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Supplementary Information

One-Electron Reduction Induced Spin Transition in Fe(II) Spin Crossover Molecules and Effect of Ligand

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S1. Details of structural and electronic properties of considered molecules

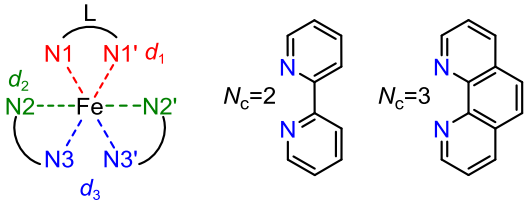
➢ Electronic configurations considered for each molecule

For each molecule, three spin configurations were considered in the neutral state (LS^0, HS^0, and MS^0). The LS^0 configuration is related to a low-spin FeII ion with S_{Fe}=0 and S=0. The HS^0 configuration is related to a high-spin FeII ion with S_{Fe}=2 and S=2. The MS^0 configuration of the whole molecule is related to a middle-spin FeII ion with S_{Fe}=1 and S=1. S_{Fe} and S denote the spin quantum number of the FeII ion and the whole molecule. In the reduced state, only one LS^- configuration is formed and related to S_{Fe}=0 and S=1/2. Two HS^- configurations can be formed: one related to S_{Fe}=2 and S=5/2; the other related to S_{Fe}=2 and S=3/2. Similarly, there are two possible MS^- configurations, that is, S_{Fe}=1 along with S=3/2 and S_{Fe}=1 along with S=1/2. In summary, eight electronic configurations are considered here. It is pointed out that only LS^0 (S_{Fe}=0,S=0), HS^0 (S_{Fe}=2,S=2), LS^- (S_{Fe}=0,S=1/2), and HS^- (S_{Fe}=2,S=3/2) were demonstrated and discussed in the main paper since they were directly associated with the spin transition under the reduction, indicated by Table S1. Figures and tables, except Table S1, in the Supplementary Information are only related to LS^0 (S_{Fe}=0,S=0), HS^0 (S_{Fe}=2,S=2), LS^- (S_{Fe}=0,S=1/2), and HS^- (S_{Fe}=2,S=3/2).

Table S1. Zero-point corrected total energies (E) of **HS^0** and **MS^0** relative to **LS^0** (S=0,S_{Fe}=0) for the neutral molecules and those of **HS^-** and **MS^-** relative to **LS^-** (S=1/2,S_{Fe}=0) for the reduced molecules. The energy unit is kcal/mol.

N_c	Neutral ($Q=0$)		Reduced ($Q=-1$)			
	δE^0(HS) S_{Fe}=2,S=2	δE^0(MS) S_{Fe}=1,S=1	δE^-(HS) S_{Fe}=2,S=3/2	δE^-(HS) S_{Fe}=2,S=5/2	δE^-(MS) S_{Fe}=1,S=1/2	δE^-(MS) S_{Fe}=1,S=3/2
2	4.5	10.8	0.1	2.8	12.0	11.4
3	4.0	10.2	−0.6	2.4	12.3	10.6
4	4.6	10.7	−0.1	3.0	11.7	19.9
5	4.6	10.7	2.3	3.6	11.3	19.7
6	4.3	10.7	3.4	3.4	10.7	10.7
7	4.3	10.7	3.3	4.0	10.6	10.6

Table S2. Comparison of selected bond lengths (unit=Å) and bond angles (unit=deg) for $Fe[H_2B(Pz)_2]_2(bpy)$ with N_c = 2 and $Fe[H_2B(Pz)_2]_2(phen)$ with N_c = 3. 'Exp' and 'Cal' mean experimental values reported in Ref. 25 and calculated values based on our DFT calculations.



Bond lengths & Bond angles	LS^0 (N_c=2)		HS^0 (N_c=2)		HS^0 (N_c=3)	
	Exp	Cal	Exp	Cal	Exp	Cal
d(Fe-N1)	2.013	1.987	2.213	2.254	2.212	2.268
d(Fe-N2)	2.046	2.029	2.190	2.192	2.184	2.186
d(Fe-N3)	2.039	2.012	2.157	2.152	2.158	2.150
∠(N1-Fe-N2)	92.3	92.0	93.9	94.4	89.8	93.6
∠(N1-Fe-N3)	97.0	95.8	97.2	96.1	97.2	95.3
∠(N2-Fe-N3)	90.1	91.0	88.7	88.7	90.9	88.9
∠(N1-Fe-N1′)	78.9	81.5	73.2	72.4	75.0	73.5
∠(N3-Fe-N3′)	87.1	86.9	92.6	95.8	90.7	96.3

Table S3. Enthalpy and Gibbs free energy differences between LS and HS at 150 K. Definitions for $\delta E_{\mathrm{H}}^{0}$, $\delta E_{\mathrm{H}}^{0}$, $\Delta(\delta E_{\mathrm{H}})$, and $\Delta(\delta E_{\mathrm{G}})$ are similar to δE^{0} and $\Delta(\delta E)$ displayed in Fig. 3 in the main paper. It shows that the LS configuration is the ground state for N_{c}=2 and 3 at 150 K, consistent with Ref. 25 in the main paper.

N_{c}	Neutral		Reduced		Reduced–Neutral	
	$\delta E_{\mathrm{H}}^{0}$	$\delta E_{\mathrm{G}}^{0}$	$\delta E_{\mathrm{H}}^{-}$	$\delta E_{\mathrm{G}}^{-}$	$\Delta(\delta E_{\mathrm{H}})$	$\Delta(\delta E_{\mathrm{G}})$
2	5.3	2.8	0.9	-1.2	-4.4	-4.0
3	4.7	2.2	0.2	-2.0	-4.5	-4.2
4	5.4	2.9	0.6	-1.6	-4.8	-4.5
5	5.4	2.9	3.1	0.9	-2.3	-2.0
6	5.1	2.7	4.2	2.0	-0.9	-0.7
7	5.1	2.6	4.0	1.8	-1.1	-0.8

Table S4. Source data for Fig. 3 in the main paper

N_{c}	Neutral ($Q=0$)			Reduced ($Q=-1$)			Reduced–Neutral	
	$\delta E_{\mathrm{e}}^{0}$	$\delta(\mathrm{ZPVE})^{0}$	δE^{0}	$\delta E_{\mathrm{e}}^{-}$	$\delta(\mathrm{ZPVE})^{-}$	δE^{-}	$\Delta(\delta E_{\mathrm{e}})$	$\Delta(\delta E)$
2	7.1	−2.6	4.5	2.6	−2.5	0.1	−4.5	−4.4
3	6.5	−2.5	4.0	1.7	−2.3	−0.6	−4.8	−4.6
4	7.1	−2.5	4.6	2.2	−2.3	−0.1	−4.9	−4.7
5	7.1	−2.5	4.6	4.7	−2.4	2.3	−2.4	−2.3
6	6.8	−2.5	4.3	6.0	−2.6	3.4	−0.8	−0.9
7	6.8	−2.5	4.3	5.8	−2.5	3.3	−1.0	−1.0

- Temperature effect on the spin transition induced by the reduction

The temperature effect is not important for the spin transition induced by the one-electron reduction, thus not discussed in the main paper. The reason is as follows.

For molecular devices of SCO molecules, it is important to switch LS and HS by voltages. For this purpose, it is necessary to retain the LS configuration when voltages are not applied. Thus related STM or similar experiments were usually conducted at low temperatures (about 5 Kelvin, Refs. 16, 18, and 19) since most SCO molecules have low transition temperatures (T_c). Once the temperature is above T_c in experiments, the HS configuration is favored in Gibbs free energy and the spin switch is out of control by voltages. In these experiments, the temperature effect is little and ignorable.

In other experiments (Refs. 17 and 20) SCO molecules with high T_c were involved. Although the temperature is lower than T_c for retaining the LS configuration, the temperature effect seems not to be neglected. We take 150 K as an example to demonstrate the temperature effect on the spin transition of our considered SCO molecules. The calculation shows that at 150 K the LS configuration is retained in Gibbs free energy ($\delta E_{\mathrm{G}}^{0} \approx 2.5$ kcal/mol) in the neutral state, and the key quantity for the spin transition induced by electron reduction is $\Delta(\delta E_{\mathrm{G}})$. However, Table S3 reveals that $\Delta(\delta E_{\mathrm{G}})$ is determined by electronic effects, i.e., $\Delta(\delta E_{\mathrm{e}})$ in Table S2. Therefore, the spin transition induced by the reduction is little affected by the temperature.

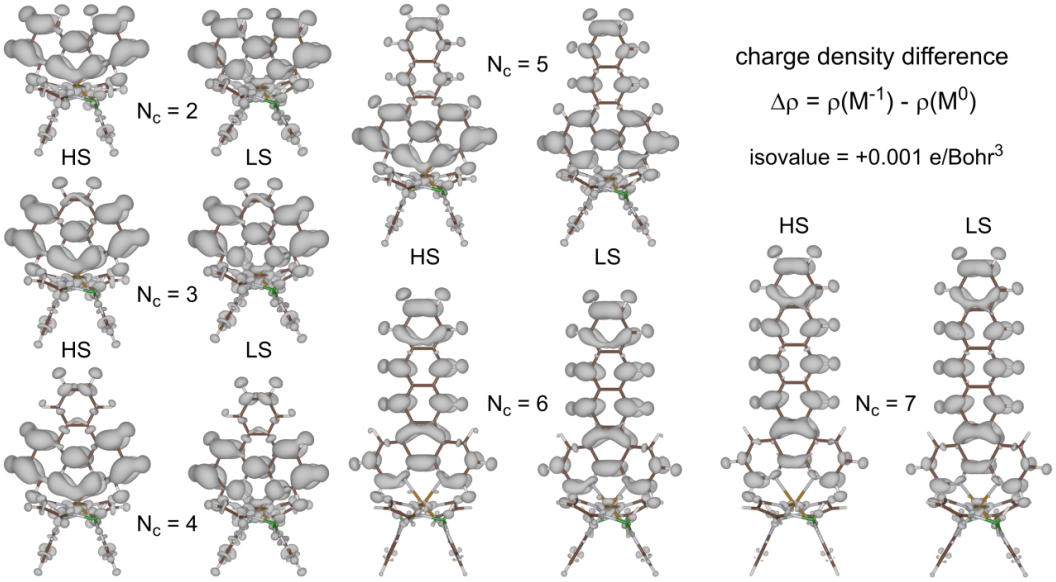


Fig. S1. Charge density difference (Δρ) between neutral and reduced molecules. Δρ surfaces are drawn with the isovalue of +0.001 e/Bohr^3, which indicate the distributions of the electron increase. Surfaces related to the isovalue of -0.001 e/Bohr^3 is trivial and not shown for clarity. The shown Δρ surfaces are calculated using the optimized structures of reduced molecules. These electron-increase distributions are well consistent with HOMOs of reduced molecules shown in Fig. 4 and Fig. S2. Δρ is also calculated using the optimized structures of neutral molecules, and the corresponding results are quite close to these displayed here.

Table S5. Mulliken charges of two fragments of considered molecules and spin density (α-β) of Fe in the HS configuration. They were calculated at the B3LYP*/Def2-TZVP level. The L ligand and $Fe[H_2B(Pz)_2]_2$ are respectively denoted by Frag1 and Frag2. The spin density equals to majority-spin (or α) electrons minus beta-spin (or β) ones.

	Neutral			Reduced			Reduced–Neutral	
Nc	Frag1	Frag2	$(\alpha-\beta)_{Fe}$	Frag1	Frag2	$(\alpha-\beta)_{Fe}$	ΔFrag1	ΔFrag2
2	0.27	-0.27	3.76	-0.40	-0.60	3.70	**-0.67**	**-0.33**
3	0.25	-0.25	3.76	-0.40	-0.60	3.70	**-0.65**	**-0.35**
4	0.26	-0.26	3.76	-0.41	-0.59	3.70	**-0.67**	**-0.33**
5	0.26	-0.26	3.82	-0.47	-0.53	3.72	**-0.73**	**-0.27**
6	0.26	-0.26	3.76	-0.59	-0.41	3.76	**-0.85**	**-0.15**
7	0.27	-0.27	3.76	-0.61	-0.39	3.76	**-0.88**	**-0.12**

Table S6. Mulliken charges of two fragments of considered complexes and spin density of Fe in the LS configuration. Other details are the same as those in Table S4.

	Neutral			Reduced			Reduced–Neutral	
Nc	Frag1	Frag2	$(\alpha-\beta)_{Fe}$	Frag1	Frag2	$(\alpha-\beta)_{Fe}$	ΔFrag1	ΔFrag2
2	0.56	-0.56	0.00	-0.21	-0.79	0.02	**-0.77**	**-0.23**
3	0.56	-0.56	0.00	-0.21	-0.79	0.03	**-0.77**	**-0.23**
4	0.57	-0.57	0.00	-0.21	-0.79	0.03	**-0.78**	**-0.22**
5	0.57	-0.57	0.00	-0.25	-0.75	0.01	**-0.82**	**-0.18**
6	0.57	-0.57	0.00	-0.30	-0.70	0.00	**-0.87**	**-0.13**
7	0.57	-0.57	0.00	-0.31	-0.69	0.00	**-0.88**	**-0.12**

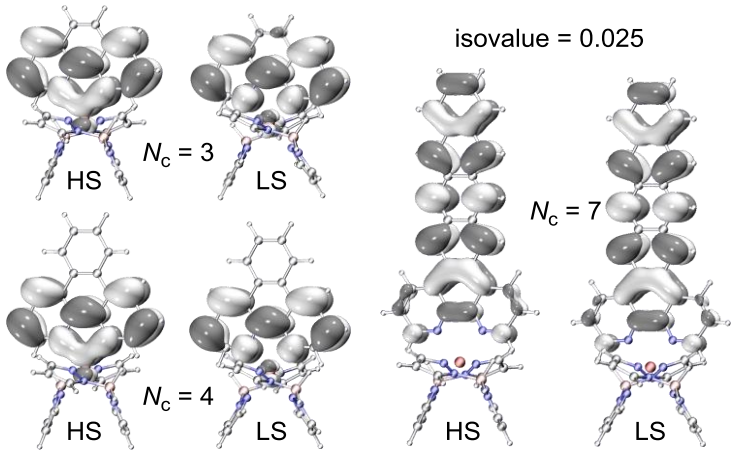


Fig. S2. Isosurfaces of HOMO for reduced HS and LS configurations.

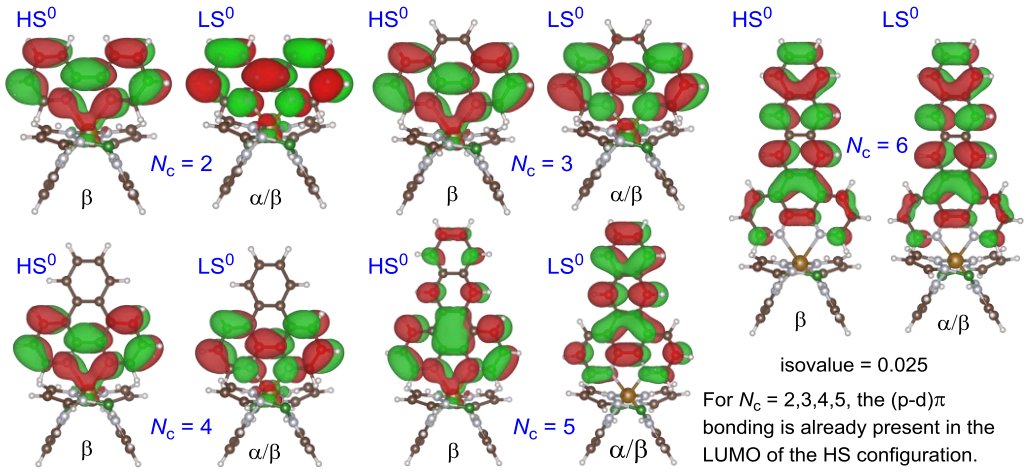


Fig. S3. Lowest unoccupied molecular orbitals (LUMOs) in the HS^0 and LS^0 configurations. These LUMOs were calculated using the optimized structures of neutral molecules. β denotes the beta-spin molecular orbitals. α/β means the spin-degenerate molecular orbitals.

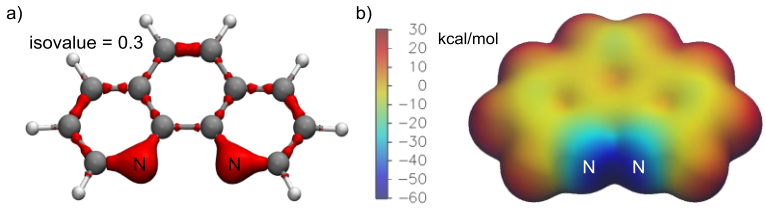


Fig. S4. a) Electron density of the gas-phase (or equilibrium) L ligand (N_c=2) in the neutral state. It shows high electron density around nitrogen atoms. b) Electrostatic potential (ESP) mapped to the electron density isosurface (isovalue = 0.002 e/au^3). It consistently shows high electric potential around nitrogen atoms.

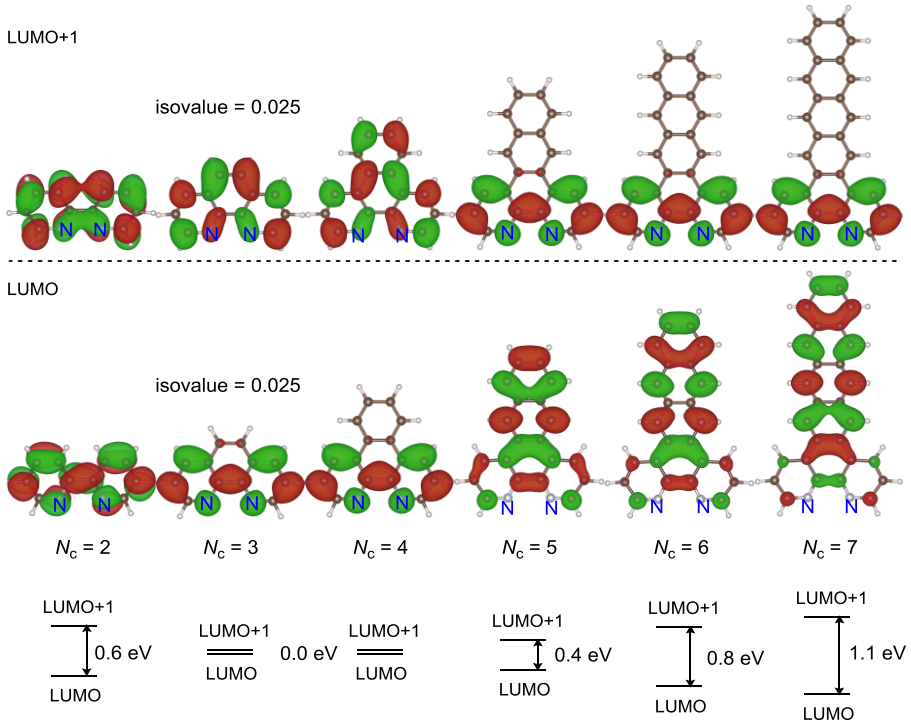


Fig. S5. LUMO and LUMO+1 of the neutral gas-phase L ligand. Energy gaps between LUMO and LUMO+1 are marked as well. These were calculated at the B3LYP*/Def2-TZVP level.

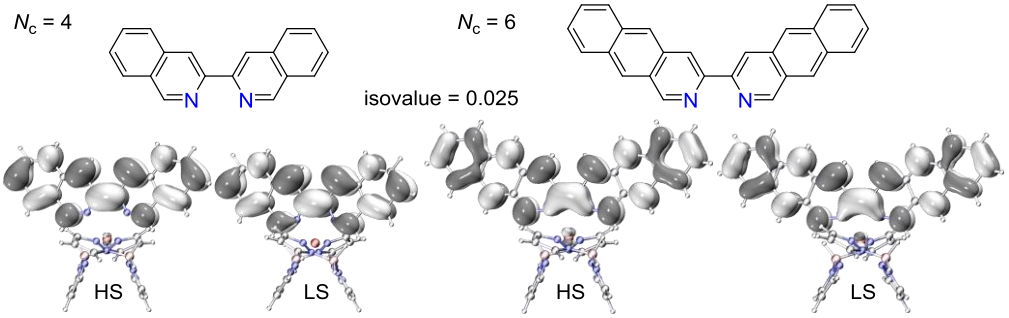
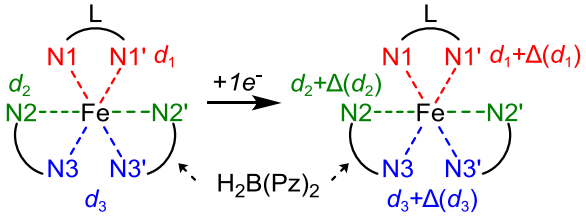


Fig. S6. Two other considered molecules for N_c = 4, 6 and HOMOs of HS^- and LS^- configurations for these two molecules. Ignorable (p-d)π bonding is witnessed in their HOMOs of the HS^- configuration.

Table S7. Energy differences between LS and HS (δE_e and δE) and variation of δE_e (δE) induced by the added electron for $N_c = 2$ and for $N_c = 4, 6$ shown in Fig. S6.

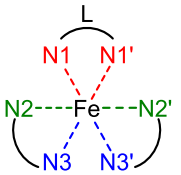
Nc	Neutral ($Q = 0$)			Reduced ($Q = -1$)			Reduced–Neutral	
	δE_e^0	$\delta(\mathrm{ZPVE})^0$	δE^0	δE_e^-	$\delta(\mathrm{ZPVE})^-$	δE^-	$\Delta(\delta E_e)$	$\Delta(\delta E)$
2	7.1	−2.6	4.5	2.6	−2.5	0.1	−4.5	−4.4
4	6.6	−2.5	4.1	5.6	−2.8	2.8	−1.0	−1.3
6	6.9	−2.5	4.4	4.9	−2.5	2.4	−2.0	−2.0

Table S8. Variations of Fe-N bond lengths induced by the added electron in different spin configurations. The Fe-N bond lengths are decreased due to the (p-d)π bonding in the HS^- configuration. As N_c increasing, the magnitude of $\Delta(d_1)$ grows smaller, consistent with the weakening of the (p-d)π bonding. Magnitudes of $\Delta(d_{1,2,3})$ in the HS state are larger than those in the LS state, consistent with larger deformation energies in the HS^- configuration (see Table S10 below).



