Supporting Information for Statistical Errors in Active-Space Reduced Density Matrices Sampled from Quantum Circuit Simulators and the Impact on Multireference Theory Calculations

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S1 Derivation of observation probability representation for elements of reduced density matrices

In this section, we present derivation of observation probability representation for elements of reduced density matrices by using an example of $\langle\Psi|a_p^\dagger a_q|\Psi\rangle$ with indices such that $p > q$ for simplicity.

With Jordan-Wigner transformation, and with the relations $P_p^X = H_p P_p^Z H_p$ and $P_p^Y = R_p^X[-\pi/2] P_p^Z R_p^X[\pi/2]$, the reduced density operator is transformed into representation with P_p^Z, H_p, and R_p^X:

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$$
\begin{aligned}
& a_p^\dagger a_q \\
&= \frac{1}{2}\left[\prod_{l=1}^{p-1} P_l^Z\right](P_p^X - jP_p^Y)\cdot\frac{1}{2}\left[\prod_{m=1}^{q-1} P_m^Z\right](P_q^X + jP_q^Y) && \text{(S1)}\\
&= \frac{1}{4}\left[\prod_{l=q}^{p-1} P_l^Z\right](P_p^X - jP_p^Y)(P_q^X + jP_q^Y) && \text{(S2)}\\
&= \frac{1}{4}\left[\prod_{l=q}^{p-1} P_l^Z\right](P_p^X P_q^X + jP_p^X P_q^Y - jP_p^Y P_q^X + P_p^Y P_q^Y) && \text{(S3)}\\
&= \frac{1}{4}\left[\prod_{l=q}^{p-1} P_l^Z\right]\Big\{(H_p P_p^Z H_p)(H_q P_q^Z H_q) + j(H_p P_p^Z H_p)(R_q^X[-\pi/2]P_q^Z R_q^X[\pi/2]) \\
&- j(R_p^X[-\pi/2]P_p^Z R_p^X[\pi/2])(H_q P_q^Z H_q) + (R_p^X[-\pi/2]P_p^Z R_p^X[\pi/2])(R_q^X[-\pi/2]P_q^Z R_q^X[\pi/2])\Big\}, && \text{(S4)}
\end{aligned}
$$

$$
\begin{aligned}
& 4a_p^\dagger a_q \\
&= H_q H_p\left[\prod_{l=q+1}^{p} P_l^Z\right]H_p H_q + j\cdot R_q^X[-\pi/2]H_p\left[\prod_{l=q+1}^{p} P_l^Z\right]H_p R_q^X[\pi/2] \\
&- j\cdot H_q R_p^X[-\pi/2]\left[\prod_{l=q+1}^{p} P_l^Z\right]R_p^X[\pi/2]H_q + R_q^X[-\pi/2]R_p^X[-\pi/2]\left[\prod_{l=q+1}^{p} P_l^Z\right]R_p^X[\pi/2]R_q^X[\pi/2]. && \text{(S5)}
\end{aligned}
$$

Therefore the matrix element for a CAS wavefunction $|\Psi_{\mathrm{CAS}}\rangle$ is written as

$$
\begin{aligned}
\langle\Psi_{\mathrm{CAS}}|a_p^\dagger a_q|\Psi_{\mathrm{CAS}}\rangle &= \frac{1}{4}\langle\Psi_{\mathrm{CAS}}|H_q H_p\left[\prod_{l=q+1}^{p} P_l^Z\right]H_p H_q|\Psi_{\mathrm{CAS}}\rangle \\
&+ \frac{j}{4}\langle\Psi_{\mathrm{CAS}}|R_q^X[-\pi/2]H_p\left[\prod_{l=q+1}^{p} P_l^Z\right]H_p R_q^X[\pi/2]|\Psi_{\mathrm{CAS}}\rangle \\
&- \frac{j}{4}\langle\Psi_{\mathrm{CAS}}|H_q R_p^X[-\pi/2]\left[\prod_{l=q+1}^{p} P_l^Z\right]R_p^X[\pi/2]H_q|\Psi_{\mathrm{CAS}}\rangle \\
&+ \frac{1}{4}\langle\Psi_{\mathrm{CAS}}|R_q^X[-\pi/2]R_p^X[-\pi/2]\left[\prod_{l=q+1}^{p} P_l^Z\right]R_p^X[\pi/2]R_q^X[\pi/2]|\Psi_{\mathrm{CAS}}\rangle. && \text{(S6)}
\end{aligned}
$$

Let $|\mathbf{k}\rangle$ be an occupation number vector,

$$|\mathbf{k}\rangle = |k_1, \cdots, k_p, \cdots, k_N\rangle \tag{S7}$$

$$= |k_1\rangle \otimes \cdots \otimes |k_p\rangle \otimes \cdots \otimes |k_N\rangle . \tag{S8}$$

