6.57619785 | 0.00000000 |
| C | -0.70085029 | -6.57619785 | 0.00000000 |
| C | -1.41929519 | -5.38663333 | 0.00000000 |
| H | -5.37736690 | -2.50103720 | 0.00000000 |
| H | -7.52133911 | -1.22916074 | 0.00000000 |
| H | -7.52133911 | 1.22916074 | 0.00000000 |
| H | -5.37736690 | 2.50103720 | 0.00000000 |
| H | -2.50103720 | 5.37736690 | 0.00000000 |
| H | -1.22916074 | 7.52133911 | 0.00000000 |
| H | 1.22916074 | 7.52133911 | 0.00000000 |
| H | 2.50103720 | 5.37736690 | 0.00000000 |
| H | 5.37736690 | 2.50103720 | 0.00000000 |
| H | 7.52133911 | 1.22916074 | 0.00000000 |
| H | 7.52133911 | -1.22916074 | 0.00000000 |
| H | 5.37736690 | -2.50103720 | 0.00000000 |
| H | 2.50103720 | -5.37736690 | 0.00000000 |
| H | 1.22916074 | -7.52133911 | 0.00000000 |
| H | -1.22916074 | -7.52133911 | 0.00000000 |
| H | -2.50103720 | -5.37736690 | 0.00000000 |

level of theory ssb-d
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39971457 | 2.39971457 | 0.00000000 |
| N | -2.39971457 | 2.39971457 | 0.00000000 |
| N | -2.39971457 | -2.39971457 | 0.00000000 |
| N | 2.39971457 | -2.39971457 | 0.00000000 |
| N | 0.00000000 | 1.94728020 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 1.12653634 | 2.76272064 | 0.00000000 |
| C | 0.70117255 | 4.14097919 | 0.00000000 |
| C | -0.70117255 | 4.14097919 | 0.00000000 |
| C | -1.12653634 | 2.76272064 | 0.00000000 |
| N | -1.94728020 | 0.00000000 | 0.00000000 |
| C | -2.76272064 | 1.12653634 | 0.00000000 |
| C | -4.14097919 | 0.70117255 | 0.00000000 |
| C | -4.14097919 | -0.70117255 | 0.00000000 |
| C | -2.76272064 | -1.12653634 | 0.00000000 |
| N | 0.00000000 | -1.94728020 | 0.00000000 |
| C | -1.12653634 | -2.76272064 | 0.00000000 |
| C | -0.70117255 | -4.14097919 | 0.00000000 |
| C | 0.70117255 | -4.14097919 | 0.00000000 |
| C | 1.12653634 | -2.76272064 | 0.00000000 |
| N | 1.94728020 | 0.00000000 | 0.00000000 |
| C | 2.76272064 | -1.12653634 | 0.00000000 |
| C | 4.14097919 | -0.70117255 | 0.00000000 |
| C | 4.14097919 | 0.70117255 | 0.00000000 |
| C | 2.76272064 | 1.12653634 | 0.00000000 |
| C | -5.33326580 | -1.42083721 | 0.00000000 |
| C | -6.52002251 | -0.70239178 | 0.00000000 |
| C | -6.52002251 | 0.70239178 | 0.00000000 |
| C | -5.33326580 | 1.42083721 | 0.00000000 |
| C | -1.42083721 | 5.33326580 | 0.00000000 |
| C | -0.70239178 | 6.52002251 | 0.00000000 |
| C | 0.70239178 | 6.52002251 | 0.00000000 |
| C | 1.42083721 | 5.33326580 | 0.00000000 |
| C | 5.33326580 | 1.42083721 | 0.00000000 |
| C | 6.52002251 | 0.70239178 | 0.00000000 |
| C | 6.52002251 | -0.70239178 | 0.00000000 |
| C | 5.33326580 | -1.42083721 | 0.00000000 |
| C | 1.42083721 | -5.33326580 | 0.00000000 |
| C | 0.70239178 | -6.52002251 | 0.00000000 |
| C | -0.70239178 | -6.52002251 | 0.00000000 |
| C | -1.42083721 | -5.33326580 | 0.00000000 |
| H | -5.32338765 | -2.50236226 | 0.00000000 |
| H | -7.46542624 | -1.23018258 | 0.00000000 |
| H | -7.46542624 | 1.23018258 | 0.00000000 |
| H | -5.32338765 | 2.50236226 | 0.00000000 |
| H | -2.50236226 | 5.32338765 | 0.00000000 |
| H | -1.23018258 | 7.46542624 | 0.00000000 |
| H | 1.23018258 | 7.46542624 | 0.00000000 |
| H | 2.50236226 | 5.32338765 | 0.00000000 |
| H | 5.32338765 | 2.50236226 | 0.00000000 |
| H | 7.46542624 | 1.23018258 | 0.00000000 |
| H | 7.46542624 | -1.23018258 | 0.00000000 |
| H | 5.32338765 | -2.50236226 | 0.00000000 |
| H | 2.50236226 | -5.32338765 | 0.00000000 |
| H | 1.23018258 | -7.46542624 | 0.00000000 |
| H | -1.23018258 | -7.46542624 | 0.00000000 |
| H | -2.50236226 | -5.32338765 | 0.00000000 |

level of theory ssb-d
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39606166 | 2.39606166 | 0.00000000 |
| N | -2.39606166 | 2.39606166 | 0.00000000 |
| N | -2.39606166 | -2.39606166 | 0.00000000 |
| N | 2.39606166 | -2.39606166 | 0.00000000 |
| N | 0.00000000 | 1.95261907 | 0.00000000 |
| C | 1.11848914 | 2.76064097 | 0.00000000 |
| C | 0.70123976 | 4.14738964 | 0.00000000 |
| C | -0.70123976 | 4.14738964 | 0.00000000 |
| C | -1.11848914 | 2.76064097 | 0.00000000 |
| N | -1.95261907 | 0.00000000 | 0.00000000 |
| C | -2.76064097 | 1.11848914 | 0.00000000 |
| C | -4.14738964 | 0.70123976 | 0.00000000 |
| C | -4.14738964 | -0.70123976 | 0.00000000 |
| C | -2.76064097 | -1.11848914 | 0.00000000 |
| N | 0.00000000 | -1.95261907 | 0.00000000 |
| C | -1.11848914 | -2.76064097 | 0.00000000 |
| C | -0.70123976 | -4.14738964 | 0.00000000 |
| C | 0.70123976 | -4.14738964 | 0.00000000 |
| C | 1.11848914 | -2.76064097 | 0.00000000 |
| N | 1.95261907 | 0.00000000 | 0.00000000 |
| C | 2.76064097 | -1.11848914 | 0.00000000 |
| C | 4.14738964 | -0.70123976 | 0.00000000 |
| C | 4.14738964 | 0.70123976 | 0.00000000 |
| C | 2.76064097 | 1.11848914 | 0.00000000 |
| C | -5.33795749 | -1.42052658 | 0.00000000 |
| C | -6.52591173 | -0.70173031 | 0.00000000 |
| C | -6.52591173 | 0.70173031 | 0.00000000 |
| C | -5.33795749 | 1.42052658 | 0.00000000 |
| C | -1.42052658 | 5.33795749 | 0.00000000 |
| C | -0.70173031 | 6.52591173 | 0.00000000 |
| C | 0.70173031 | 6.52591173 | 0.00000000 |
| C | 1.42052658 | 5.33795749 | 0.00000000 |
| C | 5.33795749 | 1.42052658 | 0.00000000 |
| C | 6.52591173 | 0.70173031 | 0.00000000 |
| C | 6.52591173 | -0.70173031 | 0.00000000 |
| C | 5.33795749 | -1.42052658 | 0.00000000 |
| C | 1.42052658 | -5.33795749 | 0.00000000 |
| C | 0.70173031 | -6.52591173 | 0.00000000 |
| C | -0.70173031 | -6.52591173 | 0.00000000 |
| C | -1.42052658 | -5.33795749 | 0.00000000 |
| H | -5.32807828 | -2.50215323 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -7.47145780 | -1.22934754 | 0.00000000 |
| H | -7.47145780 | 1.22934754 | 0.00000000 |
| H | -5.32807828 | 2.50215323 | 0.00000000 |
| H | -2.50215323 | 5.32807828 | 0.00000000 |
| H | -1.22934754 | 7.47145780 | 0.00000000 |
| H | 1.22934754 | 7.47145780 | 0.00000000 |
| H | 2.50215323 | 5.32807828 | 0.00000000 |
| H | 5.32807828 | 2.50215323 | 0.00000000 |
| H | 7.47145780 | 1.22934754 | 0.00000000 |
| H | 7.47145780 | -1.22934754 | 0.00000000 |
| H | 5.32807828 | -2.50215323 | 0.00000000 |
| H | 2.50215323 | -5.32807828 | 0.00000000 |
| H | 1.22934754 | -7.47145780 | 0.00000000 |
| H | -1.22934754 | -7.47145780 | 0.00000000 |
| H | -2.50215323 | -5.32807828 | 0.00000000 |

level of theory ssb-d
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39553513 | 2.39553513 | 0.00000000 |
| N | -2.39553513 | 2.39553513 | 0.00000000 |
| N | -2.39553513 | -2.39553513 | 0.00000000 |
| N | 2.39553513 | -2.39553513 | 0.00000000 |
| N | 0.00000000 | 1.95287254 | 0.00000000 |
| C | 1.11984225 | 2.75940111 | 0.00000000 |
| C | 0.70056770 | 4.14521367 | 0.00000000 |
| C | -0.70056770 | 4.14521367 | 0.00000000 |
| C | -1.11984225 | 2.75940111 | 0.00000000 |
| N | -1.95287254 | 0.00000000 | 0.00000000 |
| C | -2.75940111 | 1.11984225 | 0.00000000 |
| C | -4.14521367 | 0.70056770 | 0.00000000 |
| C | -4.14521367 | -0.70056770 | 0.00000000 |
| C | -2.75940111 | -1.11984225 | 0.00000000 |
| N | 0.00000000 | -1.95287254 | 0.00000000 |
| C | -1.11984225 | -2.75940111 | 0.00000000 |
| C | -0.70056770 | -4.14521367 | 0.00000000 |
| C | 0.70056770 | -4.14521367 | 0.00000000 |
| C | 1.11984225 | -2.75940111 | 0.00000000 |
| N | 1.95287254 | 0.00000000 | 0.00000000 |
| C | 2.75940111 | -1.11984225 | 0.00000000 |
| C | 4.14521367 | -0.70056770 | 0.00000000 |
| C | 4.14521367 | 0.70056770 | 0.00000000 |
| C | 2.75940111 | 1.11984225 | 0.00000000 |
| C | -5.33514703 | -1.42070068 | 0.00000000 |
| C | -6.52299702 | -0.70162341 | 0.00000000 |
| C | -6.52299702 | 0.70162341 | 0.00000000 |
| C | -5.33514703 | 1.42070068 | 0.00000000 |
| C | -1.42070068 | 5.33514703 | 0.00000000 |
| C | -0.70162341 | 6.52299702 | 0.00000000 |
| C | 0.70162341 | 6.52299702 | 0.00000000 |
| C | 1.42070068 | 5.33514703 | 0.00000000 |
| C | 5.33514703 | 1.42070068 | 0.00000000 |
| C | 6.52299702 | 0.70162341 | 0.00000000 |
| C | 6.52299702 | -0.70162341 | 0.00000000 |
| C | 5.33514703 | -1.42070068 | 0.00000000 |
| C | 1.42070068 | -5.33514703 | 0.00000000 |
| C | 0.70162341 | -6.52299702 | 0.00000000 |
| C | -0.70162341 | -6.52299702 | 0.00000000 |
| C | -1.42070068 | -5.33514703 | 0.00000000 |
| H | -5.32519585 | -2.50224108 | 0.00000000 |
| H | -7.46839546 | -1.22937770 | 0.00000000 |
| H | -7.46839546 | 1.22937770 | 0.00000000 |
| H | -5.32519585 | 2.50224108 | 0.00000000 |
| H | -2.50224108 | 5.32519585 | 0.00000000 |
| H | -1.22937770 | 7.46839546 | 0.00000000 |
| H | 1.22937770 | 7.46839546 | 0.00000000 |
| H | 2.50224108 | 5.32519585 | 0.00000000 |
| H | 5.32519585 | 2.50224108 | 0.00000000 |
| H | 7.46839546 | 1.22937770 | 0.00000000 |
| H | 7.46839546 | -1.22937770 | 0.00000000 |
| H | 5.32519585 | -2.50224108 | 0.00000000 |
| H | 2.50224108 | -5.32519585 | 0.00000000 |
| H | 1.22937770 | -7.46839546 | 0.00000000 |
| H | -1.22937770 | -7.46839546 | 0.00000000 |
| H | -2.50224108 | -5.32519585 | 0.00000000 |

level of theory ssb-d
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 20.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39558752 | 2.39558752 | 0.00000000 |
| N | -2.39558752 | 2.39558752 | 0.00000000 |
| N | -2.39558752 | -2.39558752 | 0.00000000 |

| | | | |
|---|---|---|---|
| N | 2.39558752 | -2.39558752 | 0.00000000 |
| N | 0.00000000 | 1.93897529 | 0.00000000 |
| C | 1.12279982 | 2.75721667 | 0.00000000 |
| C | 0.70049732 | 4.13760568 | 0.00000000 |
| C | -0.70049732 | 4.13760568 | 0.00000000 |
| C | -1.12279982 | 2.75721667 | 0.00000000 |
| N | -1.93897529 | 0.00000000 | 0.00000000 |
| C | -2.75721667 | 1.12279982 | 0.00000000 |
| C | -4.13760568 | 0.70049732 | 0.00000000 |
| C | -4.13760568 | -0.70049732 | 0.00000000 |
| C | -2.75721667 | -1.12279982 | 0.00000000 |
| N | 0.00000000 | -1.93897529 | 0.00000000 |
| C | -1.12279982 | -2.75721667 | 0.00000000 |
| C | -0.70049732 | -4.13760568 | 0.00000000 |
| C | 0.70049732 | -4.13760568 | 0.00000000 |
| C | 1.12279982 | -2.75721667 | 0.00000000 |
| N | 1.93897529 | 0.00000000 | 0.00000000 |
| C | 2.75721667 | -1.12279982 | 0.00000000 |
| C | 4.13760568 | -0.70049732 | 0.00000000 |
| C | 4.13760568 | 0.70049732 | 0.00000000 |
| C | 2.75721667 | 1.12279982 | 0.00000000 |
| C | -5.32894031 | -1.42085308 | 0.00000000 |
| C | -6.51610343 | -0.70212825 | 0.00000000 |
| C | -6.51610343 | 0.70212825 | 0.00000000 |
| C | -5.32894031 | 1.42085308 | 0.00000000 |
| C | -1.42085308 | 5.32894031 | 0.00000000 |
| C | -0.70212825 | 6.51610343 | 0.00000000 |
| C | 0.70212825 | 6.51610343 | 0.00000000 |
| C | 1.42085308 | 5.32894031 | 0.00000000 |
| C | 5.32894031 | 1.42085308 | 0.00000000 |
| C | 6.51610343 | 0.70212825 | 0.00000000 |
| C | 6.51610343 | -0.70212825 | 0.00000000 |
| C | 5.32894031 | -1.42085308 | 0.00000000 |
| C | 1.42085308 | -5.32894031 | 0.00000000 |
| C | 0.70212825 | -6.51610343 | 0.00000000 |
| C | -0.70212825 | -6.51610343 | 0.00000000 |
| C | -1.42085308 | -5.32894031 | 0.00000000 |
| H | -5.31818743 | -2.50230511 | 0.00000000 |
| H | -7.46135475 | -1.23002595 | 0.00000000 |
| H | -7.46135475 | 1.23002595 | 0.00000000 |
| H | -5.31818743 | 2.50230511 | 0.00000000 |
| H | -2.50230511 | 5.31818743 | 0.00000000 |
| H | -1.23002595 | 7.46135475 | 0.00000000 |
| H | 1.23002595 | 7.46135475 | 0.00000000 |
| H | 2.50230511 | 5.31818743 | 0.00000000 |
| H | 5.31818743 | 2.50230511 | 0.00000000 |
| H | 7.46135475 | 1.23002595 | 0.00000000 |
| H | 7.46135475 | -1.23002595 | 0.00000000 |
| H | 5.31818743 | -2.50230511 | 0.00000000 |
| H | 2.50230511 | -5.31818743 | 0.00000000 |
| H | 1.23002595 | -7.46135475 | 0.00000000 |
| H | -1.23002595 | -7.46135475 | 0.00000000 |
| H | -2.50230511 | -5.31818743 | 0.00000000 |