N_c	$HS^- - HS^0$			$LS^- - LS^0$		
	$\Delta(d_1)$	$\Delta(d_2)$	$\Delta(d_3)$	$\Delta(d_1)$	$\Delta(d_2)$	$\Delta(d_3)$
2	-0.099	0.031	0.081	0.006	0.002	0.019
3	-0.105	0.033	0.079	0.005	0.003	0.019
4	-0.099	0.030	0.075	0.004	0.002	0.019
5	-0.075	0.023	0.062	0.005	0.000	0.016
6	-0.038	0.011	0.036	0.007	0.000	0.012
7	-0.032	0.008	0.031	0.006	0.000	0.011

Table S9. Variations of Fe-N bond angles (α1-α6) induced by the added electron in different spin configurations. Magnitudes of Δ(α1)–Δ(α6) in the HS^- configuration are similarly larger than those in the LS configuration. Variations of Δ(α1)–Δ(α6) in the HS^- configuration are correlated with the (p-d)π bonding in HOMOs of the HS^- configuration.



α1 = ∠(N1–Fe-N2)
α2 = ∠(N1–Fe-N3)
α3 = ∠(N2–Fe-N3)
α4 = ∠(N1–Fe-N1')
α5 = ∠(N3–Fe-N3')
α6 = ∠(N2–Fe-N2')

$HS^- - HS^0$	N_c=2	N_c=3	N_c=4	N_c=5	N_c=6	N_c=7
Δ(α1)	2.1	2.7	2.3	1.5	0.5	0.4
Δ(α2)	2.6	2.6	2.6	2.3	2.2	1.9
Δ(α3)	-2.0	-2.2	-2.1	-1.5	-0.5	-0.3
Δ(α4)	3.6	3.6	3.4	3.1	1.9	1.5
Δ(α5)	-9.4	-9.4	-8.9	-8.0	-6.2	-5.5
Δ(α6)	-7.5	-8.1	-7.5	-5.9	-3.2	-2.6
$LS^- - LS^0$	N_c=2	N_c=3	N_c=4	N_c=5	N_c=6	N_c=7
Δ(α1)	-0.9	-0.8	-0.7	-1.1	-1.1	-0.9
Δ(α2)	0.3	0.5	0.3	0.3	0.4	0.4
Δ(α3)	0.4	0.4	0.3	0.4	0.5	0.4
Δ(α4)	0.8	0.5	0.6	0.7	0.3	0.2
Δ(α5)	-1.4	-1.5	-1.4	-1.3	-1.2	-1.0
Δ(α6)	0.7	0.4	0.4	0.3	0.3	0.3

S2. Details of energy composition analysis (EDA) calculations

1) Definitions of fragments for the EDA calculation and necessary explanations

a) For simplicity, the neutral HS configuration is marked by HS^0 with $S = 2$, $S_{Fe} = 2$. When performing the EDA calculation for this configuration, Frag1 directly used the L-ligand part in the HS^0 structure. This part is in the neutral state with $S = 0$, and denoted by $F1^0(HS^0)$ in the following. Frag2 directly used the $Fe[H_2B(Pz)_2]_2$ part in the HS^0 structure. This part is in the neutral state with $S = 2$, $S_{Fe} = 2$, and denoted by $F2^0(HS^0)$ in the following.

b) The neutral LS configuration is marked by $\mathrm{LS^0}$ with $\mathrm{S}=0$, $\mathrm{S_{Fe}}=0$. When performing the EDA calculation for this configuration, Frag1 directly used the L-ligand part in the $\mathrm{LS^0}$ structure. This part is in the neutral state with $\mathrm{S}=0$, and denoted by $\mathrm{F1^0(LS^0)}$ in the following. Frag2 directly used the $Fe[H_2B(Pz)_2]_2$ part in the $\mathrm{LS^0}$ structure. This part is in the neutral state with $\mathrm{S}=0$, $\mathrm{S_{Fe}}=0$, and denoted by $\mathrm{F2^0(LS^0)}$ in the following.

c) The reduced HS configuration is marked by $\mathrm{HS^-}$ with $\mathrm{S}=3/2$, $\mathrm{S_{Fe}}=2$. When performing the EDA calculation for this configuration, Frag1 used the L-ligand part in the $\mathrm{HS^-}$ structure. This part is in the reduced state (i.e. $\mathrm{L^-}$) with $\mathrm{S}=1/2$, and denoted by $\mathrm{F1^-(HS^-)}$ in the following. Frag2 used the $Fe[H_2B(Pz)_2]_2$ part in the $\mathrm{HS^-}$ structure. This part is still in the neutral state with $\mathrm{S}=2$, $\mathrm{S_{Fe}}=2$, and denoted by $\mathrm{F2^0(HS^-)}$ in the following.

d) The reduced LS configuration is marked by $\mathrm{LS^-}$ with $\mathrm{S}=1/2$, $\mathrm{S_{Fe}}=0$. When performing the EDA calculation for this configuration, Frag1 used the L-ligand part in the $\mathrm{LS^-}$ structure. This part is in the reduced state (i.e. $\mathrm{L^-}$) with $\mathrm{S}=1/2$ as well, and denoted by $\mathrm{F1^-(LS^-)}$ in the following. Frag2 used the $Fe[H_2B(Pz)_2]_2$ part in the $\mathrm{LS^-}$ structure. This part is in the neutral state with $\mathrm{S}=0$, $\mathrm{S_{Fe}}=0$, and denoted by $\mathrm{F2^0(LS^-)}$ in the following.

e) The gas-phase Frag1 and Frag2 are required for the calculation of the deformation energy. The neutral Frag1 in the gas phase is marked by $\mathrm{F1^0(GP)}$ with $\mathrm{S}=0$, and the reduced Frag1 in the gas phase is marked by $\mathrm{F1^-(GP)}$ with $\mathrm{S}=1/2$ in the following. The neutral HS Frag2 in the gas phase is marked by $\mathrm{F2^0(HS/GP)}$ with $\mathrm{S}=2$, $\mathrm{S_{Fe}}=2$ and the LS Frag2 in the gas phase is by $\mathrm{F2^0(LS/GP)}$ with $\mathrm{S}=0$, $\mathrm{S_{Fe}}=0$ in the following.

f) E_e denotes single-point or total electronic energy with the Grimme-D3(BJ) dispersion correction.

2) Energy terms given by the EDA study for the binding energy between Frag1 and Frag2

The binding energy (E_{b}) between Frag1 and Frag2 is dissected into seven energy terms in the EDA study, that is, the deformation energy (E_{deform}), the spin-excitation energy (E_{s}), the electrostatic interaction energy (E_{elstat}), the Pauli repulsion energy (E_{Pauli}), the dispersion interaction energy (E_{disp}), the polarization energy (E_{pol}) and the charge transfer energy (E_{ct}). E_{deform} is the energy consumed to deform fragments from their free (or equilibrium) geometries to combination geometries (in the overall molecular system). E_{s} is the energy increase from the HS configuration of the free Frag2 to its LS configuration. The HS configuration is the ground state of the free Frag2, while the LS configuration is an excited state of the free Frag2. E_{elstat} denotes the Coulomb interaction energy between unperturbed charge distributions of deformed fragments. E_{Pauli} accounts for the destabilizing interactions between occupied orbitals of Frag1 and Frag2. E_{disp} arises from interactions of instantaneous multipoles in fragments due to electron fluctuations in time and in this work it is calculated by the Grimme's D3 scheme with Becke-Johnson damping. E_{pol} describes the energy lowering resulting from the intra-fragment density relaxation of each fragment in response to all other fragments in the overall system. E_{ct} reflects donor-acceptor inter-fragment orbital interactions and electron-pairing bonding that bring about energy lowering in the system. The preparation energy (E_{prep} mentioned in the main paper) is the sum of E_{deform} and E_{s}. The through-space interaction energy (E_{space} mentioned in the main paper) is the sum of E_{elstat}, E_{Pauli} and E_{disp}. The orbital interaction energy (E_{orb} mentioned in the main paper) is the sum of E_{pol} and E_{ct}.

3) Calculation of deformation energy (E_{deform})

For the neutral HS configuration,

$$E_{\mathrm{deform}}(\mathrm{HS^0}) = E_e[\mathrm{F1^0(HS^0)}] - E_e[\mathrm{F1^0(GP)}] + E_e[\mathrm{F2^0(HS^0)}] - E_e[\mathrm{F2^0(HS/GP)}] \quad \text{-- (1)}$$

For the neutral LS configuration,

$$E_{\mathrm{deform}}(\mathrm{LS^0}) = E_e[\mathrm{F1^0(LS^0)}] - E_e[\mathrm{F1^0(GP)}] + E_e[\mathrm{F2^0(LS^0)}] - E_e[\mathrm{F2^0(LS/GP)}] \quad \text{-- (2)}$$

For the reduced HS configuration,

$E_{\mathrm{deform}}(\mathrm{HS}^-) = E_e[\mathrm{F1}^-(\mathrm{HS}^-)] - E_e[\mathrm{F1}^-(\mathrm{GP})] + E_e[\mathrm{F2}^0(\mathrm{HS}^-)] - E_e[\mathrm{F2}^0(\mathrm{HS/GP})]$ -- (3)

For the reduced LS configuration,

$E_{\mathrm{deform}}(\mathrm{LS}^-) = E_e[\mathrm{F1}^-(\mathrm{LS}^-)] - E_e[\mathrm{F1}^-(\mathrm{GP})] + E_e[\mathrm{F2}^0(\mathrm{LS}^-)] - E_e[\mathrm{F2}^0(\mathrm{LS/GP})]$ -- (4)

4) Calculation of spin−excitation energy (E_{s})

Since the metal ion is contained only in Frag2 (i.e. $\mathrm{Fe}[\mathrm{H_2B(Pz)_2}]_2$), the spin-excitation energy is only determined by this fragment. Our calculation showed that the HS configuration with $\mathrm{S} = 2$ and $\mathrm{S_{Fe}} = 2$ is the ground state of the neutral Frag2 in the gas phase, while the LS configuration with $\mathrm{S} = 0$ and $\mathrm{S_{Fe}} = 0$ is an excited state of the neutral Frag2 in the gas phase. Thus,

$E_{\mathrm{s}}(\mathrm{HS}^0) = E_{\mathrm{s}}(\mathrm{HS}^-) = E_e[\mathrm{F2}^0(\mathrm{HS/GP})] - E_e[\mathrm{F2}^0(\mathrm{HS/GP})] = 0$ --(5)

$E_{\mathrm{s}}(\mathrm{LS}^0) = E_{\mathrm{s}}(\mathrm{LS}^-) = E_e[\mathrm{F2}^0(\mathrm{LS/GP})] - E_e[\mathrm{F2}^0(\mathrm{HS/GP})] > 0$ --(6)

In the present work, the key quantity is the variation of energy induced by the added electron, and meanwhile, Frag2 is both $[\mathrm{Fe}[\mathrm{H_2B(Pz)_2}]_2]^0$ in the neutral and reduced configuration. Thus,

$\Delta E_{\mathrm{s}}(\mathrm{HS}) = E_{\mathrm{s}}(\mathrm{HS}^-) - E_{\mathrm{s}}(\mathrm{HS}^0) = 0$,

$\Delta E_{\mathrm{s}}(\mathrm{LS}) = E_{\mathrm{s}}(\mathrm{LS}^-) - E_{\mathrm{s}}(\mathrm{LS}^0) = 0$, and

$\Delta(\delta E_{\mathrm{s}}) = \Delta E_{\mathrm{s}}(\mathrm{HS}) - \Delta E_{\mathrm{s}}(\mathrm{LS}) = 0$.

5) Calculations of electrostatic interaction energy (E_{elstat}), Pauli repulsion energy (E_{Pauli}), dispersion interaction energy (E_{disp}), polarization energy (E_{pol}), and charge-transfer energy (E_{ct})

One can refer to references[1,2] for details about calculations of E_{elstat}, E_{Pauli}, E_{pol}, and E_{ct}. The dispersion interaction energy E_{disp} was calculated by the DFT-D3 package developed by the Grimme group.[3] Since the coefficient for B3LYP* (15%HF) is not available, E_{disp} was calculated using the coefficient for B3LYP (20% HF). Besides, it is pointed out that these EDA energy terms were calculated based on $\mathrm{F1}^0(\mathrm{HS}^0)$ and $\mathrm{F2}^0(\mathrm{HS}^0)$ for the HS^0 configuration; they were based on $\mathrm{F1}^0(\mathrm{LS}^0)$ and $\mathrm{F2}^0(\mathrm{LS}^0)$ for the LS^0 configuration; they were based on $\mathrm{F1}^-(\mathrm{HS}^-)$ and $\mathrm{F2}^0(\mathrm{HS}^-)$ for the HS^- configuration; they were based on $\mathrm{F1}^-(\mathrm{LS}^-)$ and $\mathrm{F2}^0(\mathrm{LS}^-)$ for the LS^- configuration.

6) Calculation of preparation energy (E_{prep}), through-space interaction energy (E_{space}), and through-bond interaction energy (E_{bond})

$E_{\mathrm{prep}} = E_{\mathrm{deform}} + E_{\mathrm{s}}$ --(7)

$E_{\mathrm{space}} = E_{\mathrm{elstat}} + E_{\mathrm{Pauli}} + E_{\mathrm{disp}}$ --(8)

$E_{\mathrm{orb}} = E_{\mathrm{pol}} + E_{\mathrm{ct}}$ --(9)

7) Calculation of δE_{i} and $\Delta(\delta E_{\mathrm{i}})$

$\delta E_{\mathrm{i}}^0 = E_{\mathrm{i}}(\mathrm{HS}^0) - E_{\mathrm{i}}(\mathrm{LS}^0)$ --(10-1)

$\delta E_{\mathrm{i}}^- = E_{\mathrm{i}}(\mathrm{HS}^-) - E_{\mathrm{i}}(\mathrm{LS}^-)$ --(10-2)

$\Delta(\delta E_{\mathrm{i}}) = \delta E_{\mathrm{i}}^- - \delta E_{\mathrm{i}}^0$ --(11)

or

$$\Delta E_{\mathrm{i}}(\mathrm{HS}) = E_{\mathrm{i}}(\mathrm{HS}^{-}) - E_{\mathrm{i}}(\mathrm{HS}^{0}) \quad \text{--(10′-1)}$$

$$\Delta E_{\mathrm{i}}(\mathrm{LS}) = E_{\mathrm{i}}(\mathrm{LS}^{-}) - E_{\mathrm{i}}(\mathrm{LS}^{0}) \quad \text{--(10′-2)}$$

$$\Delta(\delta E_{\mathrm{i}}) = \Delta E_{\mathrm{i}}(\mathrm{HS}) - \Delta E_{\mathrm{i}}(\mathrm{LS}) \quad \text{--(11′)}$$

References:

1 P. R. Horn, Y. Mao and M. Head−Gordon, Defining the contributions of permanent electrostatics, Pauli repulsion, and dispersion in density functional theory calculations of intermolecular interaction energies, *J. Chem. Phys.*, 2016, **144**, 114107.

2 R. Z. Khaliullin, E. A. Cobar, R. C. Lochan, A. T. Bell, and M. Head−Gordon, Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals, *J. Phys. Chem. A*, 2007, **111**, 8753–8765.

3 A. Grimme, *https://www.chemie.uni−bonn.de/pctc/mulliken−center/software/dft-d3*.

Table S10. Source data for Figure 6a. These data were calculated using equations 10′ and 11′ shown in the above and data listed in Table S10.

Energy (kcal/mol)	$N_c = 2$	$N_c = 3$	$N_c = 4$	$N_c = 5$	$N_c = 6$	$N_c = 7$
$\Delta(\delta E_b)$	−4.5	−4.8	−4.9	−2.4	−0.8	−1.0
$\Delta(\delta E_{prep})$	8.6	8.6	8.3	6.7	3.4	2.5
$\Delta(\delta E_{space})$	1.5	1.8	1.7	2.5	1.8	1.6
$\Delta(\delta E_{orb})$	−14.6	−15.2	−14.9	−11.6	−6.0	−5.1
$\Delta(\delta E_{deform})$	8.6	8.6	8.3	6.7	3.4	2.5
$\Delta(\delta E_s)$	0.0	0.0	0.0	0.0	0.0	0.0
$\Delta(\delta E_{elstat})$	−21.6	−21.8	−20.9	−16.3	−8.1	−6.6
$\Delta(\delta E_{Pauli})$	22.6	23.1	22.0	18.2	9.4	7.8
$\Delta(\delta E_{disp})$	0.5	0.5	0.6	0.6	0.5	0.4
$\Delta(\delta E_{pol})$	−7.2	−8.3	−8.1	−6.8	−3.7	−2.8
$\Delta(\delta E_{ct})$	−7.4	−6.9	−6.8	−4.8	−2.3	−2.3

Table S11. The variation of EDA energy terms (ΔE_i) induced by the extra electron in the HS and LS configurations. They were calculated by Eq. 10′-1 and 10′-2 in the above.

Energy (kcal/mol)	$N_c = 2$		$N_c = 3$		$N_c = 4$	
	HS	LS	HS	LS	HS	LS
ΔE_b	−28.9	−24.4	−26.5	−21.7	−26.3	−21.4
ΔE_{prep}	10.8	2.2	12.2	3.6	10.9	2.6
ΔE_{space}	−11.3	−12.8	−10.5	−12.3	−10.2	−11.9
ΔE_{orb}	−28.4	−13.8	−28.2	−13.0	−27.0	−12.1
ΔE_{deform}	10.8	2.2	12.2	3.6	10.9	2.6
ΔE_s	0.0	0.0	0.0	0.0	0.0	0.0
ΔE_{elstat}	−36.0	−14.4	−35.4	−13.6	−34.1	−13.2
ΔE_{Pauli}	23.7	1.1	23.9	0.8	22.8	0.8
ΔE_{disp}	1.0	0.5	1.0	0.5	1.1	0.5
ΔE_{pol}	−21.0	−13.8	−21.5	−13.2	−20.5	−12.4
ΔE_{ct}	−7.4	0.0	−6.7	0.2	−6.5	0.3
Energy (kcal/mol)	$N_c = 5$		$N_c = 6$		$N_c = 7$	
	HS	LS	HS	LS	HS	LS
ΔE_b	−16.2	−13.8	−10.7	−9.8	−9.3	−8.3

ΔE_{prep}	10.2	3.5	5.5	2.1	4.2	1.7
ΔE_{space}	−6.2	−8.7	−5.5	−7.3	−4.8	−6.4
ΔE_{orb}	−20.2	−8.6	−10.7	−4.7	−8.7	−3.6
ΔE_{deform}	10.2	3.5	5.5	2.1	4.2	1.7
ΔE_{s}	0.0	0.0	0.0	0.0	0.0	0.0
ΔE_{elstat}	−22.9	−6.6	−12.7	−4.6	−10.5	−3.9
ΔE_{Pauli}	15.7	−2.5	6.4	−3.0	5.0	−2.8
ΔE_{disp}	1.0	0.4	0.8	0.3	0.7	0.3
ΔE_{pol}	−16.2	−9.4	−9.7	−6.0	−7.8	−5.0
ΔE_{ct}	−4.0	0.8	−1.0	1.3	−0.9	1.4

Table S12. Energy decomposition analysis of $\Delta(\delta E_{\text{b}})$ for $N_{\text{c}} = 2$ and for $N_{\text{c}} = 4,\ 6$ in Fig. S6.