Here, k_p is equal to 1 if the p-th spin-orbital is occupied; otherwise k_p is equal to 0. $|0\rangle$ and $|1\rangle$ correspond to the eigenstate of P^Z for a qubit. In eq.(S6), the CAS wavefunction $|\Psi_{\mathrm{CAS}}\rangle$, which is written with expansion coefficients $c_{\mathbf{k}}$ as $|\Psi_{\mathrm{CAS}}\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}} |\mathbf{k}\rangle$, is transformed by several unitary operators. We denote these unitary-transformed wavefunctions as following:

$$|\Psi^{HH}\rangle \equiv H_p H_q |\Psi_{\mathrm{CAS}}\rangle = \sum_{\mathbf{k}} \tilde{c}^{HH}_{\mathbf{k}} |\mathbf{k}\rangle , \tag{S9}$$

$$|\Psi^{HR}\rangle \equiv H_p R^X_q[\pi/2] |\Psi_{\mathrm{CAS}}\rangle = \sum_{\mathbf{k}} \tilde{c}^{HR}_{\mathbf{k}} |\mathbf{k}\rangle , \tag{S10}$$

$$|\Psi^{RH}\rangle \equiv R^X_p[\pi/2] H_q |\Psi_{\mathrm{CAS}}\rangle = \sum_{\mathbf{k}} \tilde{c}^{RH}_{\mathbf{k}} |\mathbf{k}\rangle , \tag{S11}$$

$$|\Psi^{RR}\rangle \equiv R^X_p[\pi/2] R^X_q[\pi/2] |\Psi_{\mathrm{CAS}}\rangle = \sum_{\mathbf{k}} \tilde{c}^{RR}_{\mathbf{k}} |\mathbf{k}\rangle . \tag{S12}$$

By using eq.(S9) and $P^Z = |0\rangle\langle 0| - |1\rangle\langle 1|$, we rewrite the first term in eq.(S6) as

$$\begin{aligned}
&\frac{1}{4}\langle\Psi_{\mathrm{CAS}}|H_q H_p \left[\prod_{l=q+1}^{p} P^Z_l\right] H_p H_q|\Psi_{\mathrm{CAS}}\rangle \\
=&\frac{1}{4}\langle\Psi^{HH}| \left[\prod_{l=q+1}^{p} P^Z_l\right] |\Psi^{HH}\rangle \\
=&\frac{1}{4}\langle\Psi^{HH}| \left[\prod_{l=q+1}^{p} \Big(|0_l\rangle\langle 0_l| - |1_l\rangle\langle 1_l|\Big)\right] |\Psi^{HH}\rangle \\
=&\frac{1}{4}\langle\Psi^{HH}|(-1)^{\sum_{l=q+1}^{p} k_l}|\Psi^{HH}\rangle \\
=&\frac{1}{4}\sum_{\mathbf{k}}(-1)^{\sum_{l=q+1}^{p} k_l}|\tilde{c}^{HH}_{\mathbf{k}}|^2.
\end{aligned} \tag{S13}$$

As a result of the above transformation, the first term in eq.(S6) can be expressed as a function of $|\tilde{c}_{\mathbf{k}}^{HH}|^2$. By applying similar transformations to the remaining terms in eq.(S6), and also to one-particle reduced density operators with indices such that $p \leq q$, each component of 1RDM can be estimated based on $|\tilde{c}_{\mathbf{k}}|^2$, that is, the probability of obtaining state $|\mathbf{k}\rangle$ by observing the unitary-tranformed CAS wave function represented on the quantum circuit. Higher order RDMs can be estimated in the same way.

S2 Estimation of the N_{sample} sufficient for the chemical accuracy for polyenes