level of theory m06l

spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38867488 | 2.38867488 | 0.00000000 |
| N | -2.38867488 | 2.38867488 | 0.00000000 |
| N | -2.38867488 | -2.38867488 | 0.00000000 |
| N | 2.38867488 | -2.38867488 | 0.00000000 |
| N | 0.00000000 | 2.02188784 | 0.00000000 |
| C | 1.12364968 | 2.79708330 | 0.00000000 |
| C | 0.70248333 | 4.18556290 | 0.00000000 |
| C | -0.70248333 | 4.18556290 | 0.00000000 |
| C | -1.12364968 | 2.79708330 | 0.00000000 |
| N | -2.02188784 | 0.00000000 | 0.00000000 |
| C | -2.79708330 | 1.12364968 | 0.00000000 |
| C | -4.18556290 | 0.70248333 | 0.00000000 |
| C | -4.18556290 | -0.70248333 | 0.00000000 |
| C | -2.79708330 | -1.12364968 | 0.00000000 |
| N | 0.00000000 | -2.02188784 | 0.00000000 |
| C | -1.12364968 | -2.79708330 | 0.00000000 |
| C | -0.70248333 | -4.18556290 | 0.00000000 |
| C | 0.70248333 | -4.18556290 | 0.00000000 |
| C | 1.12364968 | -2.79708330 | 0.00000000 |
| N | 2.02188784 | 0.00000000 | 0.00000000 |
| C | 2.79708330 | -1.12364968 | 0.00000000 |
| C | 4.18556290 | -0.70248333 | 0.00000000 |
| C | 4.18556290 | 0.70248333 | 0.00000000 |
| C | 2.79708330 | 1.12364968 | 0.00000000 |
| C | -5.37475753 | -1.41284716 | 0.00000000 |
| C | -6.56093426 | -0.69815730 | 0.00000000 |
| C | -6.56093426 | 0.69815730 | 0.00000000 |
| C | -5.37475753 | 1.41284716 | 0.00000000 |
| C | -1.41284716 | 5.37475753 | 0.00000000 |
| C | -0.69815730 | 6.56093426 | 0.00000000 |
| C | 0.69815730 | 6.56093426 | 0.00000000 |
| C | 1.41284716 | 5.37475753 | 0.00000000 |
| C | 5.37475753 | 1.41284716 | 0.00000000 |
| C | 6.56093426 | 0.69815730 | 0.00000000 |
| C | 6.56093426 | -0.69815730 | 0.00000000 |
| C | 5.37475753 | -1.41284716 | 0.00000000 |
| C | 1.41284716 | -5.37475753 | 0.00000000 |
| C | 0.69815730 | -6.56093426 | 0.00000000 |
| C | -0.69815730 | -6.56093426 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -1.41284716 | -5.37475753 | 0.00000000 |
| H | -5.36786870 | -2.49280056 | 0.00000000 |
| H | -7.50360956 | -1.22624233 | 0.00000000 |
| H | -7.50360956 | 1.22624233 | 0.00000000 |
| H | -5.36786870 | 2.49280056 | 0.00000000 |
| H | -2.49280056 | 5.36786870 | 0.00000000 |
| H | -1.22624233 | 7.50360956 | 0.00000000 |
| H | 1.22624233 | 7.50360956 | 0.00000000 |
| H | 2.49280056 | 5.36786870 | 0.00000000 |
| H | 5.36786870 | 2.49280056 | 0.00000000 |
| H | 7.50360956 | 1.22624233 | 0.00000000 |
| H | 7.50360956 | -1.22624233 | 0.00000000 |
| H | 5.36786870 | -2.49280056 | 0.00000000 |
| H | 2.49280056 | -5.36786870 | 0.00000000 |
| H | 1.22624233 | -7.50360956 | 0.00000000 |
| H | -1.22624233 | -7.50360956 | 0.00000000 |
| H | -2.49280056 | -5.36786870 | 0.00000000 |

level of theory m06l
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38069806 | 2.38069806 | 0.00000000 |
| N | -2.38069806 | 2.38069806 | 0.00000000 |
| N | -2.38069806 | -2.38069806 | 0.00000000 |
| N | 2.38069806 | -2.38069806 | 0.00000000 |
| N | 0.00000000 | 1.94489572 | 0.00000000 |
| C | 1.12036772 | 2.75652398 | 0.00000000 |
| C | 0.69885899 | 4.13029245 | 0.00000000 |
| C | -0.69885899 | 4.13029245 | 0.00000000 |
| C | -1.12036772 | 2.75652398 | 0.00000000 |
| N | -1.94489572 | 0.00000000 | 0.00000000 |
| C | -2.75652398 | 1.12036772 | 0.00000000 |
| C | -4.13029245 | 0.69885899 | 0.00000000 |
| C | -4.13029245 | -0.69885899 | 0.00000000 |
| C | -2.75652398 | -1.12036772 | 0.00000000 |
| N | 0.00000000 | -1.94489572 | 0.00000000 |
| C | -1.12036772 | -2.75652398 | 0.00000000 |
| C | -0.69885899 | -4.13029245 | 0.00000000 |
| C | 0.69885899 | -4.13029245 | 0.00000000 |
| C | 1.12036772 | -2.75652398 | 0.00000000 |
| N | 1.94489572 | 0.00000000 | 0.00000000 |
| C | 2.75652398 | -1.12036772 | 0.00000000 |
| C | 4.13029245 | -0.69885899 | 0.00000000 |
| C | 4.13029245 | 0.69885899 | 0.00000000 |
| C | 2.75652398 | 1.12036772 | 0.00000000 |
| C | -5.31942993 | -1.41465113 | 0.00000000 |
| C | -6.50254538 | -0.69984379 | 0.00000000 |
| C | -6.50254538 | 0.69984379 | 0.00000000 |
| C | -5.31942993 | 1.41465113 | 0.00000000 |
| C | -1.41465113 | 5.31942993 | 0.00000000 |
| C | -0.69984379 | 6.50254538 | 0.00000000 |
| C | 0.69984379 | 6.50254538 | 0.00000000 |
| C | 1.41465113 | 5.31942993 | 0.00000000 |
| C | 5.31942993 | 1.41465113 | 0.00000000 |
| C | 6.50254538 | 0.69984379 | 0.00000000 |
| C | 6.50254538 | -0.69984379 | 0.00000000 |
| C | 5.31942993 | -1.41465113 | 0.00000000 |
| C | 1.41465113 | -5.31942993 | 0.00000000 |
| C | 0.69984379 | -6.50254538 | 0.00000000 |
| C | -0.69984379 | -6.50254538 | 0.00000000 |
| C | -1.41465113 | -5.31942993 | 0.00000000 |
| H | -5.31041487 | -2.49448863 | 0.00000000 |
| H | -7.44587526 | -1.22678844 | 0.00000000 |
| H | -7.44587526 | 1.22678844 | 0.00000000 |
| H | -5.31041487 | 2.49448863 | 0.00000000 |
| H | -2.49448863 | 5.31041487 | 0.00000000 |
| H | -1.22678844 | 7.44587526 | 0.00000000 |
| H | 1.22678844 | 7.44587526 | 0.00000000 |
| H | 2.49448863 | 5.31041487 | 0.00000000 |
| H | 5.31041487 | 2.49448863 | 0.00000000 |
| H | 7.44587526 | 1.22678844 | 0.00000000 |
| H | 7.44587526 | -1.22678844 | 0.00000000 |
| H | 5.31041487 | -2.49448863 | 0.00000000 |
| H | 2.49448863 | -5.31041487 | 0.00000000 |
| H | 1.22678844 | -7.44587526 | 0.00000000 |
| H | -1.22678844 | -7.44587526 | 0.00000000 |
| H | -2.49448863 | -5.31041487 | 0.00000000 |

level of theory m06l
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37822363 | 2.37822363 | 0.00000000 |

| | | | |
|---|---|---|---|
| N | -2.37822363 | 2.37822363 | 0.00000000 |
| N | -2.37822363 | -2.37822363 | 0.00000000 |
| N | 2.37822363 | -2.37822363 | 0.00000000 |
| N | 0.00000000 | 1.95639792 | 0.00000000 |
| C | 1.11385302 | 2.75792524 | 0.00000000 |
| C | 0.69922042 | 4.14048176 | 0.00000000 |
| C | -0.69922042 | 4.14048176 | 0.00000000 |
| C | -1.11385302 | 2.75792524 | 0.00000000 |
| N | -1.95639792 | 0.00000000 | 0.00000000 |
| C | -2.75792524 | 1.11385302 | 0.00000000 |
| C | -4.14048176 | 0.69922042 | 0.00000000 |
| C | -4.14048176 | -0.69922042 | 0.00000000 |
| C | -2.75792524 | -1.11385302 | 0.00000000 |
| N | 0.00000000 | -1.95639792 | 0.00000000 |
| C | -1.11385302 | -2.75792524 | 0.00000000 |
| C | -0.69922042 | -4.14048176 | 0.00000000 |
| C | 0.69922042 | -4.14048176 | 0.00000000 |
| C | 1.11385302 | -2.75792524 | 0.00000000 |
| N | 1.95639792 | 0.00000000 | 0.00000000 |
| C | 2.75792524 | -1.11385302 | 0.00000000 |
| C | 4.14048176 | -0.69922042 | 0.00000000 |
| C | 4.14048176 | 0.69922042 | 0.00000000 |
| C | 2.75792524 | 1.11385302 | 0.00000000 |
| C | -5.32803171 | -1.41423413 | 0.00000000 |
| C | -6.51248227 | -0.69904738 | 0.00000000 |
| C | -6.51248227 | 0.69904738 | 0.00000000 |
| C | -5.32803171 | 1.41423413 | 0.00000000 |
| C | -1.41423413 | 5.32803171 | 0.00000000 |
| C | -0.69904738 | 6.51248227 | 0.00000000 |
| C | 0.69904738 | 6.51248227 | 0.00000000 |
| C | 1.41423413 | 5.32803171 | 0.00000000 |
| C | 5.32803171 | 1.41423413 | 0.00000000 |
| C | 6.51248227 | 0.69904738 | 0.00000000 |
| C | 6.51248227 | -0.69904738 | 0.00000000 |
| C | 5.32803171 | -1.41423413 | 0.00000000 |
| C | 1.41423413 | -5.32803171 | 0.00000000 |
| C | 0.69904738 | -6.51248227 | 0.00000000 |
| C | -0.69904738 | -6.51248227 | 0.00000000 |
| C | -1.41423413 | -5.32803171 | 0.00000000 |
| H | -5.31908226 | -2.49418012 | 0.00000000 |
| H | -7.45589311 | -1.22597192 | 0.00000000 |
| H | -7.45589311 | 1.22597192 | 0.00000000 |
| H | -5.31908226 | 2.49418012 | 0.00000000 |
| H | -2.49418012 | 5.31908226 | 0.00000000 |
| H | -1.22597192 | 7.45589311 | 0.00000000 |
| H | 1.22597192 | 7.45589311 | 0.00000000 |
| H | 2.49418012 | 5.31908226 | 0.00000000 |
| H | 5.31908226 | 2.49418012 | 0.00000000 |
| H | 7.45589311 | 1.22597192 | 0.00000000 |
| H | 7.45589311 | -1.22597192 | 0.00000000 |
| H | 5.31908226 | -2.49418012 | 0.00000000 |
| H | 2.49418012 | -5.31908226 | 0.00000000 |
| H | 1.22597192 | -7.45589311 | 0.00000000 |
| H | -1.22597192 | -7.45589311 | 0.00000000 |
| H | -2.49418012 | -5.31908226 | 0.00000000 |

level of theory m06l
spin state IS3

| Occup. | alpha | // | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37738012 | 2.37738012 | 0.00000000 |
| N | -2.37738012 | 2.37738012 | 0.00000000 |
| N | -2.37738012 | -2.37738012 | 0.00000000 |
| N | 2.37738012 | -2.37738012 | 0.00000000 |
| N | 0.00000000 | 1.95346522 | 0.00000000 |
| C | 1.11414883 | 2.75453533 | 0.00000000 |
| C | 0.69827319 | 4.13628327 | 0.00000000 |
| C | -0.69827319 | 4.13628327 | 0.00000000 |
| C | -1.11414883 | 2.75453533 | 0.00000000 |
| N | -1.95346522 | 0.00000000 | 0.00000000 |
| C | -2.75453533 | 1.11414883 | 0.00000000 |
| C | -4.13628327 | 0.69827319 | 0.00000000 |
| C | -4.13628327 | -0.69827319 | 0.00000000 |
| C | -2.75453533 | -1.11414883 | 0.00000000 |
| N | 0.00000000 | -1.95346522 | 0.00000000 |
| C | -1.11414883 | -2.75453533 | 0.00000000 |
| C | -0.69827319 | -4.13628327 | 0.00000000 |
| C | 0.69827319 | -4.13628327 | 0.00000000 |
| C | 1.11414883 | -2.75453533 | 0.00000000 |
| N | 1.95346522 | 0.00000000 | 0.00000000 |
| C | 2.75453533 | -1.11414883 | 0.00000000 |
| C | 4.13628327 | -0.69827319 | 0.00000000 |
| C | 4.13628327 | 0.69827319 | 0.00000000 |
| C | 2.75453533 | 1.11414883 | 0.00000000 |
| C | -5.32291668 | -1.41441458 | 0.00000000 |
| C | -6.50724976 | -0.69891350 | 0.00000000 |
| C | -6.50724976 | 0.69891350 | 0.00000000 |
| C | -5.32291668 | 1.41441458 | 0.00000000 |
| C | -1.41441458 | 5.32291668 | 0.00000000 |
| C | -0.69891350 | 6.50724976 | 0.00000000 |
| C | 0.69891350 | 6.50724976 | 0.00000000 |
| C | 1.41441458 | 5.32291668 | 0.00000000 |
| C | 5.32291668 | 1.41441458 | 0.00000000 |
| C | 6.50724976 | 0.69891350 | 0.00000000 |
| C | 6.50724976 | -0.69891350 | 0.00000000 |
| C | 5.32291668 | -1.41441458 | 0.00000000 |
| C | 1.41441458 | -5.32291668 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 0.69891350 | -6.50724976 | 0.00000000 |
| C | -0.69891350 | -6.50724976 | 0.00000000 |
| C | -1.41441458 | -5.32291668 | 0.00000000 |
| H | -5.31477529 | -2.49417271 | 0.00000000 |
| H | -7.45047328 | -1.22598197 | 0.00000000 |
| H | -7.45047328 | 1.22598197 | 0.00000000 |
| H | -5.31477529 | 2.49417271 | 0.00000000 |
| H | -2.49417271 | 5.31477529 | 0.00000000 |
| H | -1.22598197 | 7.45047328 | 0.00000000 |
| H | 1.22598197 | 7.45047328 | 0.00000000 |
| H | 2.49417271 | 5.31477529 | 0.00000000 |
| H | 5.31477529 | 2.49417271 | 0.00000000 |
| H | 7.45047328 | 1.22598197 | 0.00000000 |
| H | 7.45047328 | -1.22598197 | 0.00000000 |
| H | 5.31477529 | -2.49417271 | 0.00000000 |
| H | 2.49417271 | -5.31477529 | 0.00000000 |
| H | 1.22598197 | -7.45047328 | 0.00000000 |
| H | -1.22598197 | -7.45047328 | 0.00000000 |
| H | -2.49417271 | -5.31477529 | 0.00000000 |