N_{c}	$\Delta(\delta E_{\text{b}})$	$\Delta(\delta E_{\text{prep}})$	$\Delta(\delta E_{\text{space}})$	$\Delta(\delta E_{\text{orb}})$
2	−4.6	8.8	1.5	−14.9
4	−1.0	3.7	1.0	−5.7
6	−2.0	3.6	1.5	−7.1

S3. Cartesian coordinates of involved molecular systems (Unit = Å)

1) Neutral LS configuration for $N_{\text{c}} = 2$, $\text{Charge} = 0$, $S = 0$ (S is the spin quantum number)

H	-0.43242700	3.59190400	0.26848300
H	-1.29363800	3.89759500	2.07607100
H	-3.11402400	-0.59216400	-0.40855600
H	-5.09092300	1.10010700	0.48013700
H	-3.65665500	3.22335400	1.56404300
H	0.63500300	3.56535400	3.66186300
H	2.58209800	1.67913500	4.27702900
H	2.30504700	-0.18137500	2.25337800
B	-0.84926700	3.06471100	1.29578400
C	-3.00902700	0.37936500	0.06530000
C	-4.01311800	1.24025600	0.53092000
C	-3.31293400	2.30947000	1.08394500
C	0.91937000	2.64974100	3.14720800
C	1.89128100	1.69515800	3.43652700
C	1.76508000	0.74949100	2.40787200
N	-1.79511100	0.89653100	0.31519400
N	0.79603800	1.11986200	1.55623800
N	-1.99240100	2.07856900	0.93940000
N	0.27793400	2.28237800	2.01820000
H	0.43372300	-3.59368300	-0.25618400
H	1.59257000	-4.11077200	1.32249000
H	3.00236000	0.66919400	-0.87110400
H	5.08457300	-1.09897800	-0.55565900
H	3.83751500	-3.35372900	0.49359100
H	-0.02710300	-3.99756000	3.24811900
H	-1.81385400	-2.22099600	4.42239900
H	-1.87178300	-0.12170900	2.62722200
B	1.02841400	-3.19284200	0.74014200
C	2.97060400	-0.35409500	-0.50868100
C	4.03068500	-1.25529200	-0.33481500
C	3.42568800	-2.39137900	0.19676800
C	-0.38600200	-3.02818300	2.90815800
C	-1.28077600	-2.12623600	3.47859100
C	-1.32467100	-1.05935700	2.56854000

N	1.81317800	-0.91039300	-0.11571600
N	-0.52403400	-1.31214300	1.52138400
N	2.10293400	-2.15803000	0.31468200
N	0.05270100	-2.51776900	1.73850700
Fe	0.00805400	-0.00576500	0.08731100
H	1.52692900	2.61436400	-0.26457300
H	2.12661500	4.06188100	-2.21446000
H	1.39317400	3.33787600	-4.52541400
H	0.11485700	1.20690800	-4.75644100
H	-0.95583300	-0.60855500	-4.77599300
H	-2.19717200	-2.76581200	-4.59214000
H	-2.52303400	-3.77996100	-2.29694200
H	-1.57604700	-2.57975600	-0.31715100
C	1.21635300	2.35137700	-1.27420000
C	1.55586000	3.14359000	-2.36921100
C	1.14960800	2.74057700	-3.64259000
C	0.43214200	1.55277000	-3.77194900
C	0.13134900	0.80543200	-2.62686600
C	-0.59557300	-0.47533800	-2.64315600
C	-1.09992000	-1.07773500	-3.80201900
C	-1.79657600	-2.28032900	-3.69810400
C	-1.97827900	-2.84318800	-2.43354900
C	-1.44408200	-2.18960200	-1.32477300
N	0.51201400	1.21780200	-1.39428300
N	-0.75948700	-1.04202800	-1.42401600

2) Reduced LS configuration for $N_{\mathrm{c}} = 2,\ \mathrm{Charge} = -1,\ S = 1/2$

H	-0.45115200	3.64902300	0.47243500
H	-1.34718200	3.77934400	2.29109500
H	-3.07013700	-0.48279900	-0.62100200
H	-5.08513500	1.17056100	0.29527400
H	-3.68138700	3.18749600	1.60532800
H	0.61512400	3.42843900	3.81067800
H	2.65297300	1.59040700	4.27671200
H	2.38931900	-0.16880000	2.15751300
B	-0.87508100	3.02510100	1.44025300
C	-2.99108800	0.44418000	-0.06054700
C	-4.00947400	1.28731800	0.41603800
C	-3.32698600	2.30202300	1.08109700
C	0.92168700	2.55142400	3.24380900
C	1.93844700	1.62397800	3.45595500
C	1.81926500	0.73015700	2.37810400
N	-1.78887000	0.92059700	0.29207100
N	0.81260900	1.10363200	1.57477600
N	-2.00198300	2.05873900	0.98801000
N	0.26541700	2.21607000	2.11229900
H	0.48644500	-3.67495300	-0.06793400
H	1.68469700	-4.01920500	1.53604600
H	2.92046000	0.58938000	-1.08073900
H	5.04589200	-1.14308000	-0.74244600
H	3.86977900	-3.32221100	0.53149100
H	0.02271600	-3.87938600	3.40675300
H	-1.88226700	-2.13532300	4.44492400
H	-1.97446900	-0.12570700	2.54552900
B	1.07967700	-3.17073400	0.88049500
C	2.93002700	-0.40092400	-0.63484100
C	4.00651400	-1.28561200	-0.45151400

C	3.43921400	-2.38241900	0.19107000
C	-0.36877900	-2.94261300	3.01476000
C	-1.32269000	-2.05962700	3.51408800
C	-1.38419900	-1.03856000	2.55048900
N	1.80244100	-0.93055200	-0.14018100
N	-0.53770600	-1.29914600	1.54365100
N	2.12103800	-2.14385300	0.36127100
N	0.08301800	-2.46322300	1.83599000
Fe	0.00674100	-0.00502100	0.07644600
H	1.49972500	2.65228000	-0.28754700
H	2.11330100	4.09237800	-2.23349000
H	1.37915900	3.33836100	-4.56358000
H	0.10971000	1.22333500	-4.79002800
H	-0.95470800	-0.62328500	-4.81183800
H	-2.18880600	-2.76350200	-4.63128200
H	-2.51474800	-3.80772200	-2.32040800
H	-1.55614400	-2.61293200	-0.34795700
C	1.20088300	2.37268200	-1.29940100
C	1.55097400	3.16863600	-2.38662100
C	1.13687800	2.74302700	-3.67641500
C	0.42810900	1.56853300	-3.80365100
C	0.11242200	0.78717900	-2.65212100
C	-0.58064200	-0.45499500	-2.66879400
C	-1.10043500	-1.09125200	-3.83549100
C	-1.78927400	-2.27994200	-3.73310000
C	-1.97740800	-2.86618900	-2.45360500
C	-1.43477700	-2.20712700	-1.35390100
N	0.50998500	1.23430500	-1.39873500
N	-0.75912000	-1.05789400	-1.43032800

3) Neutral HS configuration for $N_c = 2$, $\text{Charge} = 0$, $S = 2$

H	-0.49934500	3.48736400	0.10025900
H	-1.35090100	4.12043900	1.83875100
H	-3.26544900	-0.63236100	-0.01936300
H	-5.20462300	1.07181500	0.97380300
H	-3.73353400	3.30105700	1.74323200
H	0.34752600	3.81610100	3.67509500
H	2.37344800	2.08448400	4.45978500
H	2.37894100	0.18459800	2.43953000
B	-0.93283900	3.16183300	1.20082100
C	-3.15394600	0.37398600	0.38090900
C	-4.13214700	1.23911200	0.89432600
C	-3.41040000	2.36625600	1.28900200
C	0.72626000	2.91398000	3.19809600
C	1.74315400	2.03468400	3.57400600
C	1.75812300	1.07208500	2.55453000
N	-1.94089400	0.94077900	0.45493200
N	0.82569600	1.35993900	1.63252500
N	-2.10789800	2.16025400	1.01259300
N	0.19384200	2.48760200	2.03688000
H	0.47314900	-3.46714000	-0.38400100
H	1.62692100	-4.27974500	1.08446100
H	3.20878300	0.67085000	-0.55723300
H	5.28210600	-1.11070300	-0.13438900
H	3.95778200	-3.42757300	0.64263500
H	0.29914100	-4.20425400	3.22408700
H	-1.52616500	-2.59281700	4.56206500

H	-1.88410400	-0.47594800	2.80652800
B	1.10674200	-3.26096900	0.64610900
C	3.16380300	-0.37475400	-0.25709500
C	4.21190600	-1.28021700	-0.03218800
C	3.56503500	-2.45204800	0.36212300
C	-0.15114700	-3.25762800	2.93094800
C	-1.07052500	-2.43666800	3.58617500
C	-1.26309700	-1.36472500	2.70299600
N	1.98009800	-0.95983400	-0.02321500
N	-0.52116400	-1.53698100	1.59744300
N	2.23584700	-2.23143400	0.35571600
N	0.16168100	-2.69699600	1.74707300
Fe	0.01596300	-0.00762000	0.18122300
H	1.58148500	2.62211500	-0.52993600
H	2.23543300	3.99453100	-2.53871900
H	1.46346800	3.21405100	-4.81513800
H	0.10839600	1.13435200	-4.97767400
H	-1.03139300	-0.59773900	-4.96489600
H	-2.35491800	-2.69573100	-4.77810800
H	-2.70842400	-3.71794200	-2.49398700
H	-1.68679300	-2.55804800	-0.50470200
C	1.27897800	2.33309200	-1.53880800
C	1.63841300	3.08751200	-2.65750300
C	1.20901800	2.65290700	-3.91150200
C	0.44759100	1.48708200	-4.00324400
C	0.13351400	0.78360000	-2.83230300
C	-0.66321900	-0.47439300	-2.82586100
C	-1.19155900	-1.05398800	-3.98756600
C	-1.93514000	-2.23010800	-3.88191500
C	-2.13398000	-2.79789600	-2.62341500
C	-1.56978800	-2.16184900	-1.51575300
N	0.55018800	1.22059800	-1.63138900
N	-0.85903800	-1.03894500	-1.62180200

4) Reduced HS configuration for $N_{\mathrm{c}} = 2$, $\mathrm{Charge} = -1$, $S = 3/2$

H	-0.49739600	3.55860200	0.38279700
H	-1.37005300	3.95180000	2.18914000
H	-3.25947800	-0.48920100	-0.33565500
H	-5.22886600	1.10769400	0.79984700
H	-3.75963900	3.19862000	1.90093500
H	0.25900400	3.37525400	3.99849700
H	2.31101400	1.58162200	4.55897100
H	2.39750300	0.01698000	2.26988000
B	-0.94270000	3.08786900	1.42371100
C	-3.16128200	0.45124700	0.20457300
C	-4.15110000	1.26315700	0.78783000
C	-3.43269200	2.31893700	1.34906600
C	0.67154800	2.56439500	3.40059100
C	1.70020500	1.65896600	3.66086500
C	1.75807400	0.86689800	2.50180900
N	-1.94924400	0.98210600	0.40134700
N	0.84034900	1.27309400	1.61444200
N	-2.12106300	2.12368000	1.09816100
N	0.17706300	2.30999200	2.17209400
H	0.53490300	-3.57292200	-0.11233100
H	1.72083000	-4.15177000	1.44902800
H	3.14932700	0.56281500	-0.87476900

H	5.28138300	-1.12307700	-0.30062600
H	4.02318200	-3.34024000	0.81482800
H	0.45614000	-3.79872900	3.57860100
H	-1.44639700	-2.10590200	4.69952700
H	-1.94004800	-0.30027300	2.65206800
B	1.16710700	-3.21427400	0.87511300
C	3.14468700	-0.43223200	-0.43230400
C	4.21852400	-1.29010900	-0.13233600
C	3.60724100	-2.40987000	0.43181900
C	-0.05345800	-2.93276000	3.15957200
C	-1.01092500	-2.07561700	3.70197400
C	-1.27461200	-1.16164600	2.66789200
N	1.98529200	-0.99687100	-0.07660200
N	-0.53755300	-1.45505900	1.58840500
N	2.27332100	-2.20527000	0.44782000
N	0.20946200	-2.53799400	1.89722700
Fe	0.00073600	0.00101700	-0.01620100
H	1.53921500	2.65485200	-0.62206500
H	2.19367900	4.02997000	-2.61200100
H	1.43375100	3.23314700	-4.91808700
H	0.09905100	1.15701500	-5.08762500
H	-1.06889600	-0.59582000	-5.07247600
H	-2.36898800	-2.69185300	-4.88050900
H	-2.68533500	-3.74407900	-2.57336000
H	-1.65043900	-2.58772400	-0.60555000
C	1.24633000	2.35485500	-1.63366300
C	1.60881900	3.11548100	-2.73682400
C	1.17850800	2.66785800	-4.01534800
C	0.43301100	1.51141900	-4.10966600
C	0.10105800	0.77059000	-2.93977200
C	-0.65840600	-0.44692900	-2.93419900
C	-1.21449200	-1.05864800	-4.09363700
C	-1.94072700	-2.22617300	-3.98642800
C	-2.12498000	-2.81548600	-2.70623300
C	-1.55142800	-2.17644100	-1.61554700
N	0.52864900	1.22725800	-1.70723800
N	-0.84876800	-1.04021700	-1.70042400

5) Neutral LS configuration for $N_{\mathrm{c}} = 3,\ \mathrm{Charge} = 0,\ S = 0$

H	3.51760600	0.88438100	-0.17076500
H	3.99370100	1.99521900	1.45349800
H	-1.05288300	2.94937000	-0.35238000
H	0.47892400	5.20866200	-0.00499400
H	2.92983200	4.18148400	0.81754600
H	4.19791300	0.25037300	3.25867300
H	2.71123500	-1.79347400	4.41563200
H	0.51362200	-1.98124900	2.75007900
B	3.11231800	1.36247100	0.88520200
C	-0.01019900	3.02118600	-0.05711900
C	0.77146100	4.16981600	0.13326900
C	2.00404700	3.67519800	0.55211200
C	3.25313700	-0.19549000	2.95422100
C	2.49500300	-1.21905600	3.51716700
C	1.37987500	-1.32876400	2.67265100
N	0.70289800	1.91811200	0.22117900
N	1.47244100	-0.44348400	1.66840600
N	1.93482600	2.32914000	0.59373900

N	2.61978500	0.25204300	1.84958500
H	-3.47795100	-0.87440700	0.60520100
H	-3.60598900	-1.87141000	2.36264400
H	0.97824300	-2.97621100	-0.35770500
H	-0.43542100	-5.19750600	0.44197000
H	-2.67787700	-4.10199800	1.67072200
H	-3.45380400	-0.00782900	4.05017300
H	-1.77925300	2.09995300	4.74240500
H	0.03471500	2.16126000	2.65788300
B	-2.86309600	-1.28366000	1.58623300
C	0.01686200	-3.02159900	0.14550400
C	-0.70182100	-4.14989700	0.56623800
C	-1.82840300	-3.62051600	1.19069400
C	-2.59345500	0.41055400	3.53167300
C	-1.74482900	1.46494300	3.85949700
C	-0.82435800	1.51047500	2.80145800
N	-0.63382500	-1.89787900	0.48693200
N	-1.11149700	0.56014000	1.89855500
N	-1.76228500	-2.27516500	1.12696300
N	-2.19320800	-0.11442200	2.35445500
Fe	0.03341100	0.00982600	0.34604200
H	2.81382600	-1.23764700	-0.36648300
H	3.92875700	-1.84827400	-2.52321400
H	2.70588200	-1.47310700	-4.68909300
H	0.55099600	-0.66183700	-5.83971900
H	-1.72484400	0.28980600	-5.63831500
H	-3.60920700	1.18553800	-4.13083900
H	-4.37349800	1.70386100	-1.79109400
H	-2.84307200	1.22382700	0.13104000
C	2.31195500	-1.06940800	-1.31861000
C	2.92388700	-1.42023100	-2.53805300
C	2.24975300	-1.21324800	-3.72939300
C	0.94732400	-0.66381700	-3.69462100
C	0.41731600	-0.34727400	-2.42071900
C	0.13770100	-0.41861300	-4.85678400
C	-2.54222500	0.99237500	-0.89005700
C	-3.38944200	1.26936000	-1.98095300
C	-2.96758800	0.98361600	-3.26819400
C	-1.68131900	0.42914900	-3.46180600
C	-0.90367100	0.19013100	-2.30332300
C	-1.12062800	0.10618300	-4.74537800
N	1.09638800	-0.53527400	-1.25930800
N	-1.33608800	0.45548600	-1.04316500

6) Reduced LS configuration for $N_{\mathrm{c}} = 3,\ \mathrm{Charge} = -1,\ S = 1/2$

H	3.59412500	0.93484200	0.00788000
H	3.90954000	2.06082800	1.66880200
H	-0.98513600	2.89790000	-0.55741300
H	0.50488800	5.19287500	-0.16984300
H	2.89214500	4.21006300	0.87361900
H	4.08765900	0.27718300	3.42281700
H	2.63532700	-1.86981100	4.43719600
H	0.52182100	-2.07428500	2.66224600
B	3.09227700	1.40274200	1.02504100
C	0.02654600	2.99956200	-0.17555900
C	0.78897400	4.16162800	0.03273800
C	1.98796400	3.69118600	0.56105100

C	3.17433400	-0.19327500	3.06369300
C	2.43578400	-1.26801900	3.55213900
C	1.36366900	-1.38647000	2.65134100
N	0.71965200	1.91502100	0.19833100
N	1.46220600	-0.45813400	1.68878800
N	1.91922000	2.34527300	0.64599300
N	2.56945300	0.27102100	1.94921800
H	-3.51541700	-0.90843500	0.79613400
H	-3.48069900	-1.92019700	2.55695000
H	0.86737700	-2.93577700	-0.55390100
H	-0.49927700	-5.18983500	0.27633700
H	-2.63175400	-4.12378000	1.71499300
H	-3.31265300	-0.02366600	4.18921700
H	-1.69755200	2.17367200	4.74688400
H	0.01275200	2.24573300	2.57225500
B	-2.81493300	-1.31149100	1.71929500
C	-0.04537200	-3.00508000	0.03068600
C	-0.74272200	-4.14553700	0.46446100
C	-1.81274400	-3.63296600	1.19268900
C	-2.49351200	0.41550400	3.62300100
C	-1.67754100	1.51402800	3.88099400
C	-0.81029000	1.56541300	2.77640200
N	-0.65495500	-1.89349300	0.46561000
N	-1.09613000	0.57723700	1.91625700
N	-1.73646700	-2.28490600	1.17388500
N	-2.12368800	-0.12493600	2.44204600
Fe	0.03269000	0.01067500	0.33397700
H	2.84534100	-1.21467900	-0.40192500
H	3.94595500	-1.84995900	-2.54432300
H	2.69014400	-1.48264600	-4.73176300
H	0.54260400	-0.66877300	-5.87134300
H	-1.72568000	0.28277500	-5.67119400
H	-3.60398200	1.18464100	-4.17732300
H	-4.39425700	1.70372800	-1.81028100
H	-2.87926100	1.20370700	0.10257500
C	2.33004600	-1.06216800	-1.35253600
C	2.93946300	-1.42505100	-2.55682400
C	2.24040000	-1.21830000	-3.76868100
C	0.95695600	-0.67332800	-3.72727300
C	0.40118800	-0.34054100	-2.44685900
C	0.13317700	-0.42407400	-4.88474200
C	-2.56558200	0.98534500	-0.92038500
C	-3.40819900	1.27220100	-1.99790600
C	-2.96709500	0.98135800	-3.30972600
C	-1.69811300	0.43167400	-3.49271500
C	-0.89280500	0.18035800	-2.33194300
C	-1.12362000	0.10100300	-4.77376700
N	1.10881700	-0.53104000	-1.26932200
N	-1.34915300	0.45266700	-1.05084200

7) Neutral HS configuration for $N_{\mathrm{c}} = 3,\ \mathrm{Charge} = 0,\ S = 2$

H	3.41055800	0.86698600	-0.26672800
H	4.17259300	2.00245500	1.24168300
H	-0.99558000	3.14667300	-0.05640200
H	0.58454600	5.36849700	0.41913100
H	3.06336900	4.25162900	0.99540400
H	4.36878300	0.51955300	3.26583500

H	3.03738600	-1.55666800	4.54433700
H	0.85874200	-2.00588900	2.88767600
B	3.19221900	1.40492100	0.81436800
C	0.06384000	3.19581900	0.19022100
C	0.86796800	4.31793400	0.44146000
C	2.11961300	3.77564800	0.73586900
C	3.45512500	-0.00479900	2.99186200
C	2.77416400	-1.05028700	3.61770500
C	1.67242200	-1.28922400	2.78377300
N	0.77928600	2.06888200	0.31671000
N	1.69830300	-0.45495500	1.73247700
N	2.03673100	2.43343300	0.65131200
N	2.79119500	0.33286600	1.86970100
H	-3.39040200	-0.85985400	0.48582900
H	-3.82463400	-1.88905000	2.18797100
H	0.98204400	-3.15040900	-0.05024400
H	-0.45467400	-5.32581700	0.87846800
H	-2.77315600	-4.15716900	1.86991000
H	-3.61719000	-0.27576200	4.10881600
H	-2.06967100	1.87164900	4.95244900
H	-0.27437800	2.19727400	2.86352500
B	-2.95470300	-1.32737700	1.53335500
C	-0.00529500	-3.17620900	0.40811900
C	-0.73464900	-4.27414800	0.88919000
C	-1.90449000	-3.70543600	1.39457100
C	-2.78157300	0.22367100	3.62189800
C	-1.99565700	1.30378100	4.02702800
C	-1.08700300	1.48036200	2.97367700
N	-0.68782300	-2.03863800	0.60290500
N	-1.31895000	0.57897300	2.00643400
N	-1.84924400	-2.37217100	1.20778100
N	-2.35589700	-0.19121800	2.41329200
Fe	0.04396100	0.01451500	0.44278100
H	2.78320400	-1.36054600	-0.58542700
H	3.84798900	-2.04399600	-2.76436800
H	2.59771300	-1.62365400	-4.90505000
H	0.50532900	-0.72986100	-6.03469900
H	-1.72418400	0.33168100	-5.84203400
H	-3.55070000	1.31251800	-4.37396000
H	-4.34462800	1.88217200	-2.05716400
H	-2.85604300	1.33767900	-0.09848300
C	2.27195100	-1.19701100	-1.53710400
C	2.86005000	-1.57777300	-2.76139900
C	2.17047600	-1.34448200	-3.93713200
C	0.89344200	-0.73652100	-3.88840700
C	0.38895000	-0.39430300	-2.60705100
C	0.10144900	-0.46021400	-5.05468600
C	-2.54688400	1.10809600	-1.12100700
C	-3.37331100	1.41067000	-2.22337700
C	-2.93441700	1.09533900	-3.49625600
C	-1.66976900	0.48344800	-3.66688900
C	-0.91397000	0.22367300	-2.49437500
C	-1.12842300	0.12496600	-4.94839300
N	1.08061600	-0.62588000	-1.47048400
N	-1.36281500	0.53474900	-1.25924800

8) Reduced HS configuration for $N_c = 3,\ \text{Charge} = -1,\ S = 3/2$

H	3.50287000	0.92090400	-0.02686500
H	4.06568300	2.05476700	1.57810200
H	-0.91925900	3.12849700	-0.33635700
H	0.57739500	5.38470000	0.28932700
H	2.98274800	4.29659500	1.16813300
H	4.00158000	0.61016000	3.61984200
H	2.58545300	-1.52452700	4.70550900
H	0.68548100	-2.05333300	2.75330600
B	3.15118700	1.44492600	1.02443700
C	0.09952600	3.20053600	0.04169900
C	0.86264000	4.33663100	0.36710700
C	2.07523300	3.81091400	0.81342700
C	3.15862300	0.04692300	3.22313900
C	2.43895900	-1.02636900	3.74839900
C	1.47879000	-1.30780500	2.76184300
N	0.80250200	2.08647200	0.27409600
N	1.61961700	-0.47258600	1.72418400
N	2.00889400	2.46480700	0.74269100
N	2.64698900	0.35574800	2.01423700
H	-3.43499100	-0.88535300	0.74675300
H	-3.65517900	-1.91329600	2.49988700
H	0.84117100	-3.14561000	-0.31656800
H	-0.48929000	-5.34664300	0.73608300
H	-2.67060300	-4.18611600	2.01561700
H	-3.17695000	-0.34922100	4.39411900
H	-1.57650400	1.83523400	5.03299200
H	-0.12145800	2.22878800	2.70324300
B	-2.87485900	-1.34696300	1.73498200
C	-0.07946700	-3.18579600	0.26380300
C	-0.75668600	-4.29331400	0.80579700
C	-1.85561400	-3.73086500	1.45541300
C	-2.43626100	0.18199600	3.79883400
C	-1.62829600	1.27893400	4.09836300
C	-0.89306200	1.49200300	2.92004300
N	-0.72497700	-2.05357700	0.56507700
N	-1.24124400	0.59688500	1.98636800
N	-1.80991100	-2.39217400	1.29048800
N	-2.18333800	-0.20360900	2.53159900
Fe	0.02255000	0.01041400	0.24694000
H	2.79537700	-1.33336500	-0.67670200
H	3.85043000	-2.04016700	-2.83018500
H	2.58620200	-1.63874600	-5.00273500
H	0.49342300	-0.74097400	-6.13346500
H	-1.72819700	0.32490300	-5.94411400
H	-3.55658400	1.31300600	-4.47963200
H	-4.36006000	1.87195400	-2.12976600
H	-2.88776800	1.30871500	-0.18967200
C	2.27413200	-1.18640800	-1.62833100
C	2.85969800	-1.57857500	-2.83278900
C	2.15724700	-1.35222400	-4.03664000
C	0.89677600	-0.75006400	-3.98824300
C	0.36420600	-0.38903700	-2.70672000
C	0.09266400	-0.46924900	-5.15050500
C	-2.56747300	1.09336900	-1.21435900
C	-3.38663800	1.40499300	-2.30013500
C	-2.93953000	1.09130200	-3.60241500
C	-1.69070600	0.48554400	-3.76751600
C	-0.90806000	0.21065600	-2.59786500

C	-1.13544900	0.11919000	-5.04579000
N	1.07057700	-0.61328900	-1.54018900
N	-1.36630600	0.51997800	-1.33116600

9) Neutral LS configuration for $N_c = 4$, Charge $= 0$, $S = 0$

H	0.83200	−3.62400	−0.23700
H	2.53500	−4.09900	−1.22400
H	0.20400	0.45100	−3.09500
H	0.79300	−1.40900	−5.03500
H	1.85400	−3.52300	−3.57200
H	4.29300	−3.78200	0.55200
H	5.20200	−1.84000	2.32000
H	3.29600	0.14800	2.09100
B	1.85200	−3.19100	−0.76700
C	0.61800	−0.54500	−2.97400
C	0.93100	−1.49200	−3.95900
C	1.47100	−2.55900	−3.24500
C	3.86900	−2.81600	0.81900
C	4.30600	−1.83200	1.70200
C	3.33900	−0.82100	1.60000
N	0.94100	−1.01200	−1.75700
N	2.38400	−1.18100	0.72800
N	1.46300	−2.24600	−1.93400
N	2.71800	−2.40200	0.24900
H	0.83200	3.62400	0.23700
H	2.53500	4.09900	1.22400
H	0.20400	−0.45100	3.09500
H	0.79200	1.40900	5.03500
H	1.85400	3.52300	3.57200
H	4.29300	3.78200	−0.55200
H	5.20200	1.84000	−2.32000
H	3.29600	−0.14800	−2.09100
B	1.85200	3.19100	0.76700
C	0.61800	0.54600	2.97300
C	0.93100	1.49200	3.95900
C	1.47100	2.55900	3.24500
C	3.86900	2.81600	−0.81900
C	4.30600	1.83200	−1.70200
C	3.33900	0.82100	−1.60000
N	0.94100	1.01200	1.75700
N	2.38500	1.18100	−0.72800
N	1.46300	2.24600	1.93400
N	2.71800	2.40200	−0.24900
Fe	0.93200	−0.00000	−0.00000
H	0.50300	−2.54400	1.70700
H	−1.53300	−3.77600	2.50100
H	−3.78800	−2.91400	1.90700
H	−3.78800	2.91400	−1.90700
H	−1.53300	3.77600	−2.50100
H	0.50300	2.54400	−1.70700
C	−0.49700	−2.20100	1.44800
C	−1.64300	−2.87300	1.89600
C	−2.89800	−2.38700	1.56100
C	−3.00800	−1.21300	0.78500
C	−1.79700	−0.60900	0.38700
C	−4.27600	−0.59900	0.38700
C	−0.49700	2.20100	−1.44800

C	−1.64300	2.87300	−1.89600
C	−2.89800	2.38700	−1.56100
C	−3.00800	1.21300	−0.78500
C	−1.79700	0.60900	−0.38700
C	−4.27600	0.59800	−0.38800
N	−0.57300	−1.10200	0.70100
N	−0.57300	1.10200	−0.70100
C	−5.51400	1.16800	−0.75600
H	−5.53600	2.08400	−1.34700
C	−5.51400	−1.16800	0.75500
H	−5.53500	−2.08400	1.34700
C	−6.71800	0.58900	−0.38100
H	−7.66200	1.05300	−0.68000
C	−6.71800	−0.58900	0.38100
H	−7.66200	−1.05300	0.68000

10) Reduced LS configuration for $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = -1$, $S = 1/2$

H	−1.00700	−3.69400	0.05200
H	−2.72600	−4.08200	1.06000
H	−0.02300	0.20000	3.05400
H	−0.63700	−1.73900	4.92300
H	−1.89700	−3.69500	3.39400
H	−4.43400	−3.64000	−0.72200
H	−5.22100	−1.62100	−2.46900
H	−3.22600	0.27200	−2.15800
B	−1.98000	−3.20800	0.62000
C	−0.51300	−0.75800	2.90800
C	−0.83700	−1.74600	3.85300
C	−1.47400	−2.73400	3.10700
C	−3.96500	−2.68700	−0.96100
C	−4.33900	−1.66800	−1.83300
C	−3.32600	−0.70400	−1.68900
N	−0.92500	−1.12900	1.68700
N	−2.40900	−1.12400	−0.80600
N	−1.51000	−2.33900	1.81600
N	−2.80800	−2.33500	−0.36100
H	−1.01000	3.69400	−0.05200
H	−2.73100	4.08100	−1.05900
H	−0.02600	−0.19900	−3.05500
H	−0.64600	1.73900	−4.92400
H	−1.90500	3.69400	−3.39300
H	−4.43600	3.63700	0.72600
H	−5.21900	1.61800	2.47500
H	−3.22300	−0.27300	2.16100
B	−1.98400	3.20700	−0.61900
C	−0.51700	0.75900	−2.90900
C	−0.84400	1.74600	−3.85400
C	−1.48100	2.73300	−3.10700
C	−3.96600	2.68500	0.96500
C	−4.33800	1.66500	1.83700
C	−3.32400	0.70200	1.69200
N	−0.92800	1.12900	−1.68700
N	−2.40900	1.12200	0.80700
N	−1.51400	2.33900	−1.81600
N	−2.81000	2.33400	0.36300
Fe	−0.92700	0.00000	−0.00000
H	−0.47800	−2.47600	−1.84000

H	1.55000	−3.64000	−2.72300
H	3.82500	−2.78600	−2.07800
H	3.82400	2.78800	2.07500
H	1.55000	3.64300	2.71900
H	−0.47800	2.47700	1.83800
C	0.52300	−2.13200	−1.57100
C	1.65700	−2.77200	−2.06900
C	2.93100	−2.28500	−1.69800
C	3.03400	−1.17600	−0.86300
C	1.81800	−0.57100	−0.40800
C	4.30000	−0.57500	−0.42300
C	0.52200	2.13300	1.56800
C	1.65700	2.77500	2.06600
C	2.93100	2.28700	1.69600
C	3.03400	1.17700	0.86200
C	1.81800	0.57200	0.40700
C	4.30000	0.57700	0.42200
N	0.57400	−1.07300	−0.76400
N	0.57400	1.07400	0.76200
C	5.54400	1.11800	0.81800
H	5.55900	2.00000	1.46200
C	5.54400	−1.11700	−0.81900
H	5.55900	−1.99900	−1.46200
C	6.75200	0.56600	0.41400
H	7.69500	1.01500	0.74200
C	6.75200	−0.56600	−0.41400
H	7.69500	−1.01500	−0.74100

11) Neutral HS configuration for $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = 0$, $S = 2$

H	0.71700	−3.52800	0.04800
H	2.33100	−4.39100	−0.84300
H	0.54500	0.13300	−3.30100
H	1.25000	−1.90800	−5.03200
H	2.04200	−3.93600	−3.30500
H	4.32500	−3.96700	0.63500
H	5.39000	−2.01200	2.29600
H	3.49100	0.00700	2.16900
B	1.78600	−3.34200	−0.52400
C	0.90100	−0.87000	−3.07100
C	1.26900	−1.90500	−3.94400
C	1.67300	−2.93500	−3.09300
C	3.93800	−2.98700	0.90600
C	4.45500	−1.99400	1.74000
C	3.49800	−0.97000	1.68700
N	1.06500	−1.25100	−1.79600
N	2.48000	−1.32800	0.88900
N	1.53800	−2.51700	−1.81900
N	2.75900	−2.56400	0.41000
H	0.72400	3.52900	−0.04800
H	2.34100	4.38900	0.84100
H	0.54800	−0.13100	3.30200
H	1.26000	1.90800	5.03200
H	2.05400	3.93500	3.30400
H	4.33200	3.96200	−0.64000
H	5.39100	2.00400	−2.30200
H	3.48900	−0.01100	−2.17200
B	1.79300	3.34100	0.52300

C	0.90600	0.87100	3.07200
C	1.27700	1.90600	3.94400
C	1.68200	2.93400	3.09200
C	3.94200	2.98200	−0.91000
C	4.45600	1.98800	−1.74400
C	3.49800	0.96600	−1.69000
N	1.06900	1.25200	1.79600
N	2.48200	1.32600	−0.89000
N	1.54500	2.51600	1.81900
N	2.76400	2.56100	−0.41200
Fe	1.04000	0.00000	0.00000
H	0.29700	−2.34400	2.02100
H	−1.76700	−3.44500	2.97600
H	−4.00000	−2.62700	2.26500
H	−4.00000	2.62900	−2.26300
H	−1.76600	3.44700	−2.97400
H	0.29700	2.34700	−2.01800
C	−0.70600	−2.01700	1.73800
C	−1.85900	−2.62100	2.26500
C	−3.10100	−2.15900	1.86200
C	−3.19800	−1.09300	0.94000
C	−1.97800	−0.55300	0.47400
C	−4.46700	−0.54000	0.46400
C	−0.70600	2.01900	−1.73600
C	−1.85800	2.62300	−2.26300
C	−3.10000	2.16100	−1.86000
C	−3.19800	1.09500	−0.93800
C	−1.97700	0.55500	−0.47200
C	−4.46700	0.54200	−0.46300
N	−0.77600	−1.01800	0.87100
N	−0.77500	1.02000	−0.86900
C	−5.70600	1.05700	−0.90400
H	−5.72900	1.88600	−1.61300
C	−5.70600	−1.05500	0.90500
H	−5.72900	−1.88400	1.61400
C	−6.90900	0.53400	−0.45600
H	−7.85300	0.95400	−0.81500
C	−6.91000	−0.53200	0.45700
H	−7.85400	−0.95200	0.81500

12) Reduced HS configuration for $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = -1$, $S = 3/2$

H	1.00300	3.43300	−1.10800
H	2.69300	4.34400	−0.40700
H	0.30300	0.94900	3.11900
H	1.14400	3.35000	4.23400
H	2.23600	4.68700	2.05100
H	4.67300	3.29700	−1.52200
H	5.53500	0.85200	−2.53200
H	3.37400	−0.81400	−2.02500
B	2.02800	3.30900	−0.44600
C	0.78700	1.80100	2.64300
C	1.22200	3.01700	3.20000
C	1.77600	3.70300	2.11900
C	4.17100	2.33200	−1.55900
C	4.58300	1.09800	−2.06400
C	3.49100	0.24900	−1.82000
N	1.05900	1.76500	1.33400

N	2.50000	0.92500	−1.22300
N	1.66000	2.93000	1.01900
N	2.92400	2.19800	−1.06400
H	1.00000	−3.43200	1.10800
H	2.68800	−4.34500	0.40600
H	0.30000	−0.94800	−3.11900
H	1.13800	−3.35000	−4.23400
H	2.23000	−4.68800	−2.05200
H	4.67000	−3.30100	1.52100
H	5.53500	−0.85700	2.53000
H	3.37600	0.81200	2.02400
B	2.02400	−3.31000	0.44600
C	0.78300	−1.80000	−2.64300
C	1.21700	−3.01700	−3.20000
C	1.77100	−3.70300	−2.11900
C	4.16900	−2.33500	1.55800
C	4.58300	−1.10200	2.06200
C	3.49100	−0.25100	1.81800
N	1.05600	−1.76500	−1.33400
N	2.49900	−0.92600	1.22200
N	1.65600	−2.93000	−1.01900
N	2.92200	−2.20000	1.06300
Fe	0.88400	0.00000	0.00000
H	0.23600	1.67400	−2.61500
H	−1.80700	2.41900	−3.86400
H	−4.07000	1.83000	−2.94700
H	−4.07000	−1.82900	2.94800
H	−1.80700	−2.41700	3.86500
H	0.23600	−1.67200	2.61600
C	−0.76700	1.42700	−2.25300
C	−1.90300	1.83900	−2.94200
C	−3.17200	1.50500	−2.41700
C	−3.26400	0.77200	−1.23400
C	−2.04500	0.38000	−0.59800
C	−4.53100	0.37800	−0.60500
C	−0.76700	−1.42500	2.25400
C	−1.90300	−1.83700	2.94400
C	−3.17200	−1.50400	2.41800
C	−3.26400	−0.77100	1.23500
C	−2.04500	−0.37800	0.59900
C	−4.53100	−0.37700	0.60500
N	−0.81300	0.72000	−1.12100
N	−0.81300	−0.71800	1.12200
C	−5.77400	−0.73300	1.17600
H	−5.79000	−1.31100	2.10200
C	−5.77400	0.73400	−1.17600
H	−5.79000	1.31200	−2.10200
C	−6.98100	−0.37100	0.59600
H	−7.92500	−0.66500	1.06600
C	−6.98100	0.37200	−0.59600
H	−7.92500	0.66500	−1.06600

13) Neutral LS configuration for $N_{\mathrm{c}} = 5,\ \mathrm{Charge} = 0,\ S = 0$

H	−1.52500	−3.56800	0.66500
H	−3.22700	−3.92600	1.70300
H	−0.90000	0.81600	3.02000
H	−1.48700	−0.80000	5.16800

H	−2.54700	−3.07400	3.96600
H	−4.98800	−3.82100	−0.09500
H	−5.90000	−2.10200	−2.08000
H	−3.99400	−0.10100	−2.09100
B	−2.54500	−3.07700	1.14100
C	−1.31300	−0.18800	3.01800
C	−1.62500	−1.01100	4.10900
C	−2.16400	−2.15600	3.52700
C	−4.56500	−2.89300	−0.47500
C	−5.00300	−2.02100	−1.46900
C	−4.03600	−1.00500	−1.48900
N	−1.63600	−0.79600	1.86500
N	−3.08000	−1.25900	−0.58200
N	−2.15600	−2.00000	2.18700
N	−3.41300	−2.41500	0.04000
H	−1.52500	3.56800	−0.66500
H	−3.22700	3.92600	−1.70300
H	−0.89900	−0.81600	−3.02000
H	−1.48700	0.80000	−5.16800
H	−2.54700	3.07400	−3.96600
H	−4.98800	3.82100	0.09500
H	−5.90000	2.10200	2.08000
H	−3.99400	0.10100	2.09100
B	−2.54500	3.07800	−1.14100
C	−1.31300	0.18800	−3.01800
C	−1.62500	1.01100	−4.10900
C	−2.16400	2.15600	−3.52700
C	−4.56500	2.89300	0.47500
C	−5.00300	2.02100	1.46800
C	−4.03600	1.00500	1.48900
N	−1.63500	0.79600	−1.86500
N	−3.08000	1.25900	0.58200
N	−2.15600	2.00000	−2.18700
N	−3.41300	2.41500	−0.04000
Fe	−1.62700	0.00000	0.00000
H	−1.20400	−2.72400	−1.39400
H	0.82900	−4.04500	−2.04100
H	3.08700	−3.12100	−1.55500
H	3.08700	3.12100	1.55500
H	0.82900	4.04500	2.04200
H	−1.20400	2.72400	1.39400
C	−0.20200	−2.35600	−1.17900
C	0.94100	−3.07700	−1.54600
C	2.19700	−2.55600	−1.27200
C	2.31000	−1.30100	−0.64000
C	1.10300	−0.65200	−0.31300
C	3.58500	−0.64800	−0.31900
C	−0.20200	2.35600	1.17900
C	0.94100	3.07700	1.54600
C	2.19700	2.55600	1.27200
C	2.31000	1.30100	0.64000
C	1.10300	0.65200	0.31300
C	3.58500	0.64800	0.31900
N	−0.12200	−1.17600	−0.56500
N	−0.12200	1.17600	0.56500
C	4.80400	1.25000	0.61400
H	4.82800	2.23000	1.09400
C	4.80400	−1.25000	−0.61400

H	4.82800	−2.23000	−1.09400
C	6.04200	−0.64400	−0.31600
C	6.04200	0.64400	0.31600
C	8.47600	−0.63900	−0.31300
H	9.42800	−1.12200	−0.55000
H	7.28500	2.24600	1.10200
C	8.47600	0.63900	0.31300
H	9.42800	1.12200	0.55000
C	7.28900	1.26400	0.62000
C	7.28900	−1.26400	−0.62000
H	7.28600	−2.24600	−1.10200

14) Reduced LS configuration for $N_{\mathrm{c}} = 5,\ \mathrm{Charge} = -1,\ S = 1/2$

H	1.72600	−3.67100	−0.45500
H	3.44700	−3.93200	−1.50000
H	0.70900	0.52200	−3.01100
H	1.32600	−1.20000	−5.07900
H	2.60400	−3.30100	−3.77400
H	5.15100	−3.67700	0.32200
H	5.92100	−1.86100	2.28500
H	3.91500	0.04100	2.18400
B	2.69500	−3.11800	−0.96500
C	1.20500	−0.44300	−2.97000
C	1.53100	−1.32100	−4.01700
C	2.17700	−2.37900	−3.38400
C	4.67500	−2.76000	0.66500
C	5.04000	−1.84200	1.64600
C	4.02100	−0.87600	1.61000
N	1.62300	−0.94000	−1.79700
N	3.10700	−1.20100	0.68300
N	2.21600	−2.12600	−2.05800
N	3.51600	−2.35200	0.10500
H	1.72600	3.67100	0.45500
H	3.44700	3.93200	1.50000
H	0.70900	−0.52200	3.01100
H	1.32600	1.20000	5.07900
H	2.60400	3.30100	3.77400
H	5.15100	3.67700	−0.32200
H	5.92100	1.86100	−2.28500
H	3.91500	−0.04100	−2.18400
B	2.69500	3.11800	0.96500
C	1.20500	0.44300	2.97000
C	1.53100	1.32100	4.01700
C	2.17700	2.37900	3.38400
C	4.67500	2.76000	−0.66500
C	5.04000	1.84200	−1.64600
C	4.02100	0.87600	−1.61000
N	1.62300	0.94000	1.79700
N	3.10700	1.20100	−0.68300
N	2.21600	2.12600	2.05800
N	3.51600	2.35200	−0.10500
Fe	1.62700	−0.00000	0.00000
H	1.18500	−2.66400	1.53800
H	−0.85600	−3.93400	2.26700
H	−3.11400	−3.01200	1.72600
H	−3.11400	3.01200	−1.72600
H	−0.85600	3.93400	−2.26700

H	1.18500	2.66400	−1.53800
C	0.18600	−2.29300	1.30800
C	−0.96100	−2.99400	1.72100
C	−2.22000	−2.46900	1.41100
C	−2.33700	−1.26200	0.71100
C	−1.10900	−0.61500	0.33900
C	−3.61000	−0.63300	0.35400
C	0.18600	2.29300	−1.30800
C	−0.96100	2.99400	−1.72100
C	−2.22000	2.46900	−1.41100
C	−2.33700	1.26200	−0.71100
C	−1.10900	0.61500	−0.33900
C	−3.61000	0.63300	−0.35400
N	0.12600	−1.15300	0.63800
N	0.12600	1.15300	−0.63800
C	−4.83800	1.21500	−0.67700
H	−4.86200	2.16900	−1.20700
C	−4.83800	−1.21500	0.67700
H	−4.86200	−2.16900	1.20700
C	−6.08400	−0.62800	0.34900
C	−6.08400	0.62800	−0.34900
C	−8.53000	−0.61700	0.34300
H	−9.47900	−1.09400	0.60800
H	−7.32500	2.18300	−1.21300
C	−8.53000	0.61700	−0.34300
H	−9.47900	1.09400	−0.60800
C	−7.32900	1.22600	−0.68100
C	−7.32900	−1.22600	0.68100
H	−7.32500	−2.18300	1.21300

15) Neutral HS configuration for $N_{\mathrm{c}} = 5$, $\mathrm{Charge} = 0$, $S = 2$

H	1.43300	3.50600	0.39900
H	3.04900	4.24700	1.39200
H	1.25100	−0.54800	3.25900
H	1.96200	1.25500	5.23300
H	2.76100	3.48400	3.77700
H	5.04200	4.00900	−0.12800
H	6.10100	2.27800	−2.02600
H	4.19800	0.26500	−2.15600
B	2.50200	3.24700	0.94300
C	1.61000	0.47500	3.15700
C	1.98100	1.39100	4.15400
C	2.38800	2.51800	3.44000
C	4.65200	3.07200	−0.52100
C	5.16600	2.19200	−1.47500
C	4.20700	1.17200	−1.55300
N	1.77500	1.01400	1.94000
N	3.19100	1.42800	−0.71500
N	2.25200	2.26500	2.12300
N	3.47300	2.59200	−0.08200
H	1.43700	−3.50600	−0.40000
H	3.05500	−4.24600	−1.39100
H	1.25400	0.54700	−3.25900
H	1.96900	−1.25500	−5.23400
H	2.76800	−3.48300	−3.77600
H	5.04600	−4.00600	0.13100
H	6.10100	−2.27400	2.03100