level of theory m06l
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 12.0 |
| $A_{1u}$ | 1.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38466636 | 2.38466636 | 0.00000000 |
| N | -2.38466636 | 2.38466636 | 0.00000000 |
| N | -2.38466636 | -2.38466636 | 0.00000000 |
| N | 2.38466636 | -2.38466636 | 0.00000000 |
| N | 0.00000000 | 1.93704697 | 0.00000000 |
| C | 1.12047567 | 2.75333939 | 0.00000000 |
| C | 0.69745350 | 4.13282774 | 0.00000000 |
| C | -0.69745350 | 4.13282774 | 0.00000000 |
| C | -1.12047567 | 2.75333939 | 0.00000000 |
| N | -1.93704697 | 0.00000000 | 0.00000000 |
| C | -2.75333939 | 1.12047567 | 0.00000000 |
| C | -4.13282774 | 0.69745350 | 0.00000000 |
| C | -4.13282774 | -0.69745350 | 0.00000000 |
| C | -2.75333939 | -1.12047567 | 0.00000000 |
| N | 0.00000000 | -1.93704697 | 0.00000000 |
| C | -1.12047567 | -2.75333939 | 0.00000000 |
| C | -0.69745350 | -4.13282774 | 0.00000000 |
| C | 0.69745350 | -4.13282774 | 0.00000000 |
| C | 1.12047567 | -2.75333939 | 0.00000000 |
| N | 1.93704697 | 0.00000000 | 0.00000000 |
| C | 2.75333939 | -1.12047567 | 0.00000000 |
| C | 4.13282774 | -0.69745350 | 0.00000000 |
| C | 4.13282774 | 0.69745350 | 0.00000000 |
| C | 2.75333939 | 1.12047567 | 0.00000000 |
| C | -5.31741906 | -1.41265454 | 0.00000000 |
| C | -6.50648140 | -0.69714552 | 0.00000000 |
| C | -6.50648140 | 0.69714552 | 0.00000000 |
| C | -5.31741906 | 1.41265454 | 0.00000000 |
| C | -1.41265454 | 5.31741906 | 0.00000000 |
| C | -0.69714552 | 6.50648140 | 0.00000000 |
| C | 0.69714552 | 6.50648140 | 0.00000000 |
| C | 1.41265454 | 5.31741906 | 0.00000000 |
| C | 5.31741906 | 1.41265454 | 0.00000000 |
| C | 6.50648140 | 0.69714552 | 0.00000000 |
| C | 6.50648140 | -0.69714552 | 0.00000000 |
| C | 5.31741906 | -1.41265454 | 0.00000000 |
| C | 1.41265454 | -5.31741906 | 0.00000000 |
| C | 0.69714552 | -6.50648140 | 0.00000000 |
| C | -0.69714552 | -6.50648140 | 0.00000000 |
| C | -1.41265454 | -5.31741906 | 0.00000000 |
| H | -5.30891412 | -2.49246241 | 0.00000000 |
| H | -7.44833170 | -1.22643125 | 0.00000000 |
| H | -7.44833170 | 1.22643125 | 0.00000000 |
| H | -5.30891412 | 2.49246241 | 0.00000000 |
| H | -2.49246241 | 5.30891412 | 0.00000000 |
| H | -1.22643125 | 7.44833170 | 0.00000000 |
| H | 1.22643125 | 7.44833170 | 0.00000000 |
| H | 2.49246241 | 5.30891412 | 0.00000000 |
| H | 5.30891412 | 2.49246241 | 0.00000000 |
| H | 7.44833170 | 1.22643125 | 0.00000000 |
| H | 7.44833170 | -1.22643125 | 0.00000000 |
| H | 5.30891412 | -2.49246241 | 0.00000000 |
| H | 2.49246241 | -5.30891412 | 0.00000000 |
| H | 1.22643125 | -7.44833170 | 0.00000000 |
| H | -1.22643125 | -7.44833170 | 0.00000000 |
| H | -2.49246241 | -5.30891412 | 0.00000000 |

level of theory pbe0
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37466809 | 2.37466809 | 0.00000000 |
| N | -2.37466809 | 2.37466809 | 0.00000000 |
| N | -2.37466809 | -2.37466809 | 0.00000000 |
| N | 2.37466809 | -2.37466809 | 0.00000000 |
| N | 0.00000000 | 2.02204765 | 0.00000000 |
| C | 1.11811078 | 2.78764965 | 0.00000000 |
| C | 0.70146942 | 4.18087704 | 0.00000000 |
| C | -0.70146942 | 4.18087704 | 0.00000000 |
| C | -1.11811078 | 2.78764965 | 0.00000000 |
| N | -2.02204765 | 0.00000000 | 0.00000000 |
| C | -2.78764965 | 1.11811078 | 0.00000000 |
| C | -4.18087704 | 0.70146942 | 0.00000000 |
| C | -4.18087704 | -0.70146942 | 0.00000000 |
| C | -2.78764965 | -1.11811078 | 0.00000000 |
| N | 0.00000000 | -2.02204765 | 0.00000000 |
| C | -1.11811078 | -2.78764965 | 0.00000000 |
| C | -0.70146942 | -4.18087704 | 0.00000000 |
| C | 0.70146942 | -4.18087704 | 0.00000000 |
| C | 1.11811078 | -2.78764965 | 0.00000000 |
| N | 2.02204765 | 0.00000000 | 0.00000000 |
| C | 2.78764965 | -1.11811078 | 0.00000000 |
| C | 4.18087704 | -0.70146942 | 0.00000000 |
| C | 4.18087704 | 0.70146942 | 0.00000000 |
| C | 2.78764965 | 1.11811078 | 0.00000000 |
| C | -5.36777557 | -1.41318848 | 0.00000000 |
| C | -6.55161016 | -0.69790118 | 0.00000000 |
| C | -6.55161016 | 0.69790118 | 0.00000000 |
| C | -5.36777557 | 1.41318848 | 0.00000000 |
| C | -1.41318848 | 5.36777557 | 0.00000000 |
| C | -0.69790118 | 6.55161016 | 0.00000000 |
| C | 0.69790118 | 6.55161016 | 0.00000000 |
| C | 1.41318848 | 5.36777557 | 0.00000000 |
| C | 5.36777557 | 1.41318848 | 0.00000000 |
| C | 6.55161016 | 0.69790118 | 0.00000000 |
| C | 6.55161016 | -0.69790118 | 0.00000000 |
| C | 5.36777557 | -1.41318848 | 0.00000000 |
| C | 1.41318848 | -5.36777557 | 0.00000000 |
| C | 0.69790118 | -6.55161016 | 0.00000000 |
| C | -0.69790118 | -6.55161016 | 0.00000000 |
| C | -1.41318848 | -5.36777557 | 0.00000000 |
| H | -5.36143549 | -2.49372609 | 0.00000000 |
| H | -7.49493369 | -1.22666726 | 0.00000000 |
| H | -7.49493369 | 1.22666726 | 0.00000000 |
| H | -5.36143549 | 2.49372609 | 0.00000000 |
| H | -2.49372609 | 5.36143549 | 0.00000000 |
| H | -1.22666726 | 7.49493369 | 0.00000000 |
| H | 1.22666726 | 7.49493369 | 0.00000000 |
| H | 2.49372609 | 5.36143549 | 0.00000000 |
| H | 5.36143549 | 2.49372609 | 0.00000000 |
| H | 7.49493369 | 1.22666726 | 0.00000000 |
| H | 7.49493369 | -1.22666726 | 0.00000000 |
| H | 5.36143549 | -2.49372609 | 0.00000000 |
| H | 2.49372609 | -5.36143549 | 0.00000000 |
| H | 1.22666726 | -7.49493369 | 0.00000000 |
| H | -1.22666726 | -7.49493369 | 0.00000000 |
| H | -2.49372609 | -5.36143549 | 0.00000000 |

level of theory pbe0
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.36732416 | 2.36732416 | 0.00000000 |
| N | -2.36732416 | 2.36732416 | 0.00000000 |
| N | -2.36732416 | -2.36732416 | 0.00000000 |
| N | 2.36732416 | -2.36732416 | 0.00000000 |
| N | 0.00000000 | 1.93577377 | 0.00000000 |
| C | 1.11445628 | 2.74320511 | 0.00000000 |
| C | 0.69782339 | 4.11892149 | 0.00000000 |
| C | -0.69782339 | 4.11892149 | 0.00000000 |
| C | -1.11445628 | 2.74320511 | 0.00000000 |
| N | -1.93577377 | 0.00000000 | 0.00000000 |
| C | -2.74320511 | 1.11445628 | 0.00000000 |
| C | -4.11892149 | 0.69782339 | 0.00000000 |
| C | -4.11892149 | -0.69782339 | 0.00000000 |
| C | -2.74320511 | -1.11445628 | 0.00000000 |
| N | 0.00000000 | -1.93577377 | 0.00000000 |
| C | -1.11445628 | -2.74320511 | 0.00000000 |
| C | -0.69782339 | -4.11892149 | 0.00000000 |
| C | 0.69782339 | -4.11892149 | 0.00000000 |
| C | 1.11445628 | -2.74320511 | 0.00000000 |
| N | 1.93577377 | 0.00000000 | 0.00000000 |
| C | 2.74320511 | -1.11445628 | 0.00000000 |
| C | 4.11892149 | -0.69782339 | 0.00000000 |
| C | 4.11892149 | 0.69782339 | 0.00000000 |
| C | 2.74320511 | 1.11445628 | 0.00000000 |
| C | -5.30693077 | -1.41520041 | 0.00000000 |
| C | -6.48707752 | -0.70016341 | 0.00000000 |
| C | -6.48707752 | 0.70016341 | 0.00000000 |
| C | -5.30693077 | 1.41520041 | 0.00000000 |
| C | -1.41520041 | 5.30693077 | 0.00000000 |
| C | -0.70016341 | 6.48707752 | 0.00000000 |
| C | 0.70016341 | 6.48707752 | 0.00000000 |
| C | 1.41520041 | 5.30693077 | 0.00000000 |
| C | 5.30693077 | 1.41520041 | 0.00000000 |
| C | 6.48707752 | 0.70016341 | 0.00000000 |
| C | 6.48707752 | -0.70016341 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 5.30693077 | -1.41520041 | 0.00000000 |
| C | 1.41520041 | -5.30693077 | 0.00000000 |
| C | 0.70016341 | -6.48707752 | 0.00000000 |
| C | -0.70016341 | -6.48707752 | 0.00000000 |
| C | -1.41520041 | -5.30693077 | 0.00000000 |
| H | -5.29872164 | -2.49539776 | 0.00000000 |
| H | -7.43102760 | -1.22760972 | 0.00000000 |
| H | -7.43102760 | 1.22760972 | 0.00000000 |
| H | -5.29872164 | 2.49539776 | 0.00000000 |
| H | -2.49539776 | 5.29872164 | 0.00000000 |
| H | -1.22760972 | 7.43102760 | 0.00000000 |
| H | 1.22760972 | 7.43102760 | 0.00000000 |
| H | 2.49539776 | 5.29872164 | 0.00000000 |
| H | 5.29872164 | 2.49539776 | 0.00000000 |
| H | 7.43102760 | 1.22760972 | 0.00000000 |
| H | 7.43102760 | -1.22760972 | 0.00000000 |
| H | 5.29872164 | -2.49539776 | 0.00000000 |
| H | 2.49539776 | -5.29872164 | 0.00000000 |
| H | 1.22760972 | -7.43102760 | 0.00000000 |
| H | -1.22760972 | -7.43102760 | 0.00000000 |
| H | -2.49539776 | -5.29872164 | 0.00000000 |

level of theory pbe0
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.36397077 | 2.36397077 | 0.00000000 |
| N | -2.36397077 | 2.36397077 | 0.00000000 |
| N | -2.36397077 | -2.36397077 | 0.00000000 |
| N | 2.36397077 | -2.36397077 | 0.00000000 |
| N | 0.00000000 | 1.95414892 | 0.00000000 |
| C | 1.10717004 | 2.74718188 | 0.00000000 |
| C | 0.69796098 | 4.13461689 | 0.00000000 |
| C | -0.69796098 | 4.13461689 | 0.00000000 |
| C | -1.10717004 | 2.74718188 | 0.00000000 |
| N | -1.95414892 | 0.00000000 | 0.00000000 |
| C | -2.74718188 | 1.10717004 | 0.00000000 |
| C | -4.13461689 | 0.69796098 | 0.00000000 |
| C | -4.13461689 | -0.69796098 | 0.00000000 |
| C | -2.74718188 | -1.10717004 | 0.00000000 |
| N | 0.00000000 | -1.95414892 | 0.00000000 |
| C | -1.10717004 | -2.74718188 | 0.00000000 |
| C | -0.69796098 | -4.13461689 | 0.00000000 |
| C | 0.69796098 | -4.13461689 | 0.00000000 |
| C | 1.10717004 | -2.74718188 | 0.00000000 |
| N | 1.95414892 | 0.00000000 | 0.00000000 |
| C | 2.74718188 | -1.10717004 | 0.00000000 |
| C | 4.13461689 | -0.69796098 | 0.00000000 |
| C | 4.13461689 | 0.69796098 | 0.00000000 |
| C | 2.74718188 | 1.10717004 | 0.00000000 |
| C | -5.32013797 | -1.41457863 | 0.00000000 |
| C | -6.50204530 | -0.69894154 | 0.00000000 |
| C | -6.50204530 | 0.69894154 | 0.00000000 |
| C | -5.32013797 | 1.41457863 | 0.00000000 |
| C | -1.41457863 | 5.32013797 | 0.00000000 |
| C | -0.69894154 | 6.50204530 | 0.00000000 |
| C | 0.69894154 | 6.50204530 | 0.00000000 |
| C | 1.41457863 | 5.32013797 | 0.00000000 |
| C | 5.32013797 | 1.41457863 | 0.00000000 |
| C | 6.50204530 | 0.69894154 | 0.00000000 |
| C | 6.50204530 | -0.69894154 | 0.00000000 |
| C | 5.32013797 | -1.41457863 | 0.00000000 |
| C | 1.41457863 | -5.32013797 | 0.00000000 |
| C | 0.69894154 | -6.50204530 | 0.00000000 |
| C | -0.69894154 | -6.50204530 | 0.00000000 |
| C | -1.41457863 | -5.32013797 | 0.00000000 |
| H | -5.31162192 | -2.49479026 | 0.00000000 |
| H | -7.44599432 | -1.22623333 | 0.00000000 |
| H | -7.44599432 | 1.22623333 | 0.00000000 |
| H | -5.31162192 | 2.49479026 | 0.00000000 |
| H | -2.49479026 | 5.31162192 | 0.00000000 |
| H | -1.22623333 | 7.44599432 | 0.00000000 |
| H | 1.22623333 | 7.44599432 | 0.00000000 |
| H | 2.49479026 | 5.31162192 | 0.00000000 |
| H | 5.31162192 | 2.49479026 | 0.00000000 |
| H | 7.44599432 | 1.22623333 | 0.00000000 |
| H | 7.44599432 | -1.22623333 | 0.00000000 |
| H | 5.31162192 | -2.49479026 | 0.00000000 |
| H | 2.49479026 | -5.31162192 | 0.00000000 |
| H | 1.22623333 | -7.44599432 | 0.00000000 |
| H | -1.22623333 | -7.44599432 | 0.00000000 |
| H | -2.49479026 | -5.31162192 | 0.00000000 |