H	4.19600	−0.26300	2.15900
B	2.50600	−3.24600	−0.94300
C	1.61400	−0.47500	−3.15700
C	1.98700	−1.39100	−4.15400
C	2.39400	−2.51800	−3.43900
C	4.65500	−3.06900	0.52400
C	5.16700	−2.18900	1.47900
C	4.20700	−1.17000	1.55600
N	1.77800	−1.01400	−1.94100
N	3.19100	−1.42700	0.71600
N	2.25700	−2.26500	−2.12300
N	3.47600	−2.59100	0.08400
Fe	1.74800	−0.00000	−0.00000
H	1.01200	2.57800	−1.70600
H	−1.04800	3.79300	−2.52100
H	−3.28400	2.89500	−1.92100
H	−3.28400	−2.89600	1.92000
H	−1.04800	−3.79400	2.51900
H	1.01200	−2.57900	1.70300
C	0.00800	2.22000	−1.47000
C	−1.14200	2.88700	−1.91800
C	−2.38600	2.37900	−1.57800
C	−2.48600	1.20700	−0.79800
C	−1.26900	0.61100	−0.40200
C	−3.76200	0.60200	−0.39700
C	0.00800	−2.22100	1.46800
C	−1.14200	−2.88800	1.91700
C	−2.38600	−2.38000	1.57600
C	−2.48600	−1.20800	0.79600
C	−1.26900	−0.61200	0.40000
C	−3.76200	−0.60300	0.39600
N	−0.06700	1.11900	−0.73500
N	−0.06700	−1.12000	0.73300
C	−4.98200	−1.16400	0.76500
H	−5.00800	−2.07500	1.36400
C	−4.98200	1.16300	−0.76600
H	−5.00800	2.07500	−1.36500
C	−6.21900	−0.60000	0.39400
C	−6.21900	0.59900	−0.39400
C	−8.65400	0.59400	−0.39100
H	−9.60500	1.04500	−0.68600
C	−8.65300	−0.59500	0.39100
H	−9.60500	−1.04500	0.68700
C	−7.46600	1.17600	−0.77300
C	−7.46600	−1.17700	0.77300
H	−7.46300	2.09100	−1.37400
H	−7.46300	−2.09100	1.37400

16) Reduced HS configuration for $N_{\mathrm{c}} = 5$, $\mathrm{Charge} = -1$, $S = 3/2$

H	1.71000	3.58500	−0.37400
H	3.39600	4.33700	0.50200
H	1.01900	0.27700	3.24600
H	1.86100	2.39400	4.83400
H	2.94700	4.15600	2.97600
H	5.37300	3.56300	−0.82700
H	6.24200	1.38700	−2.32600
H	4.10000	−0.36800	−2.15500

B	2.73600	3.33100	0.24800
C	1.50100	1.20900	2.95600
C	1.93600	2.28300	3.75300
C	2.48800	3.17900	2.83700
C	4.87700	2.62200	−1.05700
C	5.29300	1.52200	−1.80900
C	4.21000	0.63100	−1.73600
N	1.76900	1.44700	1.66700
N	3.22100	1.16000	−1.00500
N	2.37000	2.65300	1.60000
N	3.63700	2.37700	−0.58900
H	1.71100	−3.58600	0.37400
H	3.39800	−4.33700	−0.50200
H	1.01900	−0.27700	−3.24600
H	1.86100	−2.39400	−4.83300
H	2.94900	−4.15600	−2.97600
H	5.37400	−3.56200	0.82700
H	6.24200	−1.38600	2.32600
H	4.10000	0.36900	2.15500
B	2.73700	−3.33100	−0.24800
C	1.50100	−1.20900	−2.95600
C	1.93700	−2.28300	−3.75300
C	2.48900	−3.17900	−2.83700
C	4.87800	−2.62100	1.05800
C	5.29300	−1.52200	1.80900
C	4.21100	−0.63000	1.73600
N	1.76900	−1.44800	−1.66700
N	3.22100	−1.16000	1.00500
N	2.37100	−2.65300	−1.60000
N	3.63700	−2.37700	0.59000
Fe	1.62600	−0.00000	0.00000
H	0.95900	2.18800	−2.20100
H	−1.09700	3.19300	−3.25500
H	−3.34400	2.41900	−2.47900
H	−3.34400	−2.41900	2.47800
H	−1.09700	−3.19300	3.25500
H	0.95900	−2.18800	2.20100
C	−0.04300	1.87200	−1.89600
C	−1.18800	2.42900	−2.48000
C	−2.44400	1.98800	−2.03400
C	−2.54700	1.01600	−1.03600
C	−1.31800	0.49600	−0.50200
C	−3.82200	0.50700	−0.51700
C	−0.04300	−1.87300	1.89600
C	−1.18800	−2.42900	2.48000
C	−2.44400	−1.98800	2.03300
C	−2.54700	−1.01700	1.03600
C	−1.31800	−0.49700	0.50200
C	−3.82200	−0.50800	0.51700
N	−0.09300	0.94500	−0.95100
N	−0.09300	−0.94600	0.95100
C	−5.04900	−0.97400	0.99100
H	−5.07300	−1.74000	1.76900
C	−5.04900	0.97400	−0.99100
H	−5.07300	1.74000	−1.76900
C	−6.29200	−0.50300	0.51200
C	−6.29200	0.50300	−0.51200
C	−8.73500	0.49700	−0.50500

H	−9.68600	0.87800	−0.89200
C	−8.73500	−0.49700	0.50500
H	−9.68600	−0.87800	0.89200
C	−7.53900	0.98400	−1.00000
C	−7.53900	−0.98400	1.00000
H	−7.53400	1.75200	−1.78100
H	−7.53400	−1.75200	1.78100

17) Neutral LS configuration for $N_{\mathrm{c}} = 6,\ \mathrm{Charge} = 0,\ S = 0$

H	2.30300	−3.49500	−0.98400
H	4.00600	−3.75400	−2.04900
H	1.67200	1.08400	−2.93500
H	2.26300	−0.33100	−5.21900
H	3.32600	−2.70300	−4.22700
H	5.76600	−3.81100	−0.24800
H	6.67400	−2.27700	1.88500
H	4.76600	−0.28700	2.07500
B	3.32200	−2.96100	−1.41400
C	2.08700	0.08400	−3.02300
C	2.40100	−0.63700	−4.18400
C	2.94200	−1.82800	−3.70600
C	5.34100	−2.92200	0.21400
C	5.77800	−2.14200	1.28200
C	4.81000	−1.13300	1.39300
N	2.40900	−0.62500	−1.92900
N	3.85500	−1.30600	0.46700
N	2.93300	−1.79400	−2.35800
N	4.18900	−2.40000	−0.25600
H	2.30300	3.49500	0.98400
H	4.00600	3.75400	2.05000
H	1.67200	−1.08400	2.93500
H	2.26300	0.33100	5.21900
H	3.32600	2.70300	4.22700
H	5.76600	3.81100	0.24800
H	6.67400	2.27700	−1.88500
H	4.76600	0.28700	−2.07400
B	3.32200	2.96100	1.41400
C	2.08700	−0.08400	3.02300
C	2.40100	0.63700	4.18400
C	2.94200	1.82800	3.70600
C	5.34100	2.92200	−0.21400
C	5.77800	2.14200	−1.28200
C	4.81000	1.13300	−1.39300
N	2.40900	0.62500	1.92900
N	3.85500	1.30600	−0.46700
N	2.93200	1.79400	2.35800
N	4.18900	2.40000	0.25700
Fe	2.40000	0.00000	0.00000
H	1.98000	−2.83600	1.14300
H	−0.05100	−4.21100	1.67300
H	−2.31000	−3.25000	1.27200
H	−2.31000	3.25000	−1.27200
H	−0.05100	4.21100	−1.67300
H	1.98000	2.83600	−1.14300
C	0.97700	−2.45200	0.96300
C	−0.16400	−3.20400	1.26600
C	−1.42100	−2.66100	1.04000

C	−1.53600	−1.35500	0.52200
C	−0.33000	−0.67800	0.25400
C	−2.81400	−0.67800	0.26200
C	0.97700	2.45200	−0.96300
C	−0.16400	3.20400	−1.26600
C	−1.42100	2.66100	−1.04000
C	−1.53600	1.35500	−0.52200
C	−0.33000	0.67800	−0.25400
C	−2.81400	0.67800	−0.26200
N	0.89500	−1.22200	0.45700
N	0.89500	1.22200	−0.45700
C	−4.02500	1.30300	−0.50200
H	−4.05000	2.32100	−0.89400
C	−4.02500	−1.30300	0.50200
H	−4.05000	−2.32100	0.89400
C	−5.27300	−0.67400	0.25900
C	−5.27300	0.67400	−0.26000
C	−7.72200	−0.67600	0.26000
H	−6.49900	2.33500	−0.89900
C	−7.72200	0.67600	−0.26000
C	−6.50000	1.31400	−0.50600
C	−6.50000	−1.31400	0.50600
H	−6.49900	−2.33500	0.89900
C	−8.97900	1.31600	−0.50700
C	−8.97900	−1.31600	0.50700
C	−10.16100	0.66700	−0.25600
H	−11.11400	1.16800	−0.44900
C	−10.16100	−0.66700	0.25700
H	−11.11400	−1.16800	0.45000
H	−8.97700	2.33700	−0.90000
H	−8.97700	−2.33700	0.89900

18) Reduced LS configuration for $N_{\mathrm{c}} = 6,\ \mathrm{Charge} = -1,\ S = 1/2$

H	2.49900	−3.60100	−0.82700
H	4.22100	−3.75900	−1.89000
H	1.48900	0.82900	−2.94600
H	2.11100	−0.67200	−5.17500
H	3.38600	−2.89500	−4.09000
H	5.92700	−3.68800	−0.05200
H	6.69600	−2.07900	2.08400
H	4.69000	−0.17900	2.17800
B	3.47100	−3.00200	−1.27700
C	1.98400	−0.13600	−3.00000
C	2.31300	−0.90100	−4.13000
C	2.95900	−2.01800	−3.60800
C	5.45000	−2.81100	0.38100
C	5.81500	−1.99600	1.45100
C	4.79500	−1.03200	1.51300
N	2.40000	−0.75100	−1.88300
N	3.88200	−1.26200	0.55800
N	2.99400	−1.90300	−2.26300
N	4.29100	−2.34900	−0.13400
H	2.49900	3.60100	0.82700
H	4.22000	3.75900	1.89000
H	1.48900	−0.82900	2.94600
H	2.11100	0.67200	5.17500
H	3.38600	2.89500	4.09000

H	5.92700	3.68800	0.05200
H	6.69600	2.07900	−2.08400
H	4.69000	0.17900	−2.17800
B	3.47100	3.00200	1.27700
C	1.98400	0.13600	3.00000
C	2.31300	0.90100	4.13000
C	2.95900	2.01800	3.60800
C	5.45000	2.81100	−0.38100
C	5.81500	1.99600	−1.45000
C	4.79500	1.03200	−1.51300
N	2.40000	0.75100	1.88300
N	3.88200	1.26200	−0.55800
N	2.99400	1.90300	2.26300
N	4.29100	2.34900	0.13400
Fe	2.40400	0.00000	0.00000
H	1.97200	−2.80200	1.25300
H	−0.07600	−4.14200	1.83900
H	−2.32600	−3.17800	1.40200
H	−2.32600	3.17800	−1.40200
H	−0.07600	4.14200	−1.83900
H	1.97200	2.80200	−1.25300
C	0.97200	−2.41300	1.06300
C	−0.18100	−3.14900	1.39500
C	−1.43200	−2.60500	1.14700
C	−1.55500	−1.31900	0.57400
C	−0.32700	−0.65600	0.28000
C	−2.82400	−0.66500	0.29000
C	0.97200	2.41300	−1.06300
C	−0.18200	3.14900	−1.39500
C	−1.43200	2.60500	−1.14700
C	−1.55500	1.31900	−0.57400
C	−0.32700	0.65600	−0.28000
C	−2.82400	0.66500	−0.29000
N	0.89700	−1.20700	0.51600
N	0.89700	1.20700	−0.51600
C	−4.05200	1.27800	−0.55800
H	−4.07700	2.28000	−0.99300
C	−4.05200	−1.27800	0.55800
H	−4.07700	−2.28000	0.99300
C	−5.30400	−0.66500	0.29100
C	−5.30400	0.66500	−0.29100
C	−7.77200	−0.66300	0.29000
H	−6.53300	2.29100	−1.00100
C	−7.77200	0.66300	−0.29000
C	−6.53300	1.28700	−0.56200
C	−6.53300	−1.28700	0.56200
H	−6.53300	−2.29100	1.00100
C	−9.02300	1.28400	−0.56100
C	−9.02300	−1.28400	0.56100
C	−10.22300	0.64800	−0.28300
H	−11.17200	1.14800	−0.50200
C	−10.22300	−0.64800	0.28300
H	−11.17200	−1.14800	0.50200
H	−9.02000	2.28800	−1.00000
H	−9.02000	−2.28800	1.00000

19) Neutral HS configuration for $N_c = 6$, Charge $= 0$, $S = 2$

H	2.23100	3.45400	0.74100
H	3.85000	4.08600	1.80300
H	2.03200	−0.86200	3.18800
H	2.74400	0.73800	5.33100
H	3.55200	3.09600	4.10100
H	5.84300	3.99000	0.26700
H	6.89500	2.45200	−1.79400
H	4.98200	0.47000	−2.12200
B	3.29900	3.13800	1.25700
C	2.39500	0.16500	3.18800
C	2.76600	0.97800	4.27000
C	3.17700	2.16900	3.67000
C	5.44900	3.09900	−0.21700
C	5.95900	2.31600	−1.25400
C	4.99500	1.31300	−1.43200
N	2.56400	0.82000	2.03000
N	3.98000	1.48900	−0.57200
N	3.04400	2.04600	2.33500
N	4.26800	2.58300	0.17300
H	2.22800	−3.45300	−0.74000
H	3.84500	−4.08700	−1.80300
H	2.03100	0.86200	−3.18800
H	2.74000	−0.73800	−5.33100
H	3.54600	−3.09600	−4.10100
H	5.84100	−3.99200	−0.27100
H	6.89600	−2.45400	1.78800
H	4.98500	−0.47100	2.11900
B	3.29500	−3.13800	−1.25700
C	2.39200	−0.16500	−3.18800
C	2.76200	−0.97800	−4.27000
C	3.17300	−2.16900	−3.67000
C	5.44800	−3.10000	0.21400
C	5.96000	−2.31700	1.25000
C	4.99700	−1.31400	1.42900
N	2.56100	−0.82000	−2.03000
N	3.98000	−1.49000	0.57100
N	3.04000	−2.04600	−2.33500
N	4.26600	−2.58400	−0.17400
Fe	2.53500	−0.00000	0.00000
H	1.80200	2.73300	−1.44000
H	−0.25600	4.02600	−2.13100
H	−2.49300	3.07400	−1.62400
H	−2.49300	−3.07300	1.62600
H	−0.25600	−4.02400	2.13400
H	1.80200	−2.73200	1.44300
C	0.79700	2.35500	−1.24100
C	−0.35100	3.06400	−1.62200
C	−1.59600	2.52600	−1.33300
C	−1.69900	1.28300	−0.67300
C	−0.48300	0.64900	−0.33800
C	−2.97700	0.64300	−0.33600
C	0.79700	−2.35400	1.24300
C	−0.35100	−3.06300	1.62400
C	−1.59600	−2.52500	1.33500
C	−1.69900	−1.28200	0.67500
C	−0.48300	−0.64800	0.34000
C	−2.97700	−0.64200	0.33800
N	0.72000	1.18600	−0.61800

N	0.72000	−1.18500	0.62000
C	−4.18900	−1.23600	0.64700
H	−4.21600	−2.20400	1.15200
C	−4.18900	1.23700	−0.64600
H	−4.21600	2.20400	−1.15100
C	−5.43800	−0.64000	0.33400
C	−5.43800	0.64000	−0.33400
C	−7.88600	0.64300	−0.33500
C	−7.88600	−0.64200	0.33500
C	−6.66400	1.24800	−0.65100
C	−6.66400	−1.24800	0.65100
H	−6.66300	2.21800	−1.15700
H	−6.66300	−2.21800	1.15800
C	−9.14300	−1.25000	0.65200
C	−9.14300	1.25000	−0.65200
C	−10.32500	−0.63400	0.33000
H	−11.27800	−1.11000	0.57800
C	−10.32500	0.63300	−0.33100
H	−11.27800	1.10900	−0.57900
H	−9.14100	−2.22100	1.15800
H	−9.14100	2.22100	−1.15800

20) Reduced HS configuration for $N_c = 6,\ \text{Charge} = -1,\ S = 3/2$

H	2.48600	3.58000	0.36500
H	4.16600	4.14500	1.37900
H	1.81400	−0.40700	3.23100
H	2.66200	1.33600	5.21500
H	3.73600	3.44700	3.75800
H	6.13700	3.69200	−0.10300
H	7.01500	1.88300	−2.02400
H	4.89900	0.09800	−2.19800
B	3.51400	3.21000	0.92200
C	2.29200	0.56700	3.13600
C	2.73100	1.45200	4.13400
C	3.27700	2.52000	3.42200
C	5.65100	2.81000	−0.51600
C	6.07200	1.89400	−1.48100
C	5.00300	0.99000	−1.58300
N	2.55100	1.06900	1.92200
N	4.01500	1.34500	−0.74900
N	3.15200	2.26400	2.10300
N	4.42000	2.45700	−0.09600
H	2.47900	−3.57900	−0.36700
H	4.15700	−4.14700	−1.38200
H	1.81100	0.41000	−3.22900
H	2.65400	−1.33300	−5.21500
H	3.72700	−3.44700	−3.76000
H	6.13000	−3.69900	0.10000
H	7.01300	−1.89200	2.02000
H	4.90100	−0.10200	2.19600
B	3.50700	−3.21100	−0.92400
C	2.28700	−0.56500	−3.13500
C	2.72400	−1.45000	−4.13500
C	3.26900	−2.51900	−3.42300
C	5.64600	−2.81600	0.51300
C	6.06900	−1.90100	1.47800
C	5.00200	−0.99500	1.58100

N	2.54600	−1.06700	−1.92200
N	4.01300	−1.34700	0.74700
N	3.14600	−2.26300	−2.10500
N	4.41500	−2.46000	0.09300
Fe	2.45800	0.00100	0.00000
H	1.76500	2.59800	−1.69400
H	−0.30900	3.80500	−2.50400
H	−2.53800	2.88800	−1.90500
H	−2.53800	−2.88700	1.90700
H	−0.30900	−3.80300	2.50700
H	1.76500	−2.59600	1.69800
C	0.76300	2.22900	−1.46200
C	−0.39600	2.89400	−1.90600
C	−1.63600	2.37700	−1.56600
C	−1.74500	1.20100	−0.78700
C	−0.50900	0.60200	−0.39200
C	−3.01600	0.60600	−0.39700
C	0.76300	−2.22700	1.46500
C	−0.39600	−2.89200	1.90900
C	−1.63600	−2.37500	1.56800
C	−1.74500	−1.19900	0.79000
C	−0.50900	−0.60000	0.39500
C	−3.01600	−0.60500	0.39800
N	0.69600	1.12600	−0.73500
N	0.69600	−1.12400	0.73800
C	−4.24400	−1.16600	0.76400
H	−4.27100	−2.08000	1.36200
C	−4.24400	1.16700	−0.76300
H	−4.27100	2.08100	−1.36100
C	−5.49600	−0.60700	0.39800
C	−5.49600	0.60800	−0.39700
C	−7.96400	0.60500	−0.39600
C	−7.96400	−0.60500	0.39600
C	−6.72500	1.17500	−0.76800
C	−6.72500	−1.17500	0.76900
H	−6.72500	2.09300	−1.36800
H	−6.72500	−2.09200	1.36800
C	−9.21400	−1.17300	0.76600
C	−9.21400	1.17300	−0.76700
C	−10.41400	−0.59200	0.38700
H	−11.36400	−1.04900	0.68500
C	−10.41400	0.59200	−0.38700
H	−11.36400	1.04900	−0.68600
H	−9.21100	−2.09000	1.36600
H	−9.21100	2.09000	−1.36600

21) Neutral LS configuration for $N_{\mathrm{c}} = 7,\ \mathrm{Charge} = 0,\ S = 0$

H	3.15100	−3.43600	−1.18300
H	4.85500	−3.62600	−2.26100
H	2.49600	1.24300	−2.86700
H	3.09000	−0.03800	−5.22800
H	4.16700	−2.45700	−4.37400
H	6.61100	−3.78400	−0.46200
H	7.51000	−2.37700	1.76100
H	5.59700	−0.40600	2.06200
B	4.16800	−2.87400	−1.58000
C	2.91600	0.25200	−3.01200

C	3.23200	−0.40100	−4.21200
C	3.78000	−1.61400	−3.80400
C	6.18300	−2.92400	0.05100
C	6.61500	−2.20900	1.16500
C	5.64400	−1.21000	1.33200
N	3.24500	−0.51600	−1.96100
N	4.69200	−1.32900	0.39400
N	3.77300	−1.65600	−2.45600
N	5.03100	−2.37800	−0.39200
H	3.15100	3.43600	1.18300
H	4.85500	3.62600	2.26100
H	2.49600	−1.24300	2.86700
H	3.09000	0.03800	5.22800
H	4.16700	2.45700	4.37400
H	6.61100	3.78400	0.46200
H	7.51000	2.37700	−1.76100
H	5.59700	0.40600	−2.06200
B	4.16800	2.87400	1.58000
C	2.91600	−0.25200	3.01200
C	3.23200	0.40100	4.21200
C	3.78000	1.61400	3.80400
C	6.18300	2.92400	−0.05100
C	6.61500	2.20900	−1.16500
C	5.64400	1.21000	−1.33200
N	3.24500	0.51600	1.96100
N	4.69200	1.32900	−0.39400
N	3.77300	1.65600	2.45600
N	5.03100	2.37800	0.39200
Fe	3.23700	0.00000	0.00000
H	2.81900	−2.89700	0.97500
H	0.78800	−4.30300	1.42100
H	−1.47100	−3.32100	1.07700
H	−1.47100	3.32100	−1.07700
H	0.78800	4.30300	−1.42100
H	2.81900	2.89700	−0.97500
C	1.81600	−2.50500	0.81800
C	0.67500	−3.27400	1.07400
C	−0.58300	−2.71900	0.88000
C	−0.69800	−1.38500	0.44100
C	0.50700	−0.69200	0.21400
C	−1.97700	−0.69500	0.22100
C	1.81600	2.50500	−0.81800
C	0.67500	3.27400	−1.07400
C	−0.58300	2.71900	−0.88000
C	−0.69800	1.38500	−0.44100
C	0.50700	0.69200	−0.21400
C	−1.97700	0.69500	−0.22100
N	1.73200	−1.24600	0.38500
N	1.73200	1.24600	−0.38500
C	−3.18600	1.33300	−0.42200
H	−3.21000	2.37300	−0.75000
C	−3.18600	−1.33300	0.42200
H	−3.21000	−2.37300	0.75000
C	−4.43900	−0.69100	0.21800
C	−4.43900	0.69100	−0.21800
C	−6.89000	−0.69400	0.21800
H	−5.65600	2.38900	−0.75200
C	−6.89000	0.69400	−0.21800

C	−5.65700	1.34500	−0.42300
C	−5.65700	−1.34500	0.42300
H	−5.65600	−2.38900	0.75200
C	−8.12700	1.34400	−0.42200
C	−8.12700	−1.34400	0.42200
C	−9.34300	0.69300	−0.21800
C	−9.34300	−0.69300	0.21800
H	−8.12800	2.38800	−0.75100
H	−8.12800	−2.38800	0.75100
C	−10.60400	−1.34700	0.42300
H	−10.60200	−2.39100	0.75100
C	−10.60400	1.34700	−0.42300
H	−10.60200	2.39100	−0.75100
C	−11.78400	−0.68300	0.21500
H	−12.73800	−1.19400	0.37500
C	−11.78400	0.68300	−0.21500
H	−12.73800	1.19400	−0.37500

22) Reduced LS configuration for $N_{\mathrm{c}} = 7,\ \mathrm{Charge} = -1,\ S = 1/2$

H	3.32100	3.52300	1.09200
H	5.04100	3.61500	2.16400
H	2.34400	−1.05800	2.87900
H	2.96400	0.27300	5.21200
H	4.22200	2.58000	4.29500
H	6.75400	3.68300	0.33000
H	7.53400	2.23500	−1.91400
H	5.53600	0.34000	−2.15100
B	4.29800	2.90000	1.49700
C	2.83200	−0.09600	3.00400
C	3.16100	0.58300	4.18800
C	3.79800	1.74000	3.74900
C	6.28100	2.83800	−0.16700
C	6.65200	2.10400	−1.29000
C	5.63600	1.14400	−1.42600
N	3.24000	0.60400	1.93500
N	4.71900	1.30100	−0.46000
N	3.82800	1.72800	2.40000
N	5.12200	2.33700	0.31000
H	3.32100	−3.52300	−1.09200
H	5.04100	−3.61500	−2.16400
H	2.34400	1.05800	−2.87900
H	2.96400	−0.27300	−5.21200
H	4.22200	−2.58000	−4.29500
H	6.75400	−3.68300	−0.33000
H	7.53400	−2.23500	1.91400
H	5.53600	−0.34000	2.15100
B	4.29800	−2.90000	−1.49700
C	2.83200	0.09600	−3.00400
C	3.16100	−0.58300	−4.18800
C	3.79800	−1.74000	−3.74900
C	6.28100	−2.83800	0.16700
C	6.65200	−2.10400	1.29000
C	5.63600	−1.14400	1.42600
N	3.24000	−0.60400	−1.93500
N	4.71900	−1.30100	0.46000
N	3.82800	−1.72800	−2.40000
N	5.12200	−2.33700	−0.31000

Fe	3.24300	−0.00000	0.00000
H	2.81600	2.88400	−1.04000
H	0.77100	4.26800	−1.52200
H	−1.48100	3.27900	−1.15800
H	−1.48100	−3.27900	1.15800
H	0.77100	−4.26800	1.52200
H	2.81600	−2.88400	1.04000
C	1.81400	2.48600	−0.88000
C	0.66400	3.24400	−1.15300
C	−0.58900	2.68800	−0.94700
C	−0.71100	1.36000	−0.47300
C	0.51200	0.68000	−0.23100
C	−1.97900	0.68500	−0.23800
C	1.81400	−2.48600	0.88000
C	0.66400	−3.24400	1.15300
C	−0.58900	−2.68800	0.94700
C	−0.71100	−1.36000	0.47300
C	0.51200	−0.68000	0.23100
C	−1.97900	−0.68500	0.23800
N	1.73500	1.24000	−0.42300
N	1.73500	−1.24000	0.42300
C	−3.20600	−1.31700	0.45800
H	−3.23000	−2.34900	0.81500
C	−3.20600	1.31700	−0.45800
H	−3.23000	2.34900	−0.81500
C	−4.45600	0.68800	−0.23900
C	−4.45600	−0.68800	0.23900
C	−6.92700	0.69000	−0.23900
H	−5.68200	−2.36400	0.82000
C	−6.92700	−0.69000	0.23900
C	−5.68200	−1.32900	0.46100
C	−5.68200	1.32900	−0.46100
H	−5.68200	2.36400	−0.82000
C	−8.16000	−1.32600	0.46000
C	−8.16000	1.32600	−0.46000
C	−9.39400	−0.68400	0.23700
C	−9.39400	0.68400	−0.23700
H	−8.16100	−2.36200	0.81800
H	−8.16100	2.36200	−0.81800
C	−10.64800	1.32500	−0.45900
H	−10.64500	2.36100	−0.81800
C	−10.64800	−1.32500	0.45900
H	−10.64500	−2.36100	0.81800
C	−11.84300	0.67100	−0.23200
H	−12.79300	1.18500	−0.41000
C	−11.84300	−0.67100	0.23200
H	−12.79300	−1.18500	0.41000

23) Neutral HS configuration for $N_{\mathrm{c}} = 7$, $\mathrm{Charge} = 0$, $S = 2$

H	3.06900	−3.36700	−1.05500
H	4.68600	−3.90800	−2.16900
H	2.89300	1.15500	−3.09700
H	3.60100	−0.24500	−5.37700
H	4.39600	−2.70900	−4.36800
H	6.68000	−3.96000	−0.63300
H	7.74000	−2.61800	1.55700
H	5.83500	−0.66700	2.06600

B	4.13900	−3.01000	−1.54000
C	3.25100	0.13000	−3.19100
C	3.62000	−0.58100	−4.34200
C	4.02500	−1.82400	−3.85400
C	6.29000	−3.11400	−0.06900
C	6.80400	−2.43000	1.03300
C	5.84500	−1.44400	1.30300
N	3.41500	−0.62900	−2.09800
N	4.82700	−1.53800	0.43200
N	3.89000	−1.82300	−2.51300
N	5.11000	−2.56100	−0.40900
H	3.06800	3.36700	1.05500
H	4.68400	3.90800	2.16900
H	2.89300	−1.15500	3.09700
H	3.59900	0.24400	5.37700
H	4.39400	2.70900	4.36800
H	6.67900	3.96000	0.63400
H	7.74000	2.61900	−1.55500
H	5.83600	0.66800	−2.06600
B	4.13700	3.01100	1.54000
C	3.25000	−0.13100	3.19000
C	3.61800	0.58100	4.34200
C	4.02300	1.82400	3.85400
C	6.28900	3.11500	0.07000
C	6.80400	2.43100	−1.03200
C	5.84500	1.44400	−1.30200
N	3.41400	0.62900	2.09800
N	4.82700	1.53800	−0.43200
N	3.88800	1.82300	2.51300
N	5.10900	2.56100	0.41000
Fe	3.38400	−0.00000	−0.00000
H	2.65200	−2.85000	1.19000
H	0.59500	−4.19800	1.76800
H	−1.64300	−3.20600	1.34900
H	−1.64300	3.20600	−1.34900
H	0.59500	4.19800	−1.76800
H	2.65200	2.84900	−1.19000
C	1.64700	−2.45600	1.02700
C	0.50000	−3.19600	1.34500
C	−0.74600	−2.63400	1.10700
C	−0.84900	−1.33800	0.56000
C	0.36600	−0.67700	0.28000
C	−2.12900	−0.67200	0.28100
C	1.64700	2.45600	−1.02700
C	0.50000	3.19500	−1.34500
C	−0.74600	2.63400	−1.10700
C	−0.84900	1.33800	−0.56000
C	0.36600	0.67700	−0.28100
C	−2.12900	0.67100	−0.28100
N	1.56900	−1.23700	0.51000
N	1.56900	1.23600	−0.51000
C	−3.33800	1.28900	−0.54000
H	−3.36400	2.29500	−0.96000
C	−3.33800	−1.28900	0.53900
H	−3.36400	−2.29600	0.96000
C	−4.59100	0.66800	−0.28000
C	−4.59100	−0.66800	0.28000
C	−7.04200	−0.67100	0.28100

C	−7.04200	0.67100	−0.28100
C	−5.80900	−1.30100	0.54400
C	−5.80900	1.30100	−0.54500
H	−5.80800	−2.31000	0.96700
H	−5.80800	2.31000	−0.96700
C	−8.28000	1.30000	−0.54400
C	−8.28000	−1.30000	0.54400
C	−9.49500	0.67000	−0.28100
C	−9.49500	−0.67100	0.28100
H	−8.28000	2.30900	−0.96700
H	−8.28000	−2.30900	0.96700
C	−10.75600	1.30200	−0.54500
H	−10.75400	2.31100	−0.96800
C	−10.75600	−1.30200	0.54500
H	−10.75400	−2.31100	0.96800
C	−11.93600	0.66100	−0.27700
H	−12.89000	1.15500	−0.48400
C	−11.93600	−0.66100	0.27700
H	−12.89000	−1.15500	0.48400

24) Reduced HS configuration for $N_{\mathrm{c}} = 7,\ \mathrm{Charge} = -1,\ S = 3/2$

H	3.29300	−3.47500	−0.89300
H	4.96400	−3.91600	−1.97900
H	2.70200	0.90500	−3.13600
H	3.52800	−0.53700	−5.35600
H	4.55900	−2.86200	−4.22900
H	6.93600	−3.73000	−0.43900
H	7.84400	−2.23500	1.72300
H	5.76600	−0.44800	2.15000
B	4.32800	−3.04600	−1.38900
C	3.16100	−0.08200	−3.18600
C	3.58900	−0.81500	−4.30500
C	4.11300	−1.98700	−3.75800
C	6.46700	−2.90600	0.09500
C	6.90300	−2.14800	1.18300
C	5.85400	−1.24400	1.41200
N	3.40500	−0.76400	−2.06000
N	4.86200	−1.45300	0.53400
N	3.98600	−1.92900	−2.41700
N	5.24600	−2.46900	−0.27200
H	3.29300	3.47500	0.89300
H	4.96400	3.91600	1.97900
H	2.70200	−0.90400	3.13700
H	3.52900	0.53800	5.35600
H	4.55900	2.86200	4.22900
H	6.93700	3.72900	0.43900
H	7.84400	2.23500	−1.72300
H	5.76600	0.44800	−2.15000
B	4.32900	3.04600	1.38900
C	3.16100	0.08200	3.18600
C	3.59000	0.81500	4.30500
C	4.11300	1.98700	3.75800
C	6.46700	2.90500	−0.09500
C	6.90300	2.14700	−1.18300
C	5.85400	1.24400	−1.41200
N	3.40500	0.76400	2.06000
N	4.86200	1.45300	−0.53400

N	3.98600	1.92900	2.41700
N	5.24700	2.46900	0.27200
Fe	3.32300	−0.00000	0.00000
H	2.62700	−2.81400	1.30000
H	0.55600	−4.12600	1.92700
H	−1.67500	−3.13800	1.46900
H	−1.67600	3.13800	−1.46900
H	0.55600	4.12600	−1.92700
H	2.62700	2.81400	−1.29900
C	1.62300	−2.41800	1.12400
C	0.46700	−3.13900	1.46700
C	−0.77400	−2.58100	1.20700
C	−0.88300	−1.30300	0.60700
C	0.34900	−0.65800	0.30500
C	−2.15200	−0.65600	0.30600
C	1.62300	2.41800	−1.12400
C	0.46700	3.13900	−1.46700
C	−0.77400	2.58100	−1.20700
C	−0.88300	1.30300	−0.60700
C	0.34900	0.65800	−0.30500
C	−2.15200	0.65600	−0.30600
N	1.55100	−1.21900	0.56300
N	1.55100	1.21900	−0.56300
C	−3.37900	1.26300	−0.59000
H	−3.40500	2.25300	−1.05100
C	−3.37900	−1.26300	0.59000
H	−3.40500	−2.25300	1.05100
C	−4.63000	0.65900	−0.30800
C	−4.63000	−0.65900	0.30800
C	−7.10000	−0.66100	0.30900
C	−7.10000	0.66100	−0.30900
C	−5.85600	−1.27400	0.59600
C	−5.85600	1.27400	−0.59600
H	−5.85500	−2.26700	1.05900
H	−5.85500	2.26700	−1.05900
C	−8.33400	1.27200	−0.59500
C	−8.33400	−1.27200	0.59500
C	−9.56700	0.65600	−0.30700
C	−9.56700	−0.65600	0.30700
H	−8.33500	2.26400	−1.05900
H	−8.33500	−2.26400	1.05900
C	−10.82100	1.27100	−0.59400
H	−10.81800	2.26300	−1.05800
C	−10.82100	−1.27100	0.59400
H	−10.81800	−2.26300	1.05800
C	−12.01600	0.64300	−0.30100
H	−12.96700	1.13600	−0.53100
C	−12.01600	−0.64300	0.30100
H	−12.96700	−1.13600	0.53100

25) Neutral gas-phase L ligand of $N_c = 2$, $\mathrm{Charge} = 0$, $S = 0$

H	0.62669200	3.14378900	-2.13182300
H	0.04512900	4.58496800	-0.16406200
H	-0.60454300	3.45099000	2.00017100
H	0.64065200	-0.95131800	2.07571100
H	-0.64065200	0.95131800	2.07571100
H	0.60454300	-3.45099000	2.00017100

H	-0.04512900	-4.58496800	-0.16406200
H	-0.62669200	-3.14378900	-2.13182300
C	0.34352400	2.68636300	-1.17461100
C	0.02177700	3.49509400	-0.07771000
C	-0.33196600	2.86580900	1.11655100
C	-0.34352400	1.47138900	1.16211400
C	-0.00027100	0.74695100	0.00643000
C	-0.34352400	-2.68636300	-1.17461100
C	-0.02177700	-3.49509400	-0.07771000
C	0.33196600	-2.86580900	1.11655100
C	0.34352400	-1.47138900	1.16211400
C	0.00027100	-0.74695100	0.00643000
N	0.33278800	1.35680700	-1.13952000
N	-0.33278800	-1.35680700	-1.13952000

26) Reduced gas-phase L ligand of $N_{\mathrm{c}} = 2,\ \mathrm{Charge} = -1,\ S = 1/2$

H	0.00061900	3.17252300	-2.21878700
H	0.00019000	4.62683000	-0.17228000
H	-0.00083300	3.45261100	2.10516300
H	0.00048400	-0.99913600	2.19009000
H	-0.00048400	0.99913600	2.19009000
H	0.00083300	-3.45261100	2.10516300
H	-0.00019000	-4.62683000	-0.17228000
H	-0.00061900	-3.17252300	-2.21878700
C	0.00042100	2.70264200	-1.21803100
C	-0.00011400	3.53596900	-0.08216000
C	-0.00033300	2.87629200	1.17067100
C	-0.00030200	1.49628100	1.21678700
C	0.00011400	0.72053000	0.00374000
C	-0.00042100	-2.70264200	-1.21803100
C	0.00011400	-3.53596900	-0.08216000
C	0.00033300	-2.87629200	1.17067100
C	0.00030200	-1.49628100	1.21678700
C	-0.00011400	-0.72053000	0.00374000
N	0.00040300	1.38474300	-1.20717600
N	-0.00040300	-1.38474300	-1.20717600

27) Neutral gas-phase L ligand of $N_{\mathrm{c}} = 3,\ \mathrm{Charge} = 0,\ S = 0$

H	0.00007400	3.19367100	-2.53576200
H	-0.00014400	4.57611600	-0.44102200
H	-0.00008900	3.39146200	1.78274000
H	0.00002200	1.23991400	3.04599500
H	-0.00002200	-1.23991400	3.04599500
H	0.00008900	-3.39146200	1.78274000
H	0.00014400	-4.57611600	-0.44102200
H	-0.00007400	-3.19367100	-2.53576200
C	0.00032300	2.70130300	-1.55370900
C	0.00000800	3.48430900	-0.37720800
C	-0.00000800	2.83280100	0.84111700
C	-0.00000800	1.41884300	0.87216000
C	-0.00017500	0.72972100	-0.37766200
C	0.00001400	0.68187100	2.10443900
C	-0.00032300	-2.70130300	-1.55370900
C	-0.00000800	-3.48430900	-0.37720800
C	0.00000800	-2.83280100	0.84111700
C	0.00000800	-1.41884300	0.87216000
C	0.00017500	-0.72972100	-0.37766200

C	-0.00001400	-0.68187100	2.10443900
N	0.00008100	1.38237400	-1.55811100
N	-0.00008100	-1.38237400	-1.55811100

28) Reduced gas-phase L ligand of $N_{\mathrm{c}} = 3$, $\mathrm{Charge} = -1$, $S = 1/2$

H	0.00000300	3.20876300	-2.55308600
H	-0.00000900	4.59868000	-0.45569900
H	-0.00001800	3.43442600	1.77428100
H	-0.00001000	1.25587100	3.05091000
H	0.00001000	-1.25587100	3.05091000
H	0.00001800	-3.43442600	1.77428100
H	0.00000900	-4.59868000	-0.45569900
H	-0.00000300	-3.20876300	-2.55308600
C	0.00000200	2.72706100	-1.56420800
C	-0.00000200	3.50290600	-0.39107200
C	-0.00000600	2.86365300	0.83776900
C	0.00000200	1.43052300	0.89736300
C	0.00002800	0.74000500	-0.37978900
C	-0.00000300	0.70392300	2.10296300
C	-0.00000200	-2.72706100	-1.56420800
C	0.00000200	-3.50290600	-0.39107200
C	0.00000600	-2.86365300	0.83776900
C	-0.00000200	-1.43052300	0.89736300
C	-0.00002800	-0.74000500	-0.37978900
C	0.00000300	-0.70392300	2.10296300
N	0.00001400	1.38659400	-1.54779400
N	-0.00001400	-1.38659400	-1.54779400

29) Neutral gas-phase L ligand of $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = 0$, $S = 0$

H	3.47152300	-3.13965500	0.00004100
H	1.39907300	-4.56860300	0.00009200
H	-0.82074200	-3.45462700	0.00008300
H	-0.82076900	3.45462000	0.00008400
H	1.39903700	4.56861300	0.00005100
H	3.47149800	3.13968300	-0.00006400
C	2.47623600	-2.67519600	0.00004900
C	1.32043800	-3.47795700	0.00005100
C	0.08717400	-2.84946100	0.00003100
C	0.01121000	-1.43876000	-0.00002400
C	1.24494600	-0.73445200	-0.00003600
C	-1.25973400	-0.71144600	-0.00005700
C	2.47621500	2.67521500	-0.00004400
C	1.32041000	3.47796700	0.00003600
C	0.08715100	2.84946100	0.00006600
C	0.01119900	1.43876000	0.00005300
C	1.24494100	0.73446100	0.00002800
C	-1.25973900	0.71143600	0.00004900
N	2.43872100	-1.35631700	0.00000800
N	2.43871100	1.35633600	-0.00003900
C	-2.50038300	1.38854700	0.00011000
H	-2.52396400	2.47902500	0.00023300
C	-2.50037300	-1.38856600	-0.00017400
H	-2.52394600	-2.47904400	-0.00031900
C	-3.70459200	0.70185400	0.00002700
H	-4.64840500	1.25458500	0.00008700
C	-3.70458700	-0.70188200	-0.00013600
H	-4.64839600	-1.25461900	-0.00024200

30) Reduced gas-phase L ligand of $N_c = 4$, $\mathrm{Charge} = -1$, $S = 1/2$

H	3.46658900	3.17234300	0.00019000
H	1.38941600	4.59439600	-0.00187900
H	-0.83718200	3.44003700	-0.00159700
H	-0.83735500	-3.43999400	0.00053000
H	1.38918400	-4.59446300	0.00102400
H	3.46643000	-3.17251300	0.00024300
C	2.47338900	2.68862900	-0.00010200
C	1.31729700	3.50260500	-0.00094200
C	0.07908800	2.84275700	-0.00080700
C	0.00925300	1.44763200	0.00009700
C	1.26104400	0.70960100	0.00021700
C	-1.26179000	0.71522800	0.00054700
C	2.47325500	-2.68874900	0.00028100
C	1.31711900	-3.50266900	0.00045200
C	0.07894500	-2.84276100	0.00020300
C	0.00917900	-1.44763000	-0.00025800
C	1.26100800	-0.70966100	0.00001300
C	-1.26182500	-0.71516800	-0.00058200
N	2.47124800	1.37811000	0.00041000
N	2.47117700	-1.37823200	0.00010800
C	-2.50916300	-1.38256100	-0.00174300
H	-2.52954400	-2.47422600	-0.00340700
C	-2.50909400	1.38268200	0.00189900
H	-2.52942200	2.47434700	0.00368400
C	-3.72261200	-0.69967600	-0.00092500
H	-4.66511700	-1.25842100	-0.00187300
C	-3.72257900	0.69985700	0.00118200
H	-4.66505600	1.25864800	0.00227000

31) Neutral gas-phase L ligand of $N_c = 5$, $\mathrm{Charge} = 0$, $S = 0$

H	-4.49323400	3.13438400	-0.00079300
H	-2.42417500	4.56983300	0.00044100
H	-0.20179500	3.46033400	0.00085700
H	-0.20179500	-3.46033400	-0.00087100
H	-2.42417500	-4.56983300	-0.00044900
H	-4.49323400	-3.13438400	0.00080000
C	-3.49599600	2.67433100	-0.00033100
C	-2.34381100	3.47936700	0.00012200
C	-1.10818900	2.85268300	0.00033400
C	-1.02847400	1.44398400	0.00005600
C	-2.25891500	0.73671100	-0.00035100
C	0.24938300	0.72035900	0.00004200
C	-3.49599600	-2.67433100	0.00033500
C	-2.34381100	-3.47936700	-0.00012600
C	-1.10818900	-2.85268300	-0.00034100
C	-1.02847400	-1.44398400	-0.00005800
C	-2.25891500	-0.73671100	0.00035400
C	0.24938300	-0.72035900	-0.00004400
N	-3.45306300	1.35416700	-0.00049600
N	-3.45306300	-1.35416700	0.00050200
C	1.46993000	-1.39103400	-0.00003700
H	1.49701400	-2.48187300	0.00000200
C	1.46993000	1.39103400	0.00003600
H	1.49701400	2.48187300	-0.00000200
C	2.70802000	0.71712300	0.00000200

C	2.70802000	-0.71712300	-0.00000200
C	5.14345100	0.71138300	-0.00000700
H	6.09535000	1.25045900	-0.00002300
H	3.95211200	-2.50155200	0.00002700
C	5.14345100	-0.71138300	0.00001000
H	6.09535000	-1.25045900	0.00002600
C	3.95562900	-1.40712800	0.00001500
C	3.95562900	1.40712800	-0.00001300
H	3.95211200	2.50155100	-0.00002500