level of theory pbe0
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.36321510 | 2.36321510 | 0.00000000 |
| N | -2.36321510 | 2.36321510 | 0.00000000 |
| N | -2.36321510 | -2.36321510 | 0.00000000 |
| N | 2.36321510 | -2.36321510 | 0.00000000 |
| N | 0.00000000 | 1.95165861 | 0.00000000 |
| C | 1.10757804 | 2.74428146 | 0.00000000 |
| C | 0.69738470 | 4.13101902 | 0.00000000 |
| C | -0.69738470 | 4.13101902 | 0.00000000 |
| C | -1.10757804 | 2.74428146 | 0.00000000 |
| N | -1.95165861 | 0.00000000 | 0.00000000 |
| C | -2.74428146 | 1.10757804 | 0.00000000 |
| C | -4.13101902 | 0.69738470 | 0.00000000 |
| C | -4.13101902 | -0.69738470 | 0.00000000 |
| C | -2.74428146 | -1.10757804 | 0.00000000 |
| N | 0.00000000 | -1.95165861 | 0.00000000 |
| C | -1.10757804 | -2.74428146 | 0.00000000 |
| C | -0.69738470 | -4.13101902 | 0.00000000 |
| C | 0.69738470 | -4.13101902 | 0.00000000 |
| C | 1.10757804 | -2.74428146 | 0.00000000 |
| N | 1.95165861 | 0.00000000 | 0.00000000 |
| C | 2.74428146 | -1.10757804 | 0.00000000 |
| C | 4.13101902 | -0.69738470 | 0.00000000 |
| C | 4.13101902 | 0.69738470 | 0.00000000 |
| C | 2.74428146 | 1.10757804 | 0.00000000 |
| C | -5.31581195 | -1.41484322 | 0.00000000 |
| C | -6.49775738 | -0.69889180 | 0.00000000 |
| C | -6.49775738 | 0.69889180 | 0.00000000 |
| C | -5.31581195 | 1.41484322 | 0.00000000 |
| C | -1.41484322 | 5.31581195 | 0.00000000 |
| C | -0.69889180 | 6.49775738 | 0.00000000 |
| C | 0.69889180 | 6.49775738 | 0.00000000 |
| C | 1.41484322 | 5.31581195 | 0.00000000 |
| C | 5.31581195 | 1.41484322 | 0.00000000 |
| C | 6.49775738 | 0.69889180 | 0.00000000 |
| C | 6.49775738 | -0.69889180 | 0.00000000 |
| C | 5.31581195 | -1.41484322 | 0.00000000 |
| C | 1.41484322 | -5.31581195 | 0.00000000 |
| C | 0.69889180 | -6.49775738 | 0.00000000 |
| C | -0.69889180 | -6.49775738 | 0.00000000 |
| C | -1.41484322 | -5.31581195 | 0.00000000 |
| H | -5.30750228 | -2.49506702 | 0.00000000 |
| H | -7.44158998 | -1.22649210 | 0.00000000 |
| H | -7.44158998 | 1.22649210 | 0.00000000 |
| H | -5.30750228 | 2.49506702 | 0.00000000 |
| H | -2.49506702 | 5.30750228 | 0.00000000 |
| H | -1.22649210 | 7.44158998 | 0.00000000 |
| H | 1.22649210 | 7.44158998 | 0.00000000 |
| H | 2.49506702 | 5.30750228 | 0.00000000 |
| H | 5.30750228 | 2.49506702 | 0.00000000 |
| H | 7.44158998 | 1.22649210 | 0.00000000 |
| H | 7.44158998 | -1.22649210 | 0.00000000 |
| H | 5.30750228 | -2.49506702 | 0.00000000 |
| H | 2.49506702 | -5.30750228 | 0.00000000 |
| H | 1.22649210 | -7.44158998 | 0.00000000 |
| H | -1.22649210 | -7.44158998 | 0.00000000 |
| H | -2.49506702 | -5.30750228 | 0.00000000 |

level of theory pbe0
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 20.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37045266 | 2.37045266 | 0.00000000 |
| N | -2.37045266 | 2.37045266 | 0.00000000 |
| N | -2.37045266 | -2.37045266 | 0.00000000 |
| N | 2.37045266 | -2.37045266 | 0.00000000 |
| N | 0.00000000 | 1.94749240 | 0.00000000 |
| C | 1.10976936 | 2.74366761 | 0.00000000 |
| C | 0.69715716 | 4.13279917 | 0.00000000 |
| C | -0.69715716 | 4.13279917 | 0.00000000 |
| C | -1.10976936 | 2.74366761 | 0.00000000 |
| N | -1.94749240 | 0.00000000 | 0.00000000 |
| C | -2.74366761 | 1.10976936 | 0.00000000 |
| C | -4.13279917 | 0.69715716 | 0.00000000 |
| C | -4.13279917 | -0.69715716 | 0.00000000 |
| C | -2.74366761 | -1.10976936 | 0.00000000 |
| N | 0.00000000 | -1.94749240 | 0.00000000 |
| C | -1.10976936 | -2.74366761 | 0.00000000 |
| C | -0.69715716 | -4.13279917 | 0.00000000 |
| C | 0.69715716 | -4.13279917 | 0.00000000 |
| C | 1.10976936 | -2.74366761 | 0.00000000 |
| N | 1.94749240 | 0.00000000 | 0.00000000 |
| C | 2.74366761 | -1.10976936 | 0.00000000 |
| C | 4.13279917 | -0.69715716 | 0.00000000 |
| C | 4.13279917 | 0.69715716 | 0.00000000 |
| C | 2.74366761 | 1.10976936 | 0.00000000 |
| C | -5.31417944 | -1.41360335 | 0.00000000 |
| C | -6.50102346 | -0.69700952 | 0.00000000 |
| C | -6.50102346 | 0.69700952 | 0.00000000 |
| C | -5.31417944 | 1.41360335 | 0.00000000 |
| C | -1.41360335 | 5.31417944 | 0.00000000 |
| C | -0.69700952 | 6.50102346 | 0.00000000 |
| C | 0.69700952 | 6.50102346 | 0.00000000 |
| C | 1.41360335 | 5.31417944 | 0.00000000 |
| C | 5.31417944 | 1.41360335 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 6.50102346 | 0.69700952 | 0.00000000 |
| C | 6.50102346 | -0.69700952 | 0.00000000 |
| C | 5.31417944 | -1.41360335 | 0.00000000 |
| C | 1.41360335 | -5.31417944 | 0.00000000 |
| C | 0.69700952 | -6.50102346 | 0.00000000 |
| C | -0.69700952 | -6.50102346 | 0.00000000 |
| C | -1.41360335 | -5.31417944 | 0.00000000 |
| H | -5.30485586 | -2.49379911 | 0.00000000 |
| H | -7.44394323 | -1.22589254 | 0.00000000 |
| H | -7.44394323 | 1.22589254 | 0.00000000 |
| H | -5.30485586 | 2.49379911 | 0.00000000 |
| H | -2.49379911 | 5.30485586 | 0.00000000 |
| H | -1.22589254 | 7.44394323 | 0.00000000 |
| H | 1.22589254 | 7.44394323 | 0.00000000 |
| H | 2.49379911 | 5.30485586 | 0.00000000 |
| H | 5.30485586 | 2.49379911 | 0.00000000 |
| H | 7.44394323 | 1.22589254 | 0.00000000 |
| H | 7.44394323 | -1.22589254 | 0.00000000 |
| H | 5.30485586 | -2.49379911 | 0.00000000 |
| H | 2.49379911 | -5.30485586 | 0.00000000 |
| H | 1.22589254 | -7.44394323 | 0.00000000 |
| H | -1.22589254 | -7.44394323 | 0.00000000 |
| H | -2.49379911 | -5.30485586 | 0.00000000 |

level of theory tpssh
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.39003275 | 2.39003275 | 0.00000000 |
| N | -2.39003275 | 2.39003275 | 0.00000000 |
| N | -2.39003275 | -2.39003275 | 0.00000000 |
| N | 2.39003275 | -2.39003275 | 0.00000000 |
| N | 0.00000000 | 2.02573390 | 0.00000000 |
| C | 1.12458473 | 2.80138127 | 0.00000000 |
| C | 0.70452860 | 4.19634224 | 0.00000000 |
| C | -0.70452860 | 4.19634224 | 0.00000000 |
| C | -1.12458473 | 2.80138127 | 0.00000000 |
| N | -2.02573390 | 0.00000000 | 0.00000000 |
| C | -2.80138127 | 1.12458473 | 0.00000000 |
| C | -4.19634224 | 0.70452860 | 0.00000000 |
| C | -4.19634224 | -0.70452860 | 0.00000000 |
| C | -2.80138127 | -1.12458473 | 0.00000000 |
| N | 0.00000000 | -2.02573390 | 0.00000000 |
| C | -1.12458473 | -2.80138127 | 0.00000000 |
| C | -0.70452860 | -4.19634224 | 0.00000000 |
| C | 0.70452860 | -4.19634224 | 0.00000000 |
| C | 1.12458473 | -2.80138127 | 0.00000000 |
| N | 2.02573390 | 0.00000000 | 0.00000000 |
| C | 2.80138127 | -1.12458473 | 0.00000000 |
| C | 4.19634224 | -0.70452860 | 0.00000000 |
| C | 4.19634224 | 0.70452860 | 0.00000000 |
| C | 2.80138127 | 1.12458473 | 0.00000000 |
| C | -5.38855530 | -1.41880358 | 0.00000000 |
| C | -6.57754567 | -0.70089685 | 0.00000000 |
| C | -6.57754567 | 0.70089685 | 0.00000000 |
| C | -5.38855530 | 1.41880358 | 0.00000000 |
| C | -1.41880358 | 5.38855530 | 0.00000000 |
| C | -0.70089685 | 6.57754567 | 0.00000000 |
| C | 0.70089685 | 6.57754567 | 0.00000000 |
| C | 1.41880358 | 5.38855530 | 0.00000000 |
| C | 5.38855530 | 1.41880358 | 0.00000000 |
| C | 6.57754567 | 0.70089685 | 0.00000000 |
| C | 6.57754567 | -0.70089685 | 0.00000000 |
| C | 5.38855530 | -1.41880358 | 0.00000000 |
| C | 1.41880358 | -5.38855530 | 0.00000000 |
| C | 0.70089685 | -6.57754567 | 0.00000000 |
| C | -0.70089685 | -6.57754567 | 0.00000000 |
| C | -1.41880358 | -5.38855530 | 0.00000000 |
| H | -5.38277774 | -2.50042653 | 0.00000000 |
| H | -7.52233555 | -1.23027572 | 0.00000000 |
| H | -7.52233555 | 1.23027572 | 0.00000000 |
| H | -5.38277774 | 2.50042653 | 0.00000000 |
| H | -2.50042653 | 5.38277774 | 0.00000000 |
| H | -1.23027572 | 7.52233555 | 0.00000000 |
| H | 1.23027572 | 7.52233555 | 0.00000000 |
| H | 2.50042653 | 5.38277774 | 0.00000000 |
| H | 5.38277774 | 2.50042653 | 0.00000000 |
| H | 7.52233555 | 1.23027572 | 0.00000000 |
| H | 7.52233555 | -1.23027572 | 0.00000000 |
| H | 5.38277774 | -2.50042653 | 0.00000000 |
| H | 2.50042653 | -5.38277774 | 0.00000000 |
| H | 1.23027572 | -7.52233555 | 0.00000000 |
| H | -1.23027572 | -7.52233555 | 0.00000000 |
| H | -2.50042653 | -5.38277774 | 0.00000000 |

level of theory tpssh
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |

| | | | |
|---|---|---|---|
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38054301 | 2.38054301 | 0.00000000 |
| N | -2.38054301 | 2.38054301 | 0.00000000 |
| N | -2.38054301 | -2.38054301 | 0.00000000 |
| N | 2.38054301 | -2.38054301 | 0.00000000 |
| N | 0.00000000 | 1.94231916 | 0.00000000 |
| C | 1.11970466 | 2.75744421 | 0.00000000 |
| C | 0.70057035 | 4.13731675 | 0.00000000 |
| C | -0.70057035 | 4.13731675 | 0.00000000 |
| C | -1.11970466 | 2.75744421 | 0.00000000 |
| N | -1.94231916 | 0.00000000 | 0.00000000 |
| C | -2.75744421 | 1.11970466 | 0.00000000 |
| C | -4.13731675 | 0.70057035 | 0.00000000 |
| C | -4.13731675 | -0.70057035 | 0.00000000 |
| C | -2.75744421 | -1.11970466 | 0.00000000 |
| N | 0.00000000 | -1.94231916 | 0.00000000 |
| C | -1.11970466 | -2.75744421 | 0.00000000 |
| C | -0.70057035 | -4.13731675 | 0.00000000 |
| C | 0.70057035 | -4.13731675 | 0.00000000 |
| C | 1.11970466 | -2.75744421 | 0.00000000 |
| N | 1.94231916 | 0.00000000 | 0.00000000 |
| C | 2.75744421 | -1.11970466 | 0.00000000 |
| C | 4.13731675 | -0.70057035 | 0.00000000 |
| C | 4.13731675 | 0.70057035 | 0.00000000 |
| C | 2.75744421 | 1.11970466 | 0.00000000 |
| C | -5.32958802 | -1.42065517 | 0.00000000 |
| C | -6.51541602 | -0.70275585 | 0.00000000 |
| C | -6.51541602 | 0.70275585 | 0.00000000 |
| C | -5.32958802 | 1.42065517 | 0.00000000 |
| C | -1.42065517 | 5.32958802 | 0.00000000 |
| C | -0.70275585 | 6.51541602 | 0.00000000 |
| C | 0.70275585 | 6.51541602 | 0.00000000 |
| C | 1.42065517 | 5.32958802 | 0.00000000 |
| C | 5.32958802 | 1.42065517 | 0.00000000 |
| C | 6.51541602 | 0.70275585 | 0.00000000 |
| C | 6.51541602 | -0.70275585 | 0.00000000 |
| C | 5.32958802 | -1.42065517 | 0.00000000 |
| C | 1.42065517 | -5.32958802 | 0.00000000 |
| C | 0.70275585 | -6.51541602 | 0.00000000 |
| C | -0.70275585 | -6.51541602 | 0.00000000 |
| C | -1.42065517 | -5.32958802 | 0.00000000 |
| H | -5.32152442 | -2.50211990 | 0.00000000 |
| H | -7.46101502 | -1.23076362 | 0.00000000 |
| H | -7.46101502 | 1.23076362 | 0.00000000 |
| H | -5.32152442 | 2.50211990 | 0.00000000 |
| H | -2.50211990 | 5.32152442 | 0.00000000 |
| H | -1.23076362 | 7.46101502 | 0.00000000 |
| H | 1.23076362 | 7.46101502 | 0.00000000 |
| H | 2.50211990 | 5.32152442 | 0.00000000 |
| H | 5.32152442 | 2.50211990 | 0.00000000 |
| H | 7.46101502 | 1.23076362 | 0.00000000 |
| H | 7.46101502 | -1.23076362 | 0.00000000 |
| H | 5.32152442 | -2.50211990 | 0.00000000 |
| H | 2.50211990 | -5.32152442 | 0.00000000 |
| H | 1.23076362 | -7.46101502 | 0.00000000 |
| H | -1.23076362 | -7.46101502 | 0.00000000 |
| H | -2.50211990 | -5.32152442 | 0.00000000 |

level of theory tpssh
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37843530 | 2.37843530 | 0.00000000 |
| N | -2.37843530 | 2.37843530 | 0.00000000 |
| N | -2.37843530 | -2.37843530 | 0.00000000 |
| N | 2.37843530 | -2.37843530 | 0.00000000 |
| N | 0.00000000 | 1.95659583 | 0.00000000 |
| C | 1.11357732 | 2.76004036 | 0.00000000 |
| C | 0.70097517 | 4.14911635 | 0.00000000 |
| C | -0.70097517 | 4.14911635 | 0.00000000 |
| C | -1.11357732 | 2.76004036 | 0.00000000 |
| N | -1.95659583 | 0.00000000 | 0.00000000 |
| C | -2.76004036 | 1.11357732 | 0.00000000 |
| C | -4.14911635 | 0.70097517 | 0.00000000 |
| C | -4.14911635 | -0.70097517 | 0.00000000 |
| C | -2.76004036 | -1.11357732 | 0.00000000 |
| N | 0.00000000 | -1.95659583 | 0.00000000 |
| C | -1.11357732 | -2.76004036 | 0.00000000 |
| C | -0.70097517 | -4.14911635 | 0.00000000 |
| C | 0.70097517 | -4.14911635 | 0.00000000 |
| C | 1.11357732 | -2.76004036 | 0.00000000 |
| N | 1.95659583 | 0.00000000 | 0.00000000 |
| C | 2.76004036 | -1.11357732 | 0.00000000 |
| C | 4.14911635 | -0.70097517 | 0.00000000 |
| C | 4.14911635 | 0.70097517 | 0.00000000 |
| C | 2.76004036 | 1.11357732 | 0.00000000 |
| C | -5.33975457 | -1.42026040 | 0.00000000 |
| C | -6.52690129 | -0.70190652 | 0.00000000 |
| C | -6.52690129 | 0.70190652 | 0.00000000 |
| C | -5.33975457 | 1.42026040 | 0.00000000 |
| C | -1.42026040 | 5.33975457 | 0.00000000 |
| C | -0.70190652 | 6.52690129 | 0.00000000 |
| C | 0.70190652 | 6.52690129 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 1.42026040 | 5.33975457 | 0.00000000 |
| C | 5.33975457 | 1.42026040 | 0.00000000 |
| C | 6.52690129 | 0.70190652 | 0.00000000 |
| C | 6.52690129 | -0.70190652 | 0.00000000 |
| C | 5.33975457 | -1.42026040 | 0.00000000 |
| C | 1.42026040 | -5.33975457 | 0.00000000 |
| C | 0.70190652 | -6.52690129 | 0.00000000 |
| C | -0.70190652 | -6.52690129 | 0.00000000 |
| C | -1.42026040 | -5.33975457 | 0.00000000 |
| H | -5.33184496 | -2.50182038 | 0.00000000 |
| H | -7.47257119 | -1.22985661 | 0.00000000 |
| H | -7.47257119 | 1.22985661 | 0.00000000 |
| H | -5.33184496 | 2.50182038 | 0.00000000 |
| H | -2.50182038 | 5.33184496 | 0.00000000 |
| H | -1.22985661 | 7.47257119 | 0.00000000 |
| H | 1.22985661 | 7.47257119 | 0.00000000 |
| H | 2.50182038 | 5.33184496 | 0.00000000 |
| H | 5.33184496 | 2.50182038 | 0.00000000 |
| H | 7.47257119 | 1.22985661 | 0.00000000 |
| H | 7.47257119 | -1.22985661 | 0.00000000 |
| H | 5.33184496 | -2.50182038 | 0.00000000 |
| H | 2.50182038 | -5.33184496 | 0.00000000 |
| H | 1.22985661 | -7.47257119 | 0.00000000 |
| H | -1.22985661 | -7.47257119 | 0.00000000 |
| H | -2.50182038 | -5.33184496 | 0.00000000 |

level of theory tpssh
spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37768228 | 2.37768228 | 0.00000000 |
| N | -2.37768228 | 2.37768228 | 0.00000000 |
| N | -2.37768228 | -2.37768228 | 0.00000000 |
| N | 2.37768228 | -2.37768228 | 0.00000000 |
| N | 0.00000000 | 1.95333081 | 0.00000000 |
| C | 1.11412184 | 2.75695526 | 0.00000000 |
| C | 0.70029730 | 4.14489404 | 0.00000000 |
| C | -0.70029730 | 4.14489404 | 0.00000000 |
| C | -1.11412184 | 2.75695526 | 0.00000000 |
| N | -1.95333081 | 0.00000000 | 0.00000000 |
| C | -2.75695526 | 1.11412184 | 0.00000000 |
| C | -4.14489404 | 0.70029730 | 0.00000000 |
| C | -4.14489404 | -0.70029730 | 0.00000000 |
| C | -2.75695526 | -1.11412184 | 0.00000000 |
| N | 0.00000000 | -1.95333081 | 0.00000000 |
| C | -1.11412184 | -2.75695526 | 0.00000000 |
| C | -0.70029730 | -4.14489404 | 0.00000000 |
| C | 0.70029730 | -4.14489404 | 0.00000000 |
| C | 1.11412184 | -2.75695526 | 0.00000000 |
| N | 1.95333081 | 0.00000000 | 0.00000000 |
| C | 2.75695526 | -1.11412184 | 0.00000000 |
| C | 4.14489404 | -0.70029730 | 0.00000000 |
| C | 4.14489404 | 0.70029730 | 0.00000000 |
| C | 2.75695526 | 1.11412184 | 0.00000000 |
| C | -5.33475967 | -1.42048001 | 0.00000000 |
| C | -6.52190427 | -0.70184143 | 0.00000000 |
| C | -6.52190427 | 0.70184143 | 0.00000000 |
| C | -5.33475967 | 1.42048001 | 0.00000000 |
| C | -1.42048001 | 5.33475967 | 0.00000000 |
| C | -0.70184143 | 6.52190427 | 0.00000000 |
| C | 0.70184143 | 6.52190427 | 0.00000000 |
| C | 1.42048001 | 5.33475967 | 0.00000000 |
| C | 5.33475967 | 1.42048001 | 0.00000000 |
| C | 6.52190427 | 0.70184143 | 0.00000000 |
| C | 6.52190427 | -0.70184143 | 0.00000000 |
| C | 5.33475967 | -1.42048001 | 0.00000000 |
| C | 1.42048001 | -5.33475967 | 0.00000000 |
| C | 0.70184143 | -6.52190427 | 0.00000000 |
| C | -0.70184143 | -6.52190427 | 0.00000000 |
| C | -1.42048001 | -5.33475967 | 0.00000000 |
| H | -5.32728345 | -2.50184525 | 0.00000000 |
| H | -7.46721962 | -1.23012914 | 0.00000000 |
| H | -7.46721962 | 1.23012914 | 0.00000000 |
| H | -5.32728345 | 2.50184525 | 0.00000000 |
| H | -2.50184525 | 5.32728345 | 0.00000000 |
| H | -1.23012914 | 7.46721962 | 0.00000000 |
| H | 1.23012914 | 7.46721962 | 0.00000000 |
| H | 2.50184525 | 5.32728345 | 0.00000000 |
| H | 5.32728345 | 2.50184525 | 0.00000000 |
| H | 7.46721962 | 1.23012914 | 0.00000000 |
| H | 7.46721962 | -1.23012914 | 0.00000000 |
| H | 5.32728345 | -2.50184525 | 0.00000000 |
| H | 2.50184525 | -5.32728345 | 0.00000000 |
| H | 1.23012914 | -7.46721962 | 0.00000000 |
| H | -1.23012914 | -7.46721962 | 0.00000000 |
| H | -2.50184525 | -5.32728345 | 0.00000000 |

level of theory tpssh
spin state LS

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38474097 | 2.38474097 | 0.00000000 |
| N | -2.38474097 | 2.38474097 | 0.00000000 |
| N | -2.38474097 | -2.38474097 | 0.00000000 |
| N | 2.38474097 | -2.38474097 | 0.00000000 |
| N | 0.00000000 | 1.96299147 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 1.11545537 | 2.77683962 | 0.00000000 |
| C | 0.69907384 | 4.16643314 | 0.00000000 |
| C | -0.69907384 | 4.16643314 | 0.00000000 |
| C | -1.11545537 | 2.77683962 | 0.00000000 |
| N | -1.96299147 | 0.00000000 | 0.00000000 |
| C | -2.77683962 | 1.11545537 | 0.00000000 |
| C | -4.16643314 | 0.69907384 | 0.00000000 |
| C | -4.16643314 | -0.69907384 | 0.00000000 |
| C | -2.77683962 | -1.11545537 | 0.00000000 |
| N | 0.00000000 | -1.96299147 | 0.00000000 |
| C | -1.11545537 | -2.77683962 | 0.00000000 |
| C | -0.69907384 | -4.16643314 | 0.00000000 |
| C | 0.69907384 | -4.16643314 | 0.00000000 |
| C | 1.11545537 | -2.77683962 | 0.00000000 |
| N | 1.96299147 | 0.00000000 | 0.00000000 |
| C | 2.77683962 | -1.11545537 | 0.00000000 |
| C | 4.16643314 | -0.69907384 | 0.00000000 |
| C | 4.16643314 | 0.69907384 | 0.00000000 |
| C | 2.77683962 | 1.11545537 | 0.00000000 |
| C | -5.35335443 | -1.41213436 | 0.00000000 |
| C | -6.52977842 | -0.69729263 | 0.00000000 |
| C | -6.52977842 | 0.69729263 | 0.00000000 |
| C | -5.35335443 | 1.41213436 | 0.00000000 |
| C | -1.41213436 | 5.35335443 | 0.00000000 |
| C | -0.69729263 | 6.52977842 | 0.00000000 |
| C | 0.69729263 | 6.52977842 | 0.00000000 |
| C | 1.41213436 | 5.35335443 | 0.00000000 |
| C | 5.35335443 | 1.41213436 | 0.00000000 |
| C | 6.52977842 | 0.69729263 | 0.00000000 |
| C | 6.52977842 | -0.69729263 | 0.00000000 |
| C | 5.35335443 | -1.41213436 | 0.00000000 |
| C | 1.41213436 | -5.35335443 | 0.00000000 |
| C | 0.69729263 | -6.52977842 | 0.00000000 |
| C | -0.69729263 | -6.52977842 | 0.00000000 |
| C | -1.41213436 | -5.35335443 | 0.00000000 |
| H | -5.34962161 | -2.44952232 | 0.00000000 |
| H | -7.44123543 | -1.20541285 | 0.00000000 |
| H | -7.44123543 | 1.20541285 | 0.00000000 |
| H | -5.34962161 | 2.44952232 | 0.00000000 |
| H | -2.44952232 | 5.34962161 | 0.00000000 |
| H | -1.20541285 | 7.44123543 | 0.00000000 |
| H | 1.20541285 | 7.44123543 | 0.00000000 |
| H | 2.44952232 | 5.34962161 | 0.00000000 |
| H | 5.34962161 | 2.44952232 | 0.00000000 |
| H | 7.44123543 | 1.20541285 | 0.00000000 |
| H | 7.44123543 | -1.20541285 | 0.00000000 |
| H | 5.34962161 | -2.44952232 | 0.00000000 |
| H | 2.44952232 | -5.34962161 | 0.00000000 |
| H | 1.20541285 | -7.44123543 | 0.00000000 |
| H | -1.20541285 | -7.44123543 | 0.00000000 |
| H | -2.44952232 | -5.34962161 | 0.00000000 |

level of theory b3lyp*
spin state HS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 16.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38643328 | 2.38643328 | 0.00000000 |
| N | -2.38643328 | 2.38643328 | 0.00000000 |
| N | -2.38643328 | -2.38643328 | 0.00000000 |
| N | 2.38643328 | -2.38643328 | 0.00000000 |
| N | 0.00000000 | 2.03183161 | 0.00000000 |
| C | 1.12523139 | 2.80363451 | 0.00000000 |
| C | 0.70503026 | 4.20146203 | 0.00000000 |
| C | -0.70503026 | 4.20146203 | 0.00000000 |
| C | -1.12523139 | 2.80363451 | 0.00000000 |
| N | -2.03183161 | 0.00000000 | 0.00000000 |
| C | -2.80363451 | 1.12523139 | 0.00000000 |
| C | -4.20146203 | 0.70503026 | 0.00000000 |
| C | -4.20146203 | -0.70503026 | 0.00000000 |
| C | -2.80363451 | -1.12523139 | 0.00000000 |
| N | 0.00000000 | -2.03183161 | 0.00000000 |
| C | -1.12523139 | -2.80363451 | 0.00000000 |
| C | -0.70503026 | -4.20146203 | 0.00000000 |
| C | 0.70503026 | -4.20146203 | 0.00000000 |
| C | 1.12523139 | -2.80363451 | 0.00000000 |
| N | 2.03183161 | 0.00000000 | 0.00000000 |
| C | 2.80363451 | -1.12523139 | 0.00000000 |
| C | 4.20146203 | -0.70503026 | 0.00000000 |
| C | 4.20146203 | 0.70503026 | 0.00000000 |
| C | 2.80363451 | 1.12523139 | 0.00000000 |
| C | -5.39358460 | -1.41703666 | 0.00000000 |
| C | -6.58290888 | -0.70022744 | 0.00000000 |
| C | -6.58290888 | 0.70022744 | 0.00000000 |
| C | -5.39358460 | 1.41703666 | 0.00000000 |
| C | -1.41703666 | 5.39358460 | 0.00000000 |
| C | -0.70022744 | 6.58290888 | 0.00000000 |
| C | 0.70022744 | 6.58290888 | 0.00000000 |
| C | 1.41703666 | 5.39358460 | 0.00000000 |
| C | 5.39358460 | 1.41703666 | 0.00000000 |
| C | 6.58290888 | 0.70022744 | 0.00000000 |
| C | 6.58290888 | -0.70022744 | 0.00000000 |
| C | 5.39358460 | -1.41703666 | 0.00000000 |
| C | 1.41703666 | -5.39358460 | 0.00000000 |
| C | 0.70022744 | -6.58290888 | 0.00000000 |
| C | -0.70022744 | -6.58290888 | 0.00000000 |
| C | -1.41703666 | -5.39358460 | 0.00000000 |
| H | -5.38851984 | -2.49811138 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -7.52624300 | -1.22998414 | 0.00000000 |
| H | -7.52624300 | 1.22998414 | 0.00000000 |
| H | -5.38851984 | 2.49811138 | 0.00000000 |
| H | -2.49811138 | 5.38851984 | 0.00000000 |
| H | -1.22998414 | 7.52624300 | 0.00000000 |
| H | 1.22998414 | 7.52624300 | 0.00000000 |
| H | 2.49811138 | 5.38851984 | 0.00000000 |
| H | 5.38851984 | 2.49811138 | 0.00000000 |
| H | 7.52624300 | 1.22998414 | 0.00000000 |
| H | 7.52624300 | -1.22998414 | 0.00000000 |
| H | 5.38851984 | -2.49811138 | 0.00000000 |
| H | 2.49811138 | -5.38851984 | 0.00000000 |
| H | 1.22998414 | -7.52624300 | 0.00000000 |
| H | -1.22998414 | -7.52624300 | 0.00000000 |
| H | -2.49811138 | -5.38851984 | 0.00000000 |