32) Reduced gas-phase L ligand of $N_{\mathrm{c}} = 5$, $\mathrm{Charge} = -1$, $S = 1/2$

H	-4.50065500	3.15887400	0.00033700
H	-2.40953500	4.57489500	0.00096800
H	-0.20022200	3.43867900	0.00094300
H	-0.20022200	-3.43867900	-0.00096100
H	-2.40953600	-4.57489500	-0.00098000
H	-4.50065500	-3.15887400	-0.00032900
C	-3.50758600	2.68369500	0.00036700
C	-2.34006600	3.48204200	0.00047500
C	-1.11472800	2.84215500	0.00042700
C	-1.03282600	1.42700000	-0.00004900
C	-2.28938800	0.72487100	0.00005900
C	0.23950900	0.71979800	-0.00029900
C	-3.50758600	-2.68369400	-0.00036400
C	-2.34006600	-3.48204200	-0.00048100
C	-1.11472800	-2.84215500	-0.00043600
C	-1.03282600	-1.42700000	0.00004600
C	-2.28938800	-0.72487100	-0.00005500
C	0.23950900	-0.71979800	0.00029800
N	-3.47938900	1.36746900	0.00021400
N	-3.47938900	-1.36746900	-0.00020600
C	1.47556300	-1.39301000	0.00093000
H	1.50423200	-2.48480300	0.00182800
C	1.47556300	1.39301000	-0.00093000
H	1.50423200	2.48480300	-0.00182500
C	2.72651600	0.72093000	-0.00055200
C	2.72651600	-0.72093000	0.00055200
C	5.18288800	0.70129300	-0.00056400
H	6.13067800	1.25178900	-0.00101500
H	3.96792800	-2.49590200	0.00196300
C	5.18288800	-0.70129300	0.00056600
H	6.13067800	-1.25178900	0.00101700
C	3.97066600	-1.39961700	0.00111100
C	3.97066500	1.39961700	-0.00111000
H	3.96792800	2.49590200	-0.00196100

33) Neutral gas-phase L ligand of $N_{\mathrm{c}} = 6$, $\mathrm{Charge} = 0$, $S = 0$

H	5.57748300	3.13176600	0.00125300
H	3.51021100	4.57041100	-0.00036700
H	1.28657200	3.46343400	-0.00102200
H	1.28657200	-3.46343400	0.00103000
H	3.51021100	-4.57041100	0.00037000
H	5.57748300	-3.13176600	-0.00125900
C	4.57932500	2.67381100	0.00059300
C	3.42882800	3.48002400	-0.00003500
C	2.19209300	2.85444200	-0.00039300
C	2.11022200	1.44637500	-0.00010100

C	3.33938800	0.73777400	0.00038900
C	0.82954600	0.72493200	-0.00010700
C	4.57932500	-2.67381100	-0.00059600
C	3.42882800	-3.48002400	0.00003700
C	2.19209300	-2.85444200	0.00039700
C	2.11022200	-1.44637500	0.00010200
C	3.33938800	-0.73777400	-0.00039100
C	0.82954600	-0.72493200	0.00011000
N	4.53373000	1.35309400	0.00072300
N	4.53373000	-1.35309400	-0.00072800
C	-0.38363600	-1.39418100	0.00019900
H	-0.41096900	-2.48494200	0.00029100
C	-0.38363600	1.39418100	-0.00019600
H	-0.41096900	2.48494200	-0.00028900
C	-1.63237100	0.72153100	-0.00009300
C	-1.63237100	-0.72153100	0.00009500
C	-4.08131500	0.72465500	-0.00008700
H	-2.85862300	-2.50176900	0.00030700
C	-4.08131500	-0.72465500	0.00008600
C	-2.85943400	-1.40714000	0.00017300
C	-2.85943400	1.40714000	-0.00017100
H	-2.85862300	2.50176900	-0.00030300
C	-5.33919500	-1.40969400	0.00016100
C	-5.33919500	1.40969400	-0.00016300
C	-6.52165500	-0.71459200	0.00007900
H	-7.47474500	-1.25162900	0.00013700
C	-6.52165500	0.71459200	-0.00008100
H	-7.47474500	1.25162900	-0.00014000
H	-5.33682000	-2.50403500	0.00028300
H	-5.33682000	2.50403500	-0.00028700

34) Reduced gas-phase L ligand of $N_{\mathrm{c}} = 6$, $\mathrm{Charge} = -1$, $S = 1/2$

H	-5.58828000	-3.15145000	0.00022400
H	-3.50459100	-4.57209700	-0.00057300
H	-1.28951700	-3.44470000	-0.00078800
H	-1.28951700	3.44470000	0.00078800
H	-3.50459100	4.57209700	0.00057300
H	-5.58828000	3.15145000	-0.00022400
C	-4.59345600	-2.68169500	-0.00003300
C	-3.43168700	-3.47960100	-0.00026000
C	-2.20192400	-2.84585000	-0.00033700
C	-2.11895700	-1.43097200	-0.00001700
C	-3.36745200	-0.73085900	0.00025300
C	-0.84752800	-0.71992100	0.00006200
C	-4.59345600	2.68169500	0.00003300
C	-3.43168700	3.47960100	0.00026000
C	-2.20192400	2.84585100	0.00033700
C	-2.11895700	1.43097200	0.00001700
C	-3.36745200	0.73085900	-0.00025300
C	-0.84752800	0.71992100	-0.00006300
N	-4.55855900	-1.36245700	0.00018300
N	-4.55855900	1.36245700	-0.00018200
C	0.38483000	1.39223700	-0.00020800
H	0.41243100	2.48411900	-0.00046500
C	0.38483000	-1.39223700	0.00020800
H	0.41243100	-2.48411900	0.00046500
C	1.63533900	-0.72633900	0.00013700

C	1.63533900	0.72633900	-0.00013700
C	4.10852500	-0.72423900	0.00016500
H	2.86795700	2.50032200	-0.00053300
C	4.10852500	0.72423900	-0.00016500
C	2.86780300	1.40411700	-0.00030500
C	2.86780300	-1.40411700	0.00030400
H	2.86795700	-2.50032200	0.00053300
C	5.35913100	1.39988000	-0.00032600
C	5.35913100	-1.39988000	0.00032600
C	6.56267200	0.70602000	-0.00016500
H	7.51170400	1.25376700	-0.00029300
C	6.56267200	-0.70602000	0.00016600
H	7.51170400	-1.25376700	0.00029500
H	5.35643800	2.49607600	-0.00058100
H	5.35643800	-2.49607600	0.00058100

35) Neutral gas-phase L ligand of $N_{\mathrm{c}} = 7$, $\mathrm{Charge} = 0$, $S = 0$

H	6.69963000	3.13049800	0.00035600
H	4.63325300	4.57073000	-0.00118100
H	2.40897600	3.46503400	-0.00141100
H	2.40897600	-3.46503400	0.00141100
H	4.63325300	-4.57073000	0.00118100
H	6.69963000	-3.13049800	-0.00035600
C	5.70101900	2.67359200	-0.00005300
C	4.55135600	3.48038100	-0.00062800
C	3.31406100	2.85537500	-0.00071000
C	3.23110300	1.44758200	-0.00014100
C	4.45970100	0.73831000	0.00027200
C	1.94922000	0.72723000	0.00005400
C	5.70101900	-2.67359200	0.00005200
C	4.55135600	-3.48038100	0.00062800
C	3.31406100	-2.85537500	0.00071100
C	3.23110300	-1.44758200	0.00014100
C	4.45970100	-0.73831000	-0.00027200
C	1.94922000	-0.72723000	-0.00005400
N	5.65410100	1.35257400	0.00029400
N	5.65410100	-1.35257400	-0.00029400
C	0.73925800	-1.39576300	-0.00034900
H	0.71202600	-2.48652800	-0.00071000
C	0.73925800	1.39576300	0.00034900
H	0.71202600	2.48652800	0.00071000
C	-0.51450200	0.72428400	0.00025700
C	-0.51450200	-0.72428400	-0.00025700
C	-2.96599400	0.72773600	0.00029200
H	-1.73205200	-2.50413500	-0.00096000
C	-2.96599400	-0.72773600	-0.00029200
C	-1.73294000	-1.40964100	-0.00054800
C	-1.73294000	1.40964100	0.00054800
H	-1.73205200	2.50413500	0.00096000
C	-4.20410600	-1.40858600	-0.00057500
C	-4.20410600	1.40858600	0.00057500
C	-5.41954200	-0.72687000	-0.00029900
C	-5.41954200	0.72687000	0.00029900
H	-4.20436500	-2.50311600	-0.00102300
H	-4.20436500	2.50311600	0.00102300
C	-6.68124000	1.41135200	0.00058300
H	-6.67900400	2.50569200	0.00103600

C	-6.68124000	-1.41135200	-0.00058300
H	-6.67900400	-2.50569200	-0.00103600
C	-7.86110600	0.71637100	0.00029600
H	-8.81490300	1.25216900	0.00051900
C	-7.86110600	-0.71637100	-0.00029600
H	-8.81490300	-1.25216900	-0.00051900

36) Neutral gas-phase L ligand of $N_{\mathrm{c}} = 7$, $\mathrm{Charge} = -1$, $S = 1/2$

H	-6.71363900	3.14623700	-0.00085200
H	-4.63434800	4.57135700	0.00141200
H	-2.41599700	3.44893300	0.00192400
H	-2.41599700	-3.44893300	-0.00192400
H	-4.63434800	-4.57135700	-0.00141200
H	-6.71363900	-3.14623700	0.00085200
C	-5.71743800	2.68004000	-0.00025600
C	-4.55931800	3.47924500	0.00076600
C	-3.32693900	2.84800000	0.00109400
C	-3.24291000	1.43490700	0.00044900
C	-4.48669700	0.73341000	0.00060100
C	-1.97029000	0.72101600	-0.00002600
C	-5.71743800	-2.68004000	0.00025600
C	-4.55931800	-3.47924600	-0.00076600
C	-3.32693900	-2.84800000	-0.00109400
C	-3.24291000	-1.43490700	-0.00044900
C	-4.48669700	-0.73341000	-0.00060100
C	-1.97029000	-0.72101600	0.00002600
N	-5.67902900	1.35983200	-0.00008900
N	-5.67902900	-1.35983200	0.00008900
C	-0.74185700	-1.39149400	0.00047500
H	-0.71460700	-2.48349100	0.00093500
C	-0.74185700	1.39149400	-0.00047500
H	-0.71460700	2.48349100	-0.00093500
C	0.50758700	0.72716900	-0.00036400
C	0.50758700	-0.72716900	0.00036400
C	2.98036600	0.73077900	-0.00043000
H	1.73689400	-2.50241400	0.00136000
C	2.98036600	-0.73077900	0.00043000
C	1.73757700	-1.40651500	0.00078500
C	1.73757700	1.40651500	-0.00078500
H	1.73689400	2.50241400	-0.00136000
C	4.21638100	-1.40379000	0.00084900
C	4.21638100	1.40379000	-0.00084900
C	5.45066900	-0.72459300	0.00044200
C	5.45066900	0.72459300	-0.00044200
H	4.21766400	-2.49982300	0.00151300
H	4.21766400	2.49982300	-0.00151300
C	6.70481300	1.40177300	-0.00086000
H	6.70166700	2.49779100	-0.00153300
C	6.70481300	-1.40177300	0.00085900
H	6.70166700	-2.49779100	0.00153300
C	7.90193800	0.70949100	-0.00043600
H	8.85226500	1.25443600	-0.00077300
C	7.90193800	-0.70949100	0.00043600
H	8.85226500	-1.25443600	0.00077300

37) Neutral gas-phase HS $\mathrm{Fe[H_2B(Pz)_2]_2}$ fragment, $\mathrm{Charge} = 0$, $S = 2$

Fe	0.00000000	0.00000000	0.22893100

H	-0.45799400	2.55358200	1.60826200
H	0.69328300	4.17744100	1.08266200
H	3.07863500	-0.74432700	1.40217100
H	4.78238700	1.34980800	2.04225000
H	3.17872200	3.58961800	1.68893300
H	0.13507700	4.74329700	-1.42268600
H	-0.84524300	3.47706300	-3.69215500
H	-1.12429200	0.84395500	-2.86454100
B	0.44027800	2.99797200	0.89245400
C	2.88990200	0.32923200	1.40885300
C	3.74210500	1.39499400	1.72661900
C	2.95100200	2.53404300	1.55149000
C	-0.12703800	3.69950900	-1.58654900
C	-0.62241100	3.04507200	-2.71862500
C	-0.76954100	1.71286400	-2.31015800
N	1.67908100	0.80179500	1.07337600
N	-0.39302000	1.58509800	-1.02738800
N	1.72391100	2.15218000	1.15901900
N	0.00000000	2.80475400	-0.59258500
H	0.45799400	-2.55358200	1.60826200
H	-0.69328300	-4.17744100	1.08266200
H	-3.07863500	0.74432700	1.40217100
H	-4.78238700	-1.34980800	2.04225000
H	-3.17872200	-3.58961800	1.68893300
H	-0.13507700	-4.74329700	-1.42268600
H	0.84524300	-3.47706300	-3.69215500
H	1.12429200	-0.84395500	-2.86454100
B	-0.44027800	-2.99797200	0.89245400
C	-2.88990200	-0.32923200	1.40885300
C	-3.74210500	-1.39499400	1.72661900
C	-2.95100200	-2.53404300	1.55149000
C	0.12703800	-3.69950900	-1.58654900
C	0.62241100	-3.04507200	-2.71862500
C	0.76954100	-1.71286400	-2.31015800
N	-1.67908100	-0.80179500	1.07337600
N	0.39302000	-1.58509800	-1.02738800
N	-1.72391100	-2.15218000	1.15901900
N	0.00000000	-2.80475400	-0.59258500

38) Neutral gas-phase LS $Fe[H_2B(Pz)_2]_2$ fragment, $\mathrm{Charge} = 0$, $S = 0$

Fe	0.00000000	0.00000000	0.41489700
H	-0.47584600	1.29867000	1.70861900
H	-0.25687600	3.32181300	2.01834100
H	3.47778400	-0.12145600	-0.05145200
H	4.76700500	2.20204300	0.76687200
H	2.68392300	3.80255500	1.66348500
H	-1.15289800	4.55922100	-0.56418200
H	-1.81788400	3.49142600	-3.03901600
H	-1.20131500	0.79436200	-2.75501200
B	0.00000000	2.39698500	1.27067100
C	3.06123700	0.79251900	0.37053700
C	3.70225900	1.97811300	0.78726800
C	2.67085600	2.79788000	1.24403100
C	-1.07875900	3.53806500	-0.93439700
C	-1.40591900	2.98132000	-2.17051900
C	-1.09560200	1.61083500	-2.04161900
N	1.74753100	0.90577500	0.57047500

N	-0.61838900	1.38144100	-0.81698300
N	1.51225700	2.12222400	1.10244400
N	-0.61223600	2.54866000	-0.14543300
H	0.47584600	-1.29867000	1.70861900
H	0.25687600	-3.32181300	2.01834100
H	-3.47778400	0.12145600	-0.05145200
H	-4.76700500	-2.20204300	0.76687200
H	-2.68392300	-3.80255500	1.66348500
H	1.15289800	-4.55922100	-0.56418200
H	1.81788400	-3.49142600	-3.03901600
H	1.20131500	-0.79436200	-2.75501200
B	0.00000000	-2.39698500	1.27067100
C	-3.06123700	-0.79251900	0.37053700
C	-3.70225900	-1.97811300	0.78726800
C	-2.67085600	-2.79788000	1.24403100
C	1.07875900	-3.53806500	-0.93439700
C	1.40591900	-2.98132000	-2.17051900
C	1.09560200	-1.61083500	-2.04161900
N	-1.74753100	-0.90577500	0.57047500
N	0.61838900	-1.38144100	-0.81698300
N	-1.51225700	-2.12222400	1.10244400
N	0.61223600	-2.54866000	-0.14543300

39) Another neutral LS complex for $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = 0$, $S = 0$

H	−3.03500	0.65100	2.00900
H	−2.93700	2.35300	3.10100
H	1.91900	−0.02500	2.46800
H	1.27000	0.56900	5.07400
H	−1.28200	1.65300	4.85200
H	−3.53600	4.11100	1.40100
H	−2.73600	5.00500	−1.10600
H	−0.91100	3.08600	−1.89600
B	−2.38400	1.66300	2.25300
C	0.99700	0.39800	2.85500
C	0.66600	0.71300	4.18100
C	−0.61000	1.26400	4.09000
C	−2.83600	3.68100	0.68800
C	−2.42500	4.11000	−0.57200
C	−1.50300	3.13600	−0.98600
N	−0.00800	0.73000	2.03000
N	−1.38300	2.18500	−0.04700
N	−0.98800	1.26000	2.79500
N	−2.19800	2.52700	0.97900
H	3.03500	0.65100	−2.00900
H	2.93700	2.35300	−3.10100
H	−1.91900	−0.02500	−2.46800
H	−1.27000	0.56900	−5.07400
H	1.28200	1.65300	−4.85200
H	3.53600	4.11100	−1.40100
H	2.73600	5.00500	1.10600
H	0.91100	3.08600	1.89600
B	2.38400	1.66300	−2.25300
C	−0.99700	0.39800	−2.85500
C	−0.66600	0.71300	−4.18100
C	0.61000	1.26400	−4.09000
C	2.83600	3.68100	−0.68800
C	2.42500	4.11000	0.57200

C	1.50300	3.13600	0.98600
N	0.00800	0.73000	−2.03000
N	1.38300	2.18500	0.04700
N	0.98800	1.26000	−2.79500
N	2.19800	2.52700	−0.97900
Fe	−0.00000	0.72400	0.00000
H	−3.00400	0.35900	−0.21600
H	−1.05200	−4.15700	−0.03500
H	1.05200	−4.15700	0.03500
H	3.00400	0.35900	0.21600
C	−2.61000	−0.65500	−0.15100
C	−3.49300	−1.76300	−0.19000
C	−2.92600	−3.07300	−0.13700
C	−1.51400	−3.16900	−0.06100
C	−0.73600	−2.02900	−0.02700
C	0.73600	−2.02900	0.02700
C	1.51400	−3.16900	0.06100
C	2.92600	−3.07300	0.13700
C	3.49300	−1.76300	0.19000
C	2.61000	−0.65500	0.15100
N	−1.30000	−0.77400	−0.05800
N	1.30000	−0.77400	0.05800
C	3.79100	−4.19800	0.17100
H	3.36100	−5.20300	0.13100
C	4.90000	−1.60500	0.27300
C	5.71800	−2.71600	0.30500
C	5.15800	−4.02000	0.25400
H	5.32000	−0.59600	0.30400
C	−3.79100	−4.19800	−0.17100
H	−3.36100	−5.20300	−0.13100
C	−4.90000	−1.60500	−0.27300
C	−5.71800	−2.71600	−0.30500
C	−5.15800	−4.02000	−0.25400
H	−5.32000	−0.59600	−0.30400
H	−6.80400	−2.59800	−0.36500
H	−5.82000	−4.89000	−0.27900
H	5.82000	−4.89000	0.27900
H	6.80400	−2.59800	0.36500

40) Another reduced LS complex for $N_{\mathrm{c}} = 4,\ \mathrm{Charge} = -1,\ S = 1/2$

H	−3.07600	0.85500	2.07000
H	−2.80800	2.57700	3.11100
H	1.80500	−0.23600	2.45600
H	1.20900	0.39500	5.07500
H	−1.23400	1.71200	4.85500
H	−3.39400	4.27600	1.36200
H	−2.66800	5.01700	−1.22000
H	−0.95000	2.99000	−1.98300
B	−2.33800	1.81400	2.26900
C	0.93200	0.27400	2.85200
C	0.62500	0.60700	4.18200
C	−0.59400	1.27400	4.09200
C	−2.73900	3.78800	0.64300
C	−2.36700	4.13900	−0.65300
C	−1.50100	3.10800	−1.05400
N	−0.03300	0.70800	2.02900
N	−1.37400	2.20200	−0.07300

N	−0.96500	1.31700	2.79500
N	−2.13000	2.62600	0.96300
H	3.07600	0.85500	−2.07000
H	2.80800	2.57700	−3.11100
H	−1.80500	−0.23600	−2.45600
H	−1.20900	0.39500	−5.07500
H	1.23400	1.71200	−4.85500
H	3.39400	4.27500	−1.36200
H	2.66800	5.01700	1.22000
H	0.95000	2.99000	1.98300
B	2.33800	1.81400	−2.26900
C	−0.93200	0.27400	−2.85200
C	−0.62500	0.60700	−4.18200
C	0.59400	1.27400	−4.09200
C	2.73900	3.78800	−0.64300
C	2.36700	4.13900	0.65300
C	1.50100	3.10800	1.05400
N	0.03300	0.70800	−2.02900
N	1.37400	2.20200	0.07300
N	0.96500	1.31700	−2.79500
N	2.13000	2.62600	−0.96300
Fe	−0.00000	0.71100	−0.00000
H	−3.00800	0.34300	−0.16900
H	−1.06300	−4.18700	−0.04200
H	1.06300	−4.18700	0.04200
H	3.00800	0.34300	0.16900
C	−2.61000	−0.67200	−0.12500
C	−3.50800	−1.78300	−0.16800
C	−2.92600	−3.09800	−0.13300
C	−1.52600	−3.19900	−0.06200
C	−0.71600	−2.04100	−0.02400
C	0.71600	−2.04100	0.02400
C	1.52600	−3.19900	0.06200
C	2.92600	−3.09800	0.13300
C	3.50800	−1.78300	0.16800
C	2.61000	−0.67200	0.12500
N	−1.30400	−0.78900	−0.04900
N	1.30400	−0.78900	0.04900
C	3.81600	−4.21500	0.17900
H	3.39500	−5.22600	0.15300
C	4.90400	−1.62200	0.24200
C	5.74800	−2.73000	0.28500
C	5.18600	−4.02700	0.25300
H	5.31500	−0.60700	0.25900
C	−3.81600	−4.21500	−0.17900
H	−3.39500	−5.22600	−0.15300
C	−4.90400	−1.62200	−0.24200
C	−5.74800	−2.73000	−0.28500
C	−5.18600	−4.02700	−0.25300
H	−5.31500	−0.60700	−0.25900
H	−5.84800	−4.90000	−0.28600
H	−6.83300	−2.60100	−0.34000
H	5.84800	−4.90000	0.28600
H	6.83300	−2.60100	0.34000