level of theory b3lyp*
spin state IS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 11.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37773467 | 2.37773467 | 0.00000000 |
| N | -2.37773467 | 2.37773467 | 0.00000000 |
| N | -2.37773467 | -2.37773467 | 0.00000000 |
| N | 2.37773467 | -2.37773467 | 0.00000000 |
| N | 0.00000000 | 1.94906511 | 0.00000000 |
| C | 1.12071856 | 2.76053355 | 0.00000000 |
| C | 0.70122124 | 4.14288211 | 0.00000000 |
| C | -0.70122124 | 4.14288211 | 0.00000000 |
| C | -1.12071856 | 2.76053355 | 0.00000000 |
| N | -1.94906511 | 0.00000000 | 0.00000000 |
| C | -2.76053355 | 1.12071856 | 0.00000000 |
| C | -4.14288211 | 0.70122124 | 0.00000000 |
| C | -4.14288211 | -0.70122124 | 0.00000000 |
| C | -2.76053355 | -1.12071856 | 0.00000000 |
| N | 0.00000000 | -1.94906511 | 0.00000000 |
| C | -1.12071856 | -2.76053355 | 0.00000000 |
| C | -0.70122124 | -4.14288211 | 0.00000000 |
| C | 0.70122124 | -4.14288211 | 0.00000000 |
| C | 1.12071856 | -2.76053355 | 0.00000000 |
| N | 1.94906511 | 0.00000000 | 0.00000000 |
| C | 2.76053355 | -1.12071856 | 0.00000000 |
| C | 4.14288211 | -0.70122124 | 0.00000000 |
| C | 4.14288211 | 0.70122124 | 0.00000000 |
| C | 2.76053355 | 1.12071856 | 0.00000000 |
| C | -5.33552010 | -1.41849242 | 0.00000000 |
| C | -6.52188575 | -0.70203988 | 0.00000000 |
| C | -6.52188575 | 0.70203988 | 0.00000000 |
| C | -5.33552010 | 1.41849242 | 0.00000000 |
| C | -1.41849242 | 5.33552010 | 0.00000000 |
| C | -0.70203988 | 6.52188575 | 0.00000000 |
| C | 0.70203988 | 6.52188575 | 0.00000000 |
| C | 1.41849242 | 5.33552010 | 0.00000000 |
| C | 5.33552010 | 1.41849242 | 0.00000000 |
| C | 6.52188575 | 0.70203988 | 0.00000000 |
| C | 6.52188575 | -0.70203988 | 0.00000000 |
| C | 5.33552010 | -1.41849242 | 0.00000000 |
| C | 1.41849242 | -5.33552010 | 0.00000000 |
| C | 0.70203988 | -6.52188575 | 0.00000000 |
| C | -0.70203988 | -6.52188575 | 0.00000000 |
| C | -1.41849242 | -5.33552010 | 0.00000000 |
| H | -5.32874028 | -2.49935018 | 0.00000000 |
| H | -7.46585593 | -1.23072658 | 0.00000000 |
| H | -7.46585593 | 1.23072658 | 0.00000000 |
| H | -5.32874028 | 2.49935018 | 0.00000000 |
| H | -2.49935018 | 5.32874028 | 0.00000000 |
| H | -1.23072658 | 7.46585593 | 0.00000000 |
| H | 1.23072658 | 7.46585593 | 0.00000000 |
| H | 2.49935018 | 5.32874028 | 0.00000000 |
| H | 5.32874028 | 2.49935018 | 0.00000000 |
| H | 7.46585593 | 1.23072658 | 0.00000000 |
| H | 7.46585593 | -1.23072658 | 0.00000000 |
| H | 5.32874028 | -2.49935018 | 0.00000000 |
| H | 2.49935018 | -5.32874028 | 0.00000000 |
| H | 1.23072658 | -7.46585593 | 0.00000000 |
| H | -1.23072658 | -7.46585593 | 0.00000000 |
| H | -2.49935018 | -5.32874028 | 0.00000000 |

level of theory b3lyp*
spin state IS2

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 14.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37580952 | 2.37580952 | 0.00000000 |
| N | -2.37580952 | 2.37580952 | 0.00000000 |
| N | -2.37580952 | -2.37580952 | 0.00000000 |

| | | | |
|---|---|---|---|
| N | 2.37580952 | -2.37580952 | 0.00000000 |
| N | 0.00000000 | 1.96485523 | 0.00000000 |
| C | 1.11472404 | 2.76371444 | 0.00000000 |
| C | 0.70155356 | 4.15561888 | 0.00000000 |
| C | -0.70155356 | 4.15561888 | 0.00000000 |
| C | -1.11472404 | 2.76371444 | 0.00000000 |
| N | -1.96485523 | 0.00000000 | 0.00000000 |
| C | -2.76371444 | 1.11472404 | 0.00000000 |
| C | -4.15561888 | 0.70155356 | 0.00000000 |
| C | -4.15561888 | -0.70155356 | 0.00000000 |
| C | -2.76371444 | -1.11472404 | 0.00000000 |
| N | 0.00000000 | -1.96485523 | 0.00000000 |
| C | -1.11472404 | -2.76371444 | 0.00000000 |
| C | -0.70155356 | -4.15561888 | 0.00000000 |
| C | 0.70155356 | -4.15561888 | 0.00000000 |
| C | 1.11472404 | -2.76371444 | 0.00000000 |
| N | 1.96485523 | 0.00000000 | 0.00000000 |
| C | 2.76371444 | -1.11472404 | 0.00000000 |
| C | 4.15561888 | -0.70155356 | 0.00000000 |
| C | 4.15561888 | 0.70155356 | 0.00000000 |
| C | 2.76371444 | 1.11472404 | 0.00000000 |
| C | -5.34648200 | -1.41809448 | 0.00000000 |
| C | -6.53421134 | -0.70113392 | 0.00000000 |
| C | -6.53421134 | 0.70113392 | 0.00000000 |
| C | -5.34648200 | 1.41809448 | 0.00000000 |
| C | -1.41809448 | 5.34648200 | 0.00000000 |
| C | -0.70113392 | 6.53421134 | 0.00000000 |
| C | 0.70113392 | 6.53421134 | 0.00000000 |
| C | 1.41809448 | 5.34648200 | 0.00000000 |
| C | 5.34648200 | 1.41809448 | 0.00000000 |
| C | 6.53421134 | 0.70113392 | 0.00000000 |
| C | 6.53421134 | -0.70113392 | 0.00000000 |
| C | 5.34648200 | -1.41809448 | 0.00000000 |
| C | 1.41809448 | -5.34648200 | 0.00000000 |
| C | 0.70113392 | -6.53421134 | 0.00000000 |
| C | -0.70113392 | -6.53421134 | 0.00000000 |
| C | -1.41809448 | -5.34648200 | 0.00000000 |
| H | -5.33973552 | -2.49915015 | 0.00000000 |
| H | -7.47822334 | -1.22995239 | 0.00000000 |
| H | -7.47822334 | 1.22995239 | 0.00000000 |
| H | -5.33973552 | 2.49915015 | 0.00000000 |
| H | -2.49915015 | 5.33973552 | 0.00000000 |
| H | -1.22995239 | 7.47822334 | 0.00000000 |
| H | 1.22995239 | 7.47822334 | 0.00000000 |
| H | 2.49915015 | 5.33973552 | 0.00000000 |
| H | 5.33973552 | 2.49915015 | 0.00000000 |
| H | 7.47822334 | 1.22995239 | 0.00000000 |
| H | 7.47822334 | -1.22995239 | 0.00000000 |
| H | 5.33973552 | -2.49915015 | 0.00000000 |
| H | 2.49915015 | -5.33973552 | 0.00000000 |
| H | 1.22995239 | -7.47822334 | 0.00000000 |
| H | -1.22995239 | -7.47822334 | 0.00000000 |
| H | -2.49915015 | -5.33973552 | 0.00000000 |

level of theory b3lyp*

spin state IS3

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 21.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 10.0 |
| $A_{1u}$ | 2.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.37466015 | 2.37466015 | 0.00000000 |
| N | -2.37466015 | 2.37466015 | 0.00000000 |
| N | -2.37466015 | -2.37466015 | 0.00000000 |
| N | 2.37466015 | -2.37466015 | 0.00000000 |
| N | 0.00000000 | 1.96180241 | 0.00000000 |
| C | 1.11512939 | 2.76066743 | 0.00000000 |
| C | 0.70085240 | 4.15151246 | 0.00000000 |
| C | -0.70085240 | 4.15151246 | 0.00000000 |
| C | -1.11512939 | 2.76066743 | 0.00000000 |
| N | -1.96180241 | 0.00000000 | 0.00000000 |
| C | -2.76066743 | 1.11512939 | 0.00000000 |
| C | -4.15151246 | 0.70085240 | 0.00000000 |
| C | -4.15151246 | -0.70085240 | 0.00000000 |
| C | -2.76066743 | -1.11512939 | 0.00000000 |
| N | 0.00000000 | -1.96180241 | 0.00000000 |
| C | -1.11512939 | -2.76066743 | 0.00000000 |
| C | -0.70085240 | -4.15151246 | 0.00000000 |
| C | 0.70085240 | -4.15151246 | 0.00000000 |
| C | 1.11512939 | -2.76066743 | 0.00000000 |
| N | 1.96180241 | 0.00000000 | 0.00000000 |
| C | 2.76066743 | -1.11512939 | 0.00000000 |
| C | 4.15151246 | -0.70085240 | 0.00000000 |
| C | 4.15151246 | 0.70085240 | 0.00000000 |
| C | 2.76066743 | 1.11512939 | 0.00000000 |
| C | -5.34165114 | -1.41830774 | 0.00000000 |
| C | -6.52925877 | -0.70112070 | 0.00000000 |
| C | -6.52925877 | 0.70112070 | 0.00000000 |
| C | -5.34165114 | 1.41830774 | 0.00000000 |
| C | -1.41830774 | 5.34165114 | 0.00000000 |
| C | -0.70112070 | 6.52925877 | 0.00000000 |
| C | 0.70112070 | 6.52925877 | 0.00000000 |
| C | 1.41830774 | 5.34165114 | 0.00000000 |
| C | 5.34165114 | 1.41830774 | 0.00000000 |
| C | 6.52925877 | 0.70112070 | 0.00000000 |
| C | 6.52925877 | -0.70112070 | 0.00000000 |
| C | 5.34165114 | -1.41830774 | 0.00000000 |
| C | 1.41830774 | -5.34165114 | 0.00000000 |
| C | 0.70112070 | -6.52925877 | 0.00000000 |
| C | -0.70112070 | -6.52925877 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -1.41830774 | -5.34165114 | 0.00000000 |
| H | -5.33481629 | -2.49916074 | 0.00000000 |
| H | -7.47306809 | -1.22993175 | 0.00000000 |
| H | -7.47306809 | 1.22993175 | 0.00000000 |
| H | -5.33481629 | 2.49916074 | 0.00000000 |
| H | -2.49916074 | 5.33481629 | 0.00000000 |
| H | -1.22993175 | 7.47306809 | 0.00000000 |
| H | 1.22993175 | 7.47306809 | 0.00000000 |
| H | 2.49916074 | 5.33481629 | 0.00000000 |
| H | 5.33481629 | 2.49916074 | 0.00000000 |
| H | 7.47306809 | 1.22993175 | 0.00000000 |
| H | 7.47306809 | -1.22993175 | 0.00000000 |
| H | 5.33481629 | -2.49916074 | 0.00000000 |
| H | 2.49916074 | -5.33481629 | 0.00000000 |
| H | 1.22993175 | -7.47306809 | 0.00000000 |
| H | -1.22993175 | -7.47306809 | 0.00000000 |
| H | -2.49916074 | -5.33481629 | 0.00000000 |

level of theory b3lyp*
spin state LS

| Occup. | alpha | | betta |
|---|---|---|---|
| $A_{1g}$ | 21.0 | // | 20.0 |
| $A_{2g}$ | 11.0 | // | 11.0 |
| $B_{1g}$ | 15.0 | // | 15.0 |
| $B_{2g}$ | 14.0 | // | 13.0 |
| $E_{1g}$ | 12.0 | // | 12.0 |
| $A_{1u}$ | 1.0 | // | 2.0 |
| $A_{2u}$ | 6.0 | // | 6.0 |
| $B_{1u}$ | 2.0 | // | 2.0 |
| $B_{2u}$ | 3.0 | // | 3.0 |
| $E_{1u}$ | 60.0 | // | 60.0 |

| | | | |
|---|---|---|---|
| Mn | 0.00000000 | 0.00000000 | 0.00000000 |
| N | 2.38111558 | 2.38111558 | 0.00000000 |
| N | -2.38111558 | 2.38111558 | 0.00000000 |
| N | -2.38111558 | -2.38111558 | 0.00000000 |
| N | 2.38111558 | -2.38111558 | 0.00000000 |
| N | 0.00000000 | 1.94270652 | 0.00000000 |
| C | 1.12064818 | 2.75748020 | 0.00000000 |
| C | 0.69977129 | 4.14703404 | 0.00000000 |
| C | -0.69977129 | 4.14703404 | 0.00000000 |
| C | -1.12064818 | 2.75748020 | 0.00000000 |
| N | -1.94270652 | 0.00000000 | 0.00000000 |
| C | -2.75748020 | 1.12064818 | 0.00000000 |
| C | -4.14703404 | 0.69977129 | 0.00000000 |
| C | -4.14703404 | -0.69977129 | 0.00000000 |
| C | -2.75748020 | -1.12064818 | 0.00000000 |
| N | 0.00000000 | -1.94270652 | 0.00000000 |
| C | -1.12064818 | -2.75748020 | 0.00000000 |
| C | -0.69977129 | -4.14703404 | 0.00000000 |
| C | 0.69977129 | -4.14703404 | 0.00000000 |
| C | 1.12064818 | -2.75748020 | 0.00000000 |
| N | 1.94270652 | 0.00000000 | 0.00000000 |
| C | 2.75748020 | -1.12064818 | 0.00000000 |
| C | 4.14703404 | -0.69977129 | 0.00000000 |
| C | 4.14703404 | 0.69977129 | 0.00000000 |
| C | 2.75748020 | 1.12064818 | 0.00000000 |
| C | -5.33448079 | -1.41635402 | 0.00000000 |
| C | -6.52735850 | -0.69902568 | 0.00000000 |
| C | -6.52735850 | 0.69902568 | 0.00000000 |
| C | -5.33448079 | 1.41635402 | 0.00000000 |
| C | -1.41635402 | 5.33448079 | 0.00000000 |
| C | -0.69902568 | 6.52735850 | 0.00000000 |
| C | 0.69902568 | 6.52735850 | 0.00000000 |
| C | 1.41635402 | 5.33448079 | 0.00000000 |
| C | 5.33448079 | 1.41635402 | 0.00000000 |
| C | 6.52735850 | 0.69902568 | 0.00000000 |
| C | 6.52735850 | -0.69902568 | 0.00000000 |
| C | 5.33448079 | -1.41635402 | 0.00000000 |
| C | 1.41635402 | -5.33448079 | 0.00000000 |
| C | 0.69902568 | -6.52735850 | 0.00000000 |
| C | -0.69902568 | -6.52735850 | 0.00000000 |
| C | -1.41635402 | -5.33448079 | 0.00000000 |
| H | -5.32736071 | -2.49736048 | 0.00000000 |
| H | -7.46990520 | -1.23024556 | 0.00000000 |
| H | -7.46990520 | 1.23024556 | 0.00000000 |
| H | -5.32736071 | 2.49736048 | 0.00000000 |
| H | -2.49736048 | 5.32736071 | 0.00000000 |
| H | -1.23024556 | 7.46990520 | 0.00000000 |
| H | 1.23024556 | 7.46990520 | 0.00000000 |
| H | 2.49736048 | 5.32736071 | 0.00000000 |
| H | 5.32736071 | 2.49736048 | 0.00000000 |
| H | 7.46990520 | 1.23024556 | 0.00000000 |
| H | 7.46990520 | -1.23024556 | 0.00000000 |
| H | 5.32736071 | -2.49736048 | 0.00000000 |
| H | 2.49736048 | -5.32736071 | 0.00000000 |
| H | 1.23024556 | -7.46990520 | 0.00000000 |
| H | -1.23024556 | -7.46990520 | 0.00000000 |
| H | -2.49736048 | -5.32736071 | 0.00000000 |

**Cartesian coordinates for $Pc^{3-}$ in HS and LS minimum structures obtained by LDA.**

**HS**

| | | | |
|---|---|---|---|
| N | 2.377060 | 2.377060 | 0.000000 |
| N | -2.377060 | 2.377060 | 0.000000 |
| N | -2.377060 | -2.377060 | 0.000000 |
| N | 2.377060 | -2.377060 | 0.000000 |
| N | 0.000000 | 1.975477 | 0.000000 |
| C | 1.096449 | 2.752524 | 0.000000 |
| C | 0.707272 | 4.153510 | 0.000000 |
| C | -0.707272 | 4.153510 | 0.000000 |
| C | -1.096449 | 2.752524 | 0.000000 |
| N | -1.975477 | 0.000000 | 0.000000 |
| C | -2.752524 | 1.096449 | 0.000000 |
| C | -4.153510 | 0.707272 | 0.000000 |
| C | -4.153510 | -0.707272 | 0.000000 |
| C | -2.752524 | -1.096449 | 0.000000 |
| N | 0.000000 | -1.975477 | 0.000000 |
| C | -1.096449 | -2.752524 | 0.000000 |
| C | -0.707272 | -4.153510 | 0.000000 |
| C | 0.707272 | -4.153510 | 0.000000 |
| C | 1.096449 | -2.752524 | 0.000000 |
| N | 1.975477 | 0.000000 | 0.000000 |
| C | 2.752524 | -1.096449 | 0.000000 |
| C | 4.153510 | -0.707272 | 0.000000 |
| C | 4.153510 | 0.707272 | 0.000000 |
| C | 2.752524 | 1.096449 | 0.000000 |
| C | -5.347039 | -1.407140 | 0.000000 |
| C | -6.543763 | -0.701259 | 0.000000 |
| C | -6.543763 | 0.701259 | 0.000000 |
| C | -5.347039 | 1.407140 | 0.000000 |
| C | -1.407140 | 5.347039 | 0.000000 |
| C | -0.701259 | 6.543763 | 0.000000 |
| C | 0.701259 | 6.543763 | 0.000000 |
| C | 1.407140 | 5.347039 | 0.000000 |
| C | 5.347039 | 1.407140 | 0.000000 |
| C | 6.543763 | 0.701259 | 0.000000 |
| C | 6.543763 | -0.701259 | 0.000000 |
| C | 5.347039 | -1.407140 | 0.000000 |
| C | 1.407140 | -5.347039 | 0.000000 |
| C | 0.701259 | -6.543763 | 0.000000 |
| C | -0.701259 | -6.543763 | 0.000000 |
| C | -1.407140 | -5.347039 | 0.000000 |
| H | -5.323716 | -2.502401 | 0.000000 |
| H | -7.499110 | -1.239699 | 0.000000 |
| H | -7.499110 | 1.239699 | 0.000000 |
| H | -5.323716 | 2.502401 | 0.000000 |
| H | -2.502401 | 5.323716 | 0.000000 |
| H | -1.239699 | 7.499110 | 0.000000 |
| H | 1.239699 | 7.499110 | 0.000000 |
| H | 2.502401 | 5.323716 | 0.000000 |
| H | 5.323716 | 2.502401 | 0.000000 |
| H | 7.499110 | 1.239699 | 0.000000 |
| H | 7.499110 | -1.239699 | 0.000000 |
| H | 5.323716 | -2.502401 | 0.000000 |
| H | 2.502401 | -5.323716 | 0.000000 |
| H | 1.239699 | -7.499110 | 0.000000 |
| H | -1.239699 | -7.499110 | 0.000000 |
| H | -2.502401 | -5.323716 | 0.000000 |

**LS min**

| | | | |
|---|---|---|---|
| N | 0.000000 | 3.374861 | 0.000000 |
| N | -3.348043 | 0.000000 | 0.000000 |
| N | 0.000000 | -3.374861 | 0.000000 |
| N | 3.348043 | 0.000000 | 0.000000 |
| N | -1.386818 | 1.404421 | 0.000000 |
| C | -1.169459 | 2.721864 | 0.000000 |
| C | -2.443845 | 3.433961 | 0.000000 |
| C | -3.439556 | 2.430502 | 0.000000 |
| C | -2.719108 | 1.172199 | 0.000000 |
| N | -1.386818 | -1.404421 | 0.000000 |
| C | -2.719108 | -1.172199 | 0.000000 |
| C | -3.439556 | -2.430502 | 0.000000 |
| C | -2.443845 | -3.433961 | 0.000000 |
| C | -1.169459 | -2.721864 | 0.000000 |
| N | 1.386818 | -1.404421 | 0.000000 |
| C | 1.169459 | -2.721864 | 0.000000 |
| C | 2.443845 | -3.433961 | 0.000000 |
| C | 3.439556 | -2.430502 | 0.000000 |
| C | 2.719108 | -1.172199 | 0.000000 |
| N | 1.386818 | 1.404421 | 0.000000 |
| C | 2.719108 | 1.172199 | 0.000000 |
| C | 3.439556 | 2.430502 | 0.000000 |
| C | 2.443845 | 3.433961 | 0.000000 |
| C | 1.169459 | 2.721864 | 0.000000 |
| C | -2.793803 | -4.770772 | 0.000000 |
| C | -4.140704 | -5.117994 | 0.000000 |
| C | -5.128537 | -4.123079 | 0.000000 |
| C | -4.780368 | -2.778801 | 0.000000 |
| C | -4.780368 | 2.778801 | 0.000000 |
| C | -5.128537 | 4.123079 | 0.000000 |
| C | -4.140704 | 5.117994 | 0.000000 |
| C | -2.793803 | 4.770772 | 0.000000 |
| C | 2.793803 | 4.770772 | 0.000000 |
| C | 4.140704 | 5.117994 | 0.000000 |
| C | 5.128537 | 4.123079 | 0.000000 |
| C | 4.780368 | 2.778801 | 0.000000 |
| C | 4.780368 | -2.778801 | 0.000000 |
| C | 5.128537 | -4.123079 | 0.000000 |
| C | 4.140704 | -5.117994 | 0.000000 |
| C | 2.793803 | -4.770772 | 0.000000 |

| | | | |
|---|---|---|---|
| H | -2.002491 | -5.528628 | 0.000000 |
| H | -4.437174 | -6.173500 | 0.000000 |
| H | -6.185788 | -4.414408 | 0.000000 |
| H | -5.538884 | -1.988307 | 0.000000 |
| H | -5.538884 | 1.988307 | 0.000000 |
| H | -6.185788 | 4.414408 | 0.000000 |
| H | -4.437174 | 6.173500 | 0.000000 |
| H | -2.002491 | 5.528628 | 0.000000 |
| H | 2.002491 | 5.528628 | 0.000000 |
| H | 4.437174 | 6.173500 | 0.000000 |
| H | 6.185788 | 4.414408 | 0.000000 |
| H | 5.538884 | 1.988307 | 0.000000 |
| H | 5.538884 | -1.988307 | 0.000000 |
| H | 6.185788 | -4.414408 | 0.000000 |
| H | 4.437174 | -6.173500 | 0.000000 |
| H | 2.002491 | -5.528628 | 0.000000 |

**LS TS**

| | | | |
|---|---|---|---|
| N | 2.372782 | 2.381236 | 0.000000 |
| N | -2.372782 | 2.381236 | 0.000000 |
| N | -2.372782 | -2.381236 | 0.000000 |
| N | 2.372782 | -2.381236 | 0.000000 |
| N | 0.000000 | 1.954888 | 0.000000 |
| C | 1.096880 | 2.733517 | 0.000000 |
| C | 0.702649 | 4.143245 | 0.000000 |
| C | -0.702649 | 4.143245 | 0.000000 |
| C | -1.096880 | 2.733517 | 0.000000 |
| N | -1.994017 | 0.000000 | 0.000000 |
| C | -2.770691 | 1.094965 | 0.000000 |
| C | -4.164122 | 0.711254 | 0.000000 |
| C | -4.164122 | -0.711254 | 0.000000 |
| C | -2.770691 | -1.094965 | 0.000000 |
| N | 0.000000 | -1.954888 | 0.000000 |
| C | -1.096880 | -2.733517 | 0.000000 |
| C | -0.702649 | -4.143245 | 0.000000 |
| C | 0.702649 | -4.143245 | 0.000000 |
| C | 1.096880 | -2.733517 | 0.000000 |
| N | 1.994017 | 0.000000 | 0.000000 |
| C | 2.770691 | -1.094965 | 0.000000 |
| C | 4.164122 | -0.711254 | 0.000000 |
| C | 4.164122 | 0.711254 | 0.000000 |
| C | 2.770691 | 1.094965 | 0.000000 |
| C | -5.361828 | -1.407932 | 0.000000 |
| C | -6.558096 | -0.703207 | 0.000000 |
| C | -6.558096 | 0.703207 | 0.000000 |
| C | -5.361828 | 1.407932 | 0.000000 |
| C | -1.406146 | 5.332906 | 0.000000 |
| C | -0.698661 | 6.530228 | 0.000000 |
| C | 0.698661 | 6.530228 | 0.000000 |
| C | 1.406146 | 5.332906 | 0.000000 |
| C | 5.361828 | 1.407932 | 0.000000 |
| C | 6.558096 | 0.703207 | 0.000000 |
| C | 6.558096 | -0.703207 | 0.000000 |
| C | 5.361828 | -1.407932 | 0.000000 |
| C | 1.406146 | -5.332906 | 0.000000 |
| C | 0.698661 | -6.530228 | 0.000000 |
| C | -0.698661 | -6.530228 | 0.000000 |
| C | -1.406146 | -5.332906 | 0.000000 |
| H | -5.342497 | -2.503615 | 0.000000 |
| H | -7.512995 | -1.242482 | 0.000000 |
| H | -7.512995 | 1.242482 | 0.000000 |
| H | -5.342497 | 2.503615 | 0.000000 |
| H | -2.501163 | 5.305584 | 0.000000 |
| H | -1.236523 | 7.485775 | 0.000000 |
| H | 1.236523 | 7.485775 | 0.000000 |
| H | 2.501163 | 5.305584 | 0.000000 |
| H | 5.342497 | 2.503615 | 0.000000 |
| H | 7.512995 | 1.242482 | 0.000000 |
| H | 7.512995 | -1.242482 | 0.000000 |
| H | 5.342497 | -2.503615 | 0.000000 |
| H | 2.501163 | -5.305584 | 0.000000 |
| H | 1.236523 | -7.485775 | 0.000000 |
| H | -1.236523 | -7.485775 | 0.000000 |
| H | -2.501163 | -5.305584 | 0.000000 |

**Cartesian coordinates for $MgPc^-$ in HS and LS minimum structures obtained by LDA.**

**HS**

| | | | |
|---|---|---|---|
| Mg | 0.000000 | 0.000000 | 0.000000 |
| N | 2.380425 | 2.380425 | 0.000000 |
| N | -2.380425 | 2.380425 | 0.000000 |
| N | -2.380425 | -2.380425 | 0.000000 |
| N | 2.380425 | -2.380425 | 0.000000 |
| N | 0.000000 | 1.989035 | 0.000000 |
| C | 1.117407 | 2.773655 | 0.000000 |
| C | 0.702697 | 4.152829 | 0.000000 |
| C | -0.702697 | 4.152829 | 0.000000 |
| C | -1.117407 | 2.773655 | 0.000000 |
| N | -1.989035 | 0.000000 | 0.000000 |
| C | -2.773655 | 1.117407 | 0.000000 |
| C | -4.152829 | 0.702697 | 0.000000 |
| C | -4.152829 | -0.702697 | 0.000000 |
| C | -2.773655 | -1.117407 | 0.000000 |
| N | 0.000000 | -1.989035 | 0.000000 |
| C | -1.117407 | -2.773655 | 0.000000 |
| C | -0.702697 | -4.152829 | 0.000000 |
| C | 0.702697 | -4.152829 | 0.000000 |
| C | 1.117407 | -2.773655 | 0.000000 |
| N | 1.989035 | 0.000000 | 0.000000 |
| C | 2.773655 | -1.117407 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 4.152829 | -0.702697 | 0.000000 |
| C | 4.152829 | 0.702697 | 0.000000 |
| C | 2.773655 | 1.117407 | 0.000000 |
| C | -5.342344 | -1.410983 | 0.000000 |
| C | -6.527566 | -0.699329 | 0.000000 |
| C | -6.527566 | 0.699329 | 0.000000 |
| C | -5.342344 | 1.410983 | 0.000000 |
| C | -1.410983 | 5.342344 | 0.000000 |
| C | -0.699329 | 6.527566 | 0.000000 |
| C | 0.699329 | 6.527566 | 0.000000 |
| C | 1.410983 | 5.342344 | 0.000000 |
| C | 5.342344 | 1.410983 | 0.000000 |
| C | 6.527566 | 0.699329 | 0.000000 |
| C | 6.527566 | -0.699329 | 0.000000 |
| C | 5.342344 | -1.410983 | 0.000000 |
| C | 1.410983 | -5.342344 | 0.000000 |
| C | 0.699329 | -6.527566 | 0.000000 |
| C | -0.699329 | -6.527566 | 0.000000 |
| C | -1.410983 | -5.342344 | 0.000000 |
| H | -5.325142 | -2.504148 | 0.000000 |
| H | -7.481291 | -1.233810 | 0.000000 |
| H | -7.481291 | 1.233810 | 0.000000 |
| H | -5.325142 | 2.504148 | 0.000000 |
| H | -2.504148 | 5.325142 | 0.000000 |
| H | -1.233810 | 7.481291 | 0.000000 |
| H | 1.233810 | 7.481291 | 0.000000 |
| H | 2.504148 | 5.325142 | 0.000000 |
| H | 5.325142 | 2.504148 | 0.000000 |
| H | 7.481291 | 1.233810 | 0.000000 |
| H | 7.481291 | -1.233810 | 0.000000 |
| H | 5.325142 | -2.504148 | 0.000000 |
| H | 2.504148 | -5.325142 | 0.000000 |
| H | 1.233810 | -7.481291 | 0.000000 |
| H | -1.233810 | -7.481291 | 0.000000 |
| H | -2.504148 | -5.325142 | 0.000000 |

**LS min**

| | | | |
|---|---|---|---|
| Mg | 0.000000 | 0.000000 | 0.000000 |
| N | 2.389324 | 2.371886 | 0.000000 |
| N | -2.389324 | 2.371886 | 0.000000 |
| N | -2.389324 | -2.371886 | 0.000000 |
| N | 2.389324 | -2.371886 | 0.000000 |
| N | 0.000000 | 1.993977 | 0.000000 |
| C | 1.114701 | 2.777098 | 0.000000 |
| C | 0.705834 | 4.147941 | 0.000000 |
| C | -0.705834 | 4.147941 | 0.000000 |
| C | -1.114701 | 2.777098 | 0.000000 |
| N | -1.982839 | 0.000000 | 0.000000 |
| C | -2.768767 | 1.119542 | 0.000000 |
| C | -4.157840 | 0.699252 | 0.000000 |
| C | -4.157840 | -0.699252 | 0.000000 |
| C | -2.768767 | -1.119542 | 0.000000 |
| N | 0.000000 | -1.993977 | 0.000000 |
| C | -1.114701 | -2.777098 | 0.000000 |
| C | -0.705834 | -4.147941 | 0.000000 |
| C | 0.705834 | -4.147941 | 0.000000 |
| C | 1.114701 | -2.777098 | 0.000000 |
| N | 1.982839 | 0.000000 | 0.000000 |
| C | 2.768767 | -1.119542 | 0.000000 |
| C | 4.157840 | -0.699252 | 0.000000 |
| C | 4.157840 | 0.699252 | 0.000000 |
| C | 2.768767 | 1.119542 | 0.000000 |
| C | -5.342426 | -1.410102 | 0.000000 |
| C | -6.529862 | -0.697316 | 0.000000 |
| C | -6.529862 | 0.697316 | 0.000000 |
| C | -5.342426 | 1.410102 | 0.000000 |
| C | -1.412460 | 5.342094 | 0.000000 |
| C | -0.701232 | 6.524225 | 0.000000 |
| C | 0.701232 | 6.524225 | 0.000000 |
| C | 1.412460 | 5.342094 | 0.000000 |
| C | 5.342426 | 1.410102 | 0.000000 |
| C | 6.529862 | 0.697316 | 0.000000 |
| C | 6.529862 | -0.697316 | 0.000000 |
| C | 5.342426 | -1.410102 | 0.000000 |
| C | 1.412460 | -5.342094 | 0.000000 |
| C | 0.701232 | -6.524225 | 0.000000 |
| C | -0.701232 | -6.524225 | 0.000000 |
| C | -1.412460 | -5.342094 | 0.000000 |
| H | -5.321824 | -2.502853 | 0.000000 |
| H | -7.483364 | -1.231729 | 0.000000 |
| H | -7.483364 | 1.231729 | 0.000000 |
| H | -5.321824 | 2.502853 | 0.000000 |
| H | -2.505470 | 5.326988 | 0.000000 |
| H | -1.234479 | 7.478506 | 0.000000 |
| H | 1.234479 | 7.478506 | 0.000000 |
| H | 2.505470 | 5.326988 | 0.000000 |
| H | 5.321824 | 2.502853 | 0.000000 |
| H | 7.483364 | 1.231729 | 0.000000 |
| H | 7.483364 | -1.231729 | 0.000000 |
| H | 5.321824 | -2.502853 | 0.000000 |
| H | 2.505470 | -5.326988 | 0.000000 |
| H | 1.234479 | -7.478506 | 0.000000 |
| H | -1.234479 | -7.478506 | 0.000000 |
| H | -2.505470 | -5.326988 | 0.000000 |