41) Another neutral HS complex for $N_{\mathrm{c}} = 4,\ \mathrm{Charge} = 0,\ S = 2$

H	−2.89300	−0.55900	−2.04800

H	−3.04700	−2.18500	−3.26300
H	2.03700	−0.33700	−2.60000
H	1.40900	−1.05300	−5.19800
H	−1.23700	−1.87600	−4.99000
H	−3.55600	−4.17100	−1.80500
H	−2.94900	−5.20900	0.70000
H	−1.26400	−3.28500	1.77300
B	−2.39300	−1.62600	−2.39200
C	1.09400	−0.70600	−3.00100
C	0.77300	−1.07900	−4.31500
C	−0.55500	−1.49800	−4.23100
C	−2.92900	−3.77100	−1.01100
C	−2.61600	−4.27400	0.25300
C	−1.76700	−3.30500	0.80700
N	0.03900	−0.88100	−2.19300
N	−1.59400	−2.29300	−0.05700
N	−0.96600	−1.36600	−2.95400
N	−2.30500	−2.58800	−1.17100
H	2.89200	−0.55500	2.04800
H	3.04800	−2.18000	3.26500
H	−2.03700	−0.33500	2.59900
H	−1.41000	−1.04900	5.19800
H	1.23700	−1.87100	4.99100
H	3.55800	−4.16800	1.80800
H	2.95200	−5.20800	−0.69600
H	1.26500	−3.28700	−1.77100
B	2.39300	−1.62200	2.39200
C	−1.09500	−0.70300	3.00100
C	−0.77300	−1.07500	4.31500
C	0.55500	−1.49400	4.23100
C	2.93100	−3.76800	1.01300
C	2.61700	−4.27300	−0.25000
C	1.76800	−3.30500	−0.80500
N	−0.04000	−0.87900	2.19300
N	1.59400	−2.29200	0.05900
N	0.96600	−1.36300	2.95400
N	2.30600	−2.58600	1.17300
Fe	−0.00000	−0.83900	−0.00000
H	−3.03100	−0.16800	0.24100
H	−1.04100	4.33300	0.03500
H	1.04000	4.33300	−0.03600
H	3.03100	−0.16800	−0.24300
C	−2.63100	0.84800	0.19400
C	−3.50600	1.96400	0.23900
C	−2.91800	3.26500	0.17900
C	−1.50700	3.34700	0.08100
C	−0.74100	2.19500	0.04600
C	0.74100	2.19500	−0.04700
C	1.50600	3.34700	−0.08200
C	2.91800	3.26500	−0.18000
C	3.50600	1.96400	−0.24100
C	2.63100	0.84800	−0.19600
N	−1.32600	0.96000	0.09900
N	1.32600	0.96100	−0.10100
C	3.76900	4.40300	−0.22000
H	3.32600	5.40200	−0.17400
C	4.91400	1.82600	−0.33600
C	5.71600	2.94800	−0.37200

C	5.13600	4.24300	−0.31500
H	5.34700	0.82200	−0.37200
C	−3.76900	4.40300	0.21900
H	−3.32600	5.40200	0.17300
C	−4.91500	1.82600	0.33400
C	−5.71600	2.94800	0.37100
C	−5.13700	4.24300	0.31400
H	−5.34800	0.82200	0.37100
H	−5.78600	5.12300	0.34400
H	−6.80300	2.84600	0.44200
H	6.80200	2.84600	−0.44300
H	5.78600	5.12300	−0.34500

42) Another reduced HS complex for $N_{\mathrm{c}} = 4$, $\mathrm{Charge} = -1$, $S = 3/2$

H	2.85000	−0.81800	2.21400
H	2.77300	−2.50600	3.36100
H	−2.04100	−0.09300	2.53500
H	−1.62100	−0.95700	5.13800
H	0.92900	−2.06100	5.01300
H	3.15400	−4.46900	1.85400
H	2.63100	−5.32600	−0.74100
H	1.23300	−3.18800	−1.82200
B	2.23000	−1.84000	2.48200
C	−1.17100	−0.58400	2.96800
C	−0.95200	−1.03100	4.28200
C	0.32500	−1.59100	4.24000
C	2.63100	−3.97300	1.03800
C	2.36300	−4.38200	−0.26800
C	1.66200	−3.30200	−0.82800
N	−0.10600	−0.85300	2.20200
N	1.53000	−2.31900	0.07400
N	0.80500	−1.46800	2.98500
N	2.12200	−2.73800	1.21400
H	−2.85000	−0.81800	−2.21400
H	−2.77300	−2.50600	−3.36100
H	2.04100	−0.09300	−2.53500
H	1.62100	−0.95700	−5.13800
H	−0.92900	−2.06200	−5.01300
H	−3.15400	−4.47000	−1.85300
H	−2.63100	−5.32600	0.74100
H	−1.23300	−3.18800	1.82200
B	−2.23000	−1.84000	−2.48200
C	1.17100	−0.58400	−2.96800
C	0.95200	−1.03100	−4.28200
C	−0.32500	−1.59200	−4.24000
C	−2.63100	−3.97300	−1.03800
C	−2.36300	−4.38200	0.26900
C	−1.66200	−3.30200	0.82800
N	0.10600	−0.85400	−2.20200
N	−1.53000	−2.31900	−0.07400
N	−0.80500	−1.46800	−2.98500
N	−2.12200	−2.73800	−1.21400
Fe	−0.00000	−0.73700	−0.00000
H	3.04900	−0.11600	−0.08600
H	1.04300	4.39100	−0.06600
H	−1.04300	4.39100	0.06600
H	−3.04900	−0.11600	0.08600

C	2.64100	0.90000	−0.08600
C	3.52700	2.02300	−0.13300
C	2.91900	3.32600	−0.12600
C	1.51500	3.40700	−0.07000
C	0.72200	2.23600	−0.02700
C	−0.72200	2.23600	0.02700
C	−1.51400	3.40800	0.07000
C	−2.91900	3.32600	0.12600
C	−3.52700	2.02300	0.13300
C	−2.64100	0.90000	0.08600
N	1.33500	1.00700	−0.03800
N	−1.33500	1.00700	0.03800
C	−3.78800	4.45900	0.17700
H	−3.34700	5.46100	0.17300
C	−4.92600	1.88700	0.18400
C	−5.74900	3.01200	0.23300
C	−5.16400	4.29600	0.23000
H	−5.35700	0.88000	0.18100
C	3.78800	4.45900	−0.17700
H	3.34700	5.46100	−0.17300
C	4.92600	1.88700	−0.18400
C	5.75000	3.01200	−0.23300
C	5.16400	4.29600	−0.23000
H	5.35700	0.88000	−0.18200
H	5.80900	5.18100	−0.26800
H	6.83700	2.90300	−0.27200
H	−5.80900	5.18100	0.26800
H	−6.83700	2.90300	0.27200

43) Another neutral LS complex for $N_c = 6$, Charge $= 0$, $S = 0$

H	−2.98600	−1.24300	−2.08800
H	−2.85400	−2.94500	−3.17600
H	1.98000	−0.55900	−2.41700
H	1.39800	−1.15000	−5.04000
H	−1.15800	−2.23800	−4.88400
H	−3.49500	−4.70300	−1.49200
H	−2.76000	−5.59500	1.03600
H	−0.95900	−3.67200	1.87300
B	−2.32500	−2.25400	−2.31400
C	1.06900	−0.98300	−2.82900
C	0.77100	−1.29600	−4.16300
C	−0.50600	−1.84900	−4.10500
C	−2.81500	−4.27100	−0.76000
C	−2.43600	−4.69900	0.51000
C	−1.52700	−3.72400	0.94700
N	0.04300	−1.31700	−2.02900
N	−1.38300	−2.77300	0.01100
N	−0.91600	−1.84700	−2.82000
N	−2.17100	−3.11700	−1.03500
H	2.98600	−1.24300	2.08800
H	2.85400	−2.94500	3.17600
H	−1.98000	−0.55900	2.41700
H	−1.39800	−1.15000	5.04000
H	1.15800	−2.23800	4.88400
H	3.49500	−4.70200	1.49200
H	2.76000	−5.59400	−1.03600
H	0.95900	−3.67200	−1.87300

B	2.32500	−2.25400	2.31400
C	−1.06900	−0.98300	2.82900
C	−0.77100	−1.29700	4.16300
C	0.50600	−1.84900	4.10500
C	2.81500	−4.27100	0.76000
C	2.43600	−4.69900	−0.51000
C	1.52700	−3.72400	−0.94700
N	−0.04300	−1.31700	2.02900
N	1.38300	−2.77300	−0.01100
N	0.91600	−1.84700	2.82000
N	2.17100	−3.11700	1.03500
Fe	−0.00000	−1.31000	−0.00000
H	−3.00400	−0.95300	0.13700
H	−1.05100	3.57000	−0.01200
H	1.05100	3.57000	0.01300
H	3.00400	−0.95300	−0.13700
C	−2.60800	0.06100	0.07600
C	−3.50300	1.17000	0.08100
C	−2.93400	2.49000	0.03700
C	−1.51300	2.58200	0.00400
C	−0.73600	1.44700	0.00300
C	0.73600	1.44700	−0.00300
C	1.51300	2.58200	−0.00400
C	2.93400	2.49100	−0.03700
C	3.50300	1.17000	−0.08100
C	2.60800	0.06100	−0.07600
N	−1.30300	0.18100	0.02200
N	1.30300	0.18100	−0.02200
C	3.78700	3.60100	−0.03600
H	3.36100	4.60800	−0.00200
C	4.89100	1.00400	−0.12000
C	5.75000	2.11400	−0.11800
C	5.18200	3.44500	−0.07600
H	5.31000	−0.00600	−0.14400
C	−3.78700	3.60100	0.03600
H	−3.36100	4.60800	0.00200
C	−4.89100	1.00400	0.12000
C	−5.75000	2.11400	0.11800
C	−5.18200	3.44500	0.07600
H	−5.31000	−0.00600	0.14400
C	6.07100	4.56600	−0.07500
H	5.64200	5.57300	−0.04300
C	7.17200	1.97300	−0.15400
C	7.99000	3.07500	−0.15100
H	9.07700	2.95400	−0.17900
C	7.43200	4.38800	−0.11100
H	8.09800	5.25500	−0.11000
C	−6.07100	4.56600	0.07500
H	−5.64200	5.57300	0.04300
C	−7.17300	1.97200	0.15400
C	−7.99000	3.07500	0.15100
H	−9.07700	2.95400	0.17900
C	−7.43200	4.38800	0.11200
H	−8.09800	5.25500	0.11000
H	−7.59600	0.96400	0.18300
H	7.59600	0.96400	−0.18300

44) Another reduced LS complex for $N_{\mathrm{c}} = 6,\ \mathrm{Charge} = -1,\ S = 1/2$

H	−2.98500	1.40400	2.17400
H	−2.71500	3.12500	3.21600
H	1.92400	0.40200	2.38700
H	1.42100	1.03000	5.02400
H	−1.05400	2.29900	4.89800
H	−3.37300	4.83200	1.50000
H	−2.73000	5.60700	−1.09500
H	−1.01500	3.60400	−1.92800
B	−2.25900	2.37700	2.35500
C	1.05700	0.89500	2.81500
C	0.79700	1.22700	4.15400
C	−0.43700	1.87000	4.11200
C	−2.73500	4.35800	0.75700
C	−2.40500	4.72500	−0.54500
C	−1.54000	3.70800	−0.98200
N	0.05100	1.30700	2.02900
N	−1.37700	2.79300	−0.01400
N	−0.86000	1.90100	2.83000
N	−2.10700	3.20000	1.04800
H	2.98500	1.40500	−2.17400
H	2.71500	3.12500	−3.21600
H	−1.92400	0.40200	−2.38700
H	−1.42100	1.03000	−5.02400
H	1.05400	2.29900	−4.89800
H	3.37300	4.83300	−1.50000
H	2.73000	5.60700	1.09500
H	1.01500	3.60400	1.92800
B	2.25900	2.37700	−2.35500
C	−1.05700	0.89500	−2.81500
C	−0.79700	1.22800	−4.15400
C	0.43700	1.87000	−4.11200
C	2.73500	4.35800	−0.75700
C	2.40500	4.72500	0.54500
C	1.54000	3.70800	0.98200
N	−0.05100	1.30700	−2.02900
N	1.37700	2.79300	0.01400
N	0.86000	1.90200	−2.83000
N	2.10700	3.20000	−1.04800
Fe	0.00000	1.30800	0.00000
H	−3.01100	0.93600	−0.06500
H	−1.05200	−3.58400	−0.01300
H	1.05200	−3.58400	0.01300
H	3.01100	0.93600	0.06500
C	−2.61100	−0.07800	−0.03400
C	−3.51000	−1.18700	−0.04600
C	−2.93300	−2.51200	−0.03400
C	−1.51900	−2.59800	−0.01200
C	−0.72500	−1.45000	−0.00000
C	0.72500	−1.45000	0.00000
C	1.51900	−2.59800	0.01200
C	2.93300	−2.51200	0.03300
C	3.51000	−1.18700	0.04600
C	2.61100	−0.07800	0.03400
N	−1.30100	−0.19500	−0.00200
N	1.30100	−0.19500	0.00200
C	3.79900	−3.62000	0.05000
H	3.37500	−4.62900	0.04100
C	4.89600	−1.02400	0.07200

C	5.76900	−2.13500	0.08800
C	5.20000	−3.46600	0.07700
H	5.31400	−0.01200	0.07400
C	−3.79900	−3.62000	−0.05000
H	−3.37500	−4.62900	−0.04100
C	−4.89600	−1.02400	−0.07200
C	−5.76900	−2.13500	−0.08800
C	−5.20000	−3.46600	−0.07700
H	−5.31400	−0.01200	−0.07400
C	6.09300	−4.57900	0.09500
H	5.66600	−5.58700	0.08700
C	7.18400	−1.99300	0.11400
C	8.01800	−3.09700	0.13000
H	9.10400	−2.96600	0.14900
C	7.46300	−4.40100	0.12100
H	8.12600	−5.27300	0.13300
C	−6.09300	−4.57900	−0.09500
H	−5.66600	−5.58700	−0.08700
C	−7.18400	−1.99300	−0.11400
C	−8.01800	−3.09700	−0.13000
H	−9.10400	−2.96600	−0.14900
C	−7.46300	−4.40100	−0.12100
H	−8.12600	−5.27300	−0.13300
H	−7.60400	−0.98200	−0.11900
H	7.60400	−0.98200	0.11900

45) Another neutral HS complex for $N_{\mathrm{c}} = 6,\ \mathrm{Charge} = 0,\ S = 2$

H	−2.83900	−1.19400	−2.13400
H	−2.94800	−2.82400	−3.34800
H	2.10400	−0.94400	−2.54200
H	1.55500	−1.66600	−5.15600
H	−1.09200	−2.50400	−5.02300
H	−3.48900	−4.80800	−1.90000
H	−2.95100	−5.83600	0.62500
H	−1.30700	−3.90100	1.74100
B	−2.32200	−2.25800	−2.45900
C	1.17600	−1.31900	−2.97000
C	0.89400	−1.69500	−4.29200
C	−0.43400	−2.12200	−4.24500
C	−2.88800	−4.40300	−1.08800
C	−2.60900	−4.90100	0.18500
C	−1.78200	−3.92600	0.76100
N	0.09900	−1.50100	−2.19100
N	−1.58800	−2.91500	−0.10100
N	−0.88100	−1.99200	−2.98000
N	−2.26500	−3.21700	−1.23400
H	2.84000	−1.19200	2.13300
H	2.94900	−2.82100	3.34900
H	−2.10300	−0.94200	2.54200
H	−1.55400	−1.66100	5.15700
H	1.09300	−2.49900	5.02400
H	3.48900	−4.80600	1.90200
H	2.95100	−5.83700	−0.62100
H	1.30600	−3.90300	−1.73900
B	2.32300	−2.25600	2.46000
C	−1.17500	−1.31700	2.97000
C	−0.89300	−1.69100	4.29300

C	0.43500	−2.11800	4.24600
C	2.88800	−4.40200	1.09100
C	2.60900	−4.90100	−0.18300
C	1.78200	−3.92600	−0.75900
N	−0.09900	−1.49900	2.19200
N	1.58800	−2.91500	0.10200
N	0.88200	−1.99000	2.98100
N	2.26500	−3.21600	1.23500
Fe	−0.00000	−1.45500	−0.00000
H	−3.02900	−0.79700	0.14700
H	−1.04200	3.71400	−0.02700
H	1.04200	3.71400	0.02600
H	3.02900	−0.79700	−0.14800
C	−2.62900	0.22000	0.10500
C	−3.51800	1.33600	0.10700
C	−2.92900	2.64900	0.05600
C	−1.50800	2.72700	0.01200
C	−0.74100	1.58300	0.01700
C	0.74100	1.58300	−0.01700
C	1.50700	2.72800	−0.01200
C	2.92900	2.64900	−0.05700
C	3.51700	1.33600	−0.10800
C	2.62900	0.22000	−0.10600
N	−1.32800	0.33600	0.05800
N	1.32800	0.33600	−0.05900
C	3.77000	3.77000	−0.05300
H	3.33200	4.77200	−0.01500
C	4.90700	1.18800	−0.14900
C	5.75200	2.30800	−0.14500
C	5.16600	3.63100	−0.09800
H	5.33800	0.18200	−0.17800
C	−3.77000	3.77000	0.05300
H	−3.33300	4.77200	0.01400
C	−4.90700	1.18700	0.14800
C	−5.75200	2.30700	0.14400
C	−5.16700	3.63100	0.09700
H	−5.33800	0.18200	0.17700
C	6.04100	4.76400	−0.09500
H	5.60000	5.76400	−0.05900
C	7.17600	2.18400	−0.18500
C	7.97900	3.29700	−0.18100
H	9.06800	3.19000	−0.21200
C	7.40400	4.60200	−0.13600
H	8.05900	5.47800	−0.13300
C	−6.04100	4.76300	0.09400
H	−5.60000	5.76400	0.05900
C	−7.17600	2.18400	0.18500
C	−7.98000	3.29700	0.18000
H	−9.06800	3.19000	0.21100
C	−7.40400	4.60200	0.13500
H	−8.05900	5.47800	0.13200
H	−7.61200	1.18100	0.21800
H	7.61200	1.18100	−0.21900

46) Another reduced HS complex for $N_{\mathrm{c}} = 6,\ \mathrm{Charge} = -1,\ S = 3/2$

H	−2.72600	−1.39200	−2.33700
H	−2.63800	−3.06800	−3.50000

H	2.19300	−0.78700	−2.43000
H	1.87300	−1.61500	−5.05600
H	−0.70800	−2.65300	−5.06300
H	−3.11700	−5.04500	−2.03400
H	−2.71500	−5.94300	0.56700
H	−1.32800	−3.84300	1.73400
B	−2.11900	−2.42600	−2.59000
C	1.33000	−1.25000	−2.90700
C	1.16300	−1.67900	−4.23400
C	−0.12900	−2.20600	−4.25700
C	−2.62000	−4.56700	−1.19100
C	−2.41200	−4.99800	0.11900
C	−1.71700	−3.93700	0.72100
N	0.22400	−1.49700	−2.19400
N	−1.53300	−2.94500	−0.16100
N	−0.66400	−2.08100	−3.02500
N	−2.08400	−3.33900	−1.33000
H	2.72700	−1.39600	2.33700
H	2.63700	−3.07300	3.49900
H	−2.19200	−0.78800	2.43100
H	−1.87300	−1.61900	5.05700
H	0.70800	−2.65800	5.06200
H	3.11500	−5.04900	2.03100
H	2.71200	−5.94400	−0.57200
H	1.32700	−3.84200	−1.73600
B	2.11900	−2.42900	2.59000
C	−1.33000	−1.25200	2.90700
C	−1.16200	−1.68200	4.23400
C	0.12900	−2.21000	4.25700
C	2.61900	−4.57000	1.18900
C	2.41000	−5.00000	−0.12300
C	1.71600	−3.93700	−0.72400
N	−0.22400	−1.49900	2.19400
N	1.53200	−2.94600	0.15900
N	0.66400	−2.08400	3.02500
N	2.08300	−3.34100	1.32900
Fe	0.00000	−1.37900	0.00000
H	−3.04600	−0.76000	−0.04500
H	−1.03400	3.73800	0.06000
H	1.03400	3.73800	−0.06000
H	3.04700	−0.76000	0.04700
C	−2.63900	0.25500	−0.02000
C	−3.52700	1.37400	0.00800
C	−2.92700	2.68800	0.04000
C	−1.50800	2.75600	0.03300
C	−0.73200	1.59900	0.00300
C	0.73300	1.59900	−0.00200
C	1.50900	2.75600	−0.03300
C	2.92700	2.68800	−0.03900
C	3.52700	1.37400	−0.00700
C	2.63900	0.25500	0.02200
N	−1.32900	0.36200	−0.02100
N	1.32900	0.36200	0.02300
C	3.77200	3.80900	−0.07600
H	3.33100	4.81100	−0.10100
C	4.91600	1.23400	−0.00900
C	5.77000	2.36000	−0.04600
C	5.17800	3.68000	−0.08100

H	5.35200	0.23000	0.02200
C	−3.77200	3.80900	0.07600
H	−3.33000	4.81100	0.10100
C	−4.91600	1.23400	0.01000
C	−5.76900	2.36000	0.04700
C	−5.17700	3.68000	0.08200
H	−5.35200	0.23100	−0.02000
C	6.04900	4.80800	−0.12000
H	5.60400	5.80800	−0.14700
C	7.18700	2.24400	−0.04900
C	8.00000	3.36200	−0.08700
H	9.08900	3.25100	−0.08900
C	7.42300	4.65600	−0.12300
H	8.07000	5.53800	−0.15300
C	−6.04900	4.80800	0.12000
H	−5.60300	5.80800	0.14700
C	−7.18700	2.24400	0.05000
C	−8.00000	3.36200	0.08800
H	−9.08900	3.25100	0.08900
C	−7.42200	4.65600	0.12300
H	−8.07000	5.53800	0.15300
H	−7.62600	1.24100	0.02200
H	7.62600	1.24100	−0.02000