**LS TS**

| | | | |
|---|---|---|---|
| Mg | 0.000002 | -0.000001 | 0.000000 |
| N | 2.388073 | 2.388082 | 0.000000 |
| N | -2.372506 | 2.372542 | 0.000000 |
| N | -2.388081 | -2.388088 | 0.000000 |
| N | 2.372508 | -2.372535 | 0.000000 |
| N | 0.011233 | 1.988443 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 1.117089 | 2.770140 | 0.000000 |
| C | 0.699122 | 4.153663 | 0.000000 |
| C | -0.705695 | 4.152166 | 0.000000 |
| C | -1.117946 | 2.776411 | 0.000000 |
| N | -1.988450 | -0.011216 | 0.000000 |
| C | -2.776411 | 1.117972 | 0.000000 |
| C | -4.152142 | 0.705694 | 0.000000 |
| C | -4.153684 | -0.699141 | 0.000000 |
| C | -2.770143 | -1.117073 | 0.000000 |
| N | -0.011238 | -1.988447 | 0.000000 |
| C | -1.117093 | -2.770145 | 0.000000 |
| C | -0.699123 | -4.153669 | 0.000000 |
| C | 0.705698 | -4.152167 | 0.000000 |
| C | 1.117947 | -2.776410 | 0.000000 |
| N | 1.988452 | 0.011221 | 0.000000 |
| C | 2.776413 | -1.117967 | 0.000000 |
| C | 4.152143 | -0.705689 | 0.000000 |
| C | 4.153681 | 0.699143 | 0.000000 |
| C | 2.770141 | 1.117073 | 0.000000 |
| C | -5.338008 | -1.412435 | 0.000000 |
| C | -6.526971 | -0.705500 | 0.000000 |
| C | -6.527476 | 0.692991 | 0.000000 |
| C | -5.346324 | 1.409803 | 0.000000 |
| C | -1.409787 | 5.346335 | 0.000000 |
| C | -0.692985 | 6.527481 | 0.000000 |
| C | 0.705497 | 6.526940 | 0.000000 |
| C | 1.412427 | 5.337968 | 0.000000 |
| C | 5.337999 | 1.412438 | 0.000000 |
| C | 6.526964 | 0.705509 | 0.000000 |
| C | 6.527474 | -0.692981 | 0.000000 |
| C | 5.346323 | -1.409796 | 0.000000 |
| C | 1.409794 | -5.346337 | 0.000000 |
| C | 0.692995 | -6.527485 | 0.000000 |
| C | -0.705488 | -6.526951 | 0.000000 |
| C | -1.412425 | -5.337981 | 0.000000 |
| H | -5.313015 | -2.505269 | 0.000000 |
| H | -7.479451 | -1.241384 | 0.000000 |
| H | -7.482466 | 1.225248 | 0.000000 |
| H | -5.335467 | 2.502704 | 0.000000 |
| H | -2.502685 | 5.335472 | 0.000000 |
| H | -1.225226 | 7.482474 | 0.000000 |
| H | 1.241400 | 7.479407 | 0.000000 |
| H | 2.505257 | 5.312969 | 0.000000 |
| H | 5.313000 | 2.505269 | 0.000000 |
| H | 7.479441 | 1.241396 | 0.000000 |
| H | 7.482464 | -1.225235 | 0.000000 |
| H | 5.335468 | -2.502696 | 0.000000 |
| H | 2.502692 | -5.335472 | 0.000000 |
| H | 1.225240 | -7.482477 | 0.000000 |
| H | -1.241386 | -7.479422 | 0.000000 |
| H | -2.505257 | -5.312987 | 0.000000 |

**Cartesian coordinates for MnPc in HS and LS minimum structures obtained by LDA.**

**HS**

| | | | |
|---|---|---|---|
| Mn | 0.000000 | 0.000000 | 0.000000 |
| N | 2.362463 | 2.362463 | 0.000000 |
| N | -2.362463 | 2.362463 | 0.000000 |
| N | -2.362463 | -2.362463 | 0.000000 |
| N | 2.362463 | -2.362463 | 0.000000 |
| N | 0.000000 | 1.916937 | 0.000000 |
| C | 1.110628 | 2.733992 | 0.000000 |
| C | 0.696744 | 4.106978 | 0.000000 |
| C | -0.696744 | 4.106978 | 0.000000 |
| C | -1.110628 | 2.733992 | 0.000000 |
| N | -1.916937 | 0.000000 | 0.000000 |
| C | -2.733992 | 1.110628 | 0.000000 |
| C | -4.106978 | 0.696744 | 0.000000 |
| C | -4.106978 | -0.696744 | 0.000000 |
| C | -2.733992 | -1.110628 | 0.000000 |
| N | 0.000000 | -1.916937 | 0.000000 |
| C | -1.110628 | -2.733992 | 0.000000 |
| C | -0.696744 | -4.106978 | 0.000000 |
| C | 0.696744 | -4.106978 | 0.000000 |
| C | 1.110628 | -2.733992 | 0.000000 |
| N | 1.916937 | 0.000000 | 0.000000 |
| C | 2.733992 | -1.110628 | 0.000000 |
| C | 4.106978 | -0.696744 | 0.000000 |
| C | 4.106978 | 0.696744 | 0.000000 |
| C | 2.733992 | 1.110628 | 0.000000 |
| C | -5.289468 | -1.414528 | 0.000000 |
| C | -6.471333 | -0.698379 | 0.000000 |
| C | -6.471333 | 0.698379 | 0.000000 |
| C | -5.289468 | 1.414528 | 0.000000 |
| C | -1.414528 | 5.289468 | 0.000000 |
| C | -0.698379 | 6.471333 | 0.000000 |
| C | 0.698379 | 6.471333 | 0.000000 |
| C | 1.414528 | 5.289468 | 0.000000 |
| C | 5.289468 | 1.414528 | 0.000000 |
| C | 6.471333 | 0.698379 | 0.000000 |
| C | 6.471333 | -0.698379 | 0.000000 |
| C | 5.289468 | -1.414528 | 0.000000 |
| C | 1.414528 | -5.289468 | 0.000000 |
| C | 0.698379 | -6.471333 | 0.000000 |
| C | -0.698379 | -6.471333 | 0.000000 |
| C | -1.414528 | -5.289468 | 0.000000 |
| H | -5.273312 | -2.506737 | 0.000000 |
| H | -7.425400 | -1.230362 | 0.000000 |
| H | -7.425400 | 1.230362 | 0.000000 |
| H | -5.273312 | 2.506737 | 0.000000 |
| H | -2.506737 | 5.273312 | 0.000000 |
| H | -1.230362 | 7.425400 | 0.000000 |
| H | 1.230362 | 7.425400 | 0.000000 |
| H | 2.506737 | 5.273312 | 0.000000 |
| H | 5.273312 | 2.506737 | 0.000000 |
| H | 7.425400 | 1.230362 | 0.000000 |
| H | 7.425400 | -1.230362 | 0.000000 |
| H | 5.273312 | -2.506737 | 0.000000 |
| H | 2.506737 | -5.273312 | 0.000000 |
| H | 1.230362 | -7.425400 | 0.000000 |
| H | -1.230362 | -7.425400 | 0.000000 |
| H | -2.506737 | -5.273312 | 0.000000 |

**LS min**

| | | | |
|---|---|---|---|
| Mn | 0.000000 | 0.000000 | 0.000000 |
| N | 2.367787 | 2.357219 | 0.000000 |
| N | -2.367787 | 2.357219 | 0.000000 |
| N | -2.367787 | -2.357219 | 0.000000 |
| N | 2.367787 | -2.357219 | 0.000000 |
| N | 0.000000 | 1.921394 | 0.000000 |
| C | 1.110962 | 2.733604 | 0.000000 |
| C | 0.698588 | 4.100287 | 0.000000 |
| C | -0.698588 | 4.100287 | 0.000000 |
| C | -1.110962 | 2.733604 | 0.000000 |
| N | -1.912189 | 0.000000 | 0.000000 |
| C | -2.734500 | 1.110339 | 0.000000 |
| C | -4.113358 | 0.694734 | 0.000000 |
| C | -4.113358 | -0.694734 | 0.000000 |
| C | -2.734500 | -1.110339 | 0.000000 |
| N | 0.000000 | -1.921394 | 0.000000 |
| C | -1.110962 | -2.733604 | 0.000000 |
| C | -0.698588 | -4.100287 | 0.000000 |
| C | 0.698588 | -4.100287 | 0.000000 |
| C | 1.110962 | -2.733604 | 0.000000 |
| N | 1.912189 | 0.000000 | 0.000000 |
| C | 2.734500 | -1.110339 | 0.000000 |
| C | 4.113358 | -0.694734 | 0.000000 |
| C | 4.113358 | 0.694734 | 0.000000 |
| C | 2.734500 | 1.110339 | 0.000000 |
| C | -5.292593 | -1.412902 | 0.000000 |
| C | -6.477660 | -0.696684 | 0.000000 |
| C | -6.477660 | 0.696684 | 0.000000 |
| C | -5.292593 | 1.412902 | 0.000000 |
| C | -1.416287 | 5.286315 | 0.000000 |
| C | -0.700297 | 6.464248 | 0.000000 |
| C | 0.700297 | 6.464248 | 0.000000 |
| C | 1.416287 | 5.286315 | 0.000000 |
| C | 5.292593 | 1.412902 | 0.000000 |
| C | 6.477660 | 0.696684 | 0.000000 |
| C | 6.477660 | -0.696684 | 0.000000 |
| C | 5.292593 | -1.412902 | 0.000000 |
| C | 1.416287 | -5.286315 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 0.700297 | -6.464248 | 0.000000 |
| C | -0.700297 | -6.464248 | 0.000000 |
| C | -1.416287 | -5.286315 | 0.000000 |
| H | -5.275478 | -2.504883 | 0.000000 |
| H | -7.430866 | -1.229806 | 0.000000 |
| H | -7.430866 | 1.229806 | 0.000000 |
| H | -5.275478 | 2.504883 | 0.000000 |
| H | -2.508237 | 5.270706 | 0.000000 |
| H | -1.230663 | 7.419076 | 0.000000 |
| H | 1.230663 | 7.419076 | 0.000000 |
| H | 2.508237 | 5.270706 | 0.000000 |
| H | 5.275478 | 2.504883 | 0.000000 |
| H | 7.430866 | 1.229806 | 0.000000 |
| H | 7.430866 | -1.229806 | 0.000000 |
| H | 5.275478 | -2.504883 | 0.000000 |
| H | 2.508237 | -5.270706 | 0.000000 |
| H | 1.230663 | -7.419076 | 0.000000 |
| H | -1.230663 | -7.419076 | 0.000000 |
| H | -2.508237 | -5.270706 | 0.000000 |

**LS TS**

| | | | |
|---|---|---|---|
| Mn | 0.000000 | 0.000000 | 0.000000 |
| N | 0.000000 | 3.345902 | 0.000000 |
| N | -3.338278 | 0.000000 | 0.000000 |
| N | 0.000000 | -3.345902 | 0.000000 |
| N | 3.338278 | 0.000000 | 0.000000 |
| N | -1.354121 | 1.356543 | 0.000000 |
| C | -1.146518 | 2.718400 | 0.000000 |
| C | -2.408593 | 3.398508 | 0.000000 |
| C | -3.394259 | 2.413799 | 0.000000 |
| C | -2.718595 | 1.148897 | 0.000000 |
| N | -1.354121 | -1.356543 | 0.000000 |
| C | -2.718595 | -1.148897 | 0.000000 |
| C | -3.394259 | -2.413799 | 0.000000 |
| C | -2.408593 | -3.398508 | 0.000000 |
| C | -1.146518 | -2.718400 | 0.000000 |
| N | 1.354121 | -1.356543 | 0.000000 |
| C | 1.146518 | -2.718400 | 0.000000 |
| C | 2.408593 | -3.398508 | 0.000000 |
| C | 3.394259 | -2.413799 | 0.000000 |
| C | 2.718595 | -1.148897 | 0.000000 |
| N | 1.354121 | 1.356543 | 0.000000 |
| C | 2.718595 | 1.148897 | 0.000000 |
| C | 3.394259 | 2.413799 | 0.000000 |
| C | 2.408593 | 3.398508 | 0.000000 |
| C | 1.146518 | 2.718400 | 0.000000 |
| C | -2.729511 | -4.743948 | 0.000000 |
| C | -4.069253 | -5.080432 | 0.000000 |
| C | -5.058528 | -4.094108 | 0.000000 |
| C | -4.736199 | -2.750332 | 0.000000 |
| C | -4.736199 | 2.750332 | 0.000000 |
| C | -5.058528 | 4.094108 | 0.000000 |
| C | -4.069253 | 5.080432 | 0.000000 |
| C | -2.729511 | 4.743948 | 0.000000 |
| C | 2.729511 | 4.743948 | 0.000000 |
| C | 4.069253 | 5.080432 | 0.000000 |
| C | 5.058528 | 4.094108 | 0.000000 |
| C | 4.736199 | 2.750332 | 0.000000 |
| C | 4.736199 | -2.750332 | 0.000000 |
| C | 5.058528 | -4.094108 | 0.000000 |
| C | 4.069253 | -5.080432 | 0.000000 |
| C | 2.729511 | -4.743948 | 0.000000 |
| H | -1.940631 | -5.499220 | 0.000000 |
| H | -4.364235 | -6.131839 | 0.000000 |
| H | -6.108517 | -4.395485 | 0.000000 |
| H | -5.502249 | -1.972021 | 0.000000 |
| H | -5.502249 | 1.972021 | 0.000000 |
| H | -6.108517 | 4.395485 | 0.000000 |
| H | -4.364235 | 6.131839 | 0.000000 |
| H | -1.940631 | 5.499220 | 0.000000 |
| H | 1.940631 | 5.499220 | 0.000000 |
| H | 4.364235 | 6.131839 | 0.000000 |
| H | 6.108517 | 4.395485 | 0.000000 |
| H | 5.502249 | 1.972021 | 0.000000 |
| H | 5.502249 | -1.972021 | 0.000000 |
| H | 6.108517 | -4.395485 | 0.000000 |
| H | 4.364235 | -6.131839 | 0.000000 |
| H | 1.940631 | -5.499220 | 0.000000 |