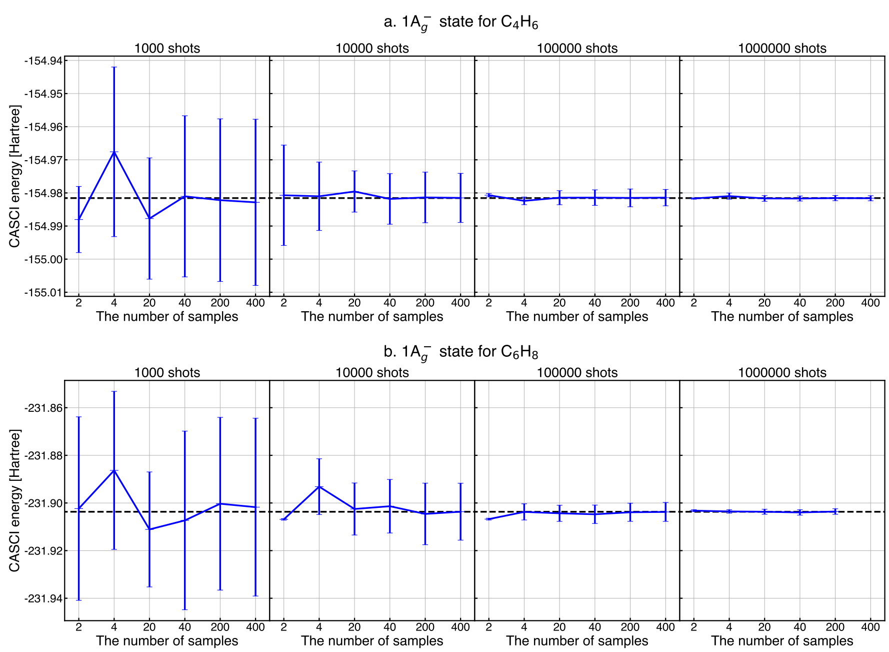

Figure S1: The convergence behaviour of the sample-mean CASCI energy of $1A_g^-$ state for C_4H_6 and C_6H_8.

We chose the value of N_{sample} as the number of sample that is sufficient for the sample-mean CASCI energy of the $1A_g^-$ state to converge within the chemical accuracy (1.0 kcal/mol) to the exact energy. As Fig. S1 shows, the values of N_{sample} are determined to be 100 for $N_{\text{shot}} = 10^3$ and 10^4, and 20 for $N_{\text{shot}} = 10^5, 10^6$.

S3 Least square fitting for the sampled CASCI energies and the sampled CASPT2 energies

Table S1: Least square fitting for the sampled CASCI energies

		A	B	R^2
	$1A_g^-$	0.8806	-0.0005	0.9994
C_4H_6	$2A_g^-$	1.8318	-0.0006	0.9984
	$1B_u^+$	1.3736	+0.0004	0.9995
	$1A_g^-$	1.2475	-0.0002	1.0000
C_6H_8	$2A_g^-$	2.0686	-0.0002	0.9970
	$1B_u^+$	2.0031	-0.0012	0.9982

The parameters A and B are defined as

$$\sigma(E) = A/\sqrt{N_{\text{shot}}} + B, \tag{S14}$$

and R^2 is the coefficient of determination.

S4 Expected value of the sum of squared errors between the classical CI vector and the observed vector

A set of squared CI coefficients in a CAS wavefunction $|\Psi\rangle = \sum_i c_i |\psi_i\rangle$ can be considered as a set of probabilities P where a configuration $|\psi_i\rangle$ is observed in the simulation of the present work,

Table S2: Least square fitting for the sampled cu(4)-CASPT2 energies

		A	B	R^2
	$1A_g^-$	0.8860	-0.0005	0.9995
C_4H_6	$2A_g^-$	1.8433	-0.0005	0.9985
	$1B_u^+$	1.3628	+0.0004	0.9995
	$1A_g^-$	1.3138	-0.0008	0.9977
C_6H_8	$2A_g^-$	2.0022	-0.0000	0.9973
	$1B_u^+$	1.1464	+0.0028	0.9593

Table S3: Least square fitting for the sampled cu(3,4)-CASPT2 energies

		A	B	R^2
	$1A_g^-$	0.9522	-0.0007	0.9980
C_4H_6	$2A_g^-$	1.8392	-0.0005	0.9984
	$1B_u^+$	1.3923	+0.0006	0.9994
	$1A_g^-$	1.2946	-0.0008	0.9989
C_6H_8	$2A_g^-$	2.0621	-0.0002	0.9972
	$1B_u^+$	1.2153	+0.0024	0.9685

$$P = \{|c_1|^2, |c_2|^2, \cdots, |c_k|^2\} \tag{S15}$$

$$= \{p_1, p_2, \cdots, p_k\}. \tag{S16}$$

By definition, the sum of p_i is equal to 1,

$$\sum_i^k p_k = 1. \tag{S17}$$

Let us assume that we perform the sampling with N_{shot} and obtain an results R where $|\psi_i\rangle$ is observed n_i times,

$$R = \{n_1, n_2, \cdots, n_k\}, \tag{S18}$$

and that R follows multinomial distribution with parameters N_{shot} and P. The probability mass function (PMF) is given as

$$\mathrm{PMF}(R; N_{\mathrm{shot}}, P) = \frac{N_{\mathrm{shot}}!}{n_1!n_2!\cdots n_k!} p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k}. \tag{S19}$$

The expected value for n_i, $\mathbb{E}[n_i]$, and the variance for n_i, $\mathrm{var}[n_i]$, are given as

$$\mathbb{E}[n_i] = N_{\mathrm{shot}} p_i, \tag{S20}$$

$$\mathrm{var}[n_i] = N_{\mathrm{shot}} p_i (1 - p_i). \tag{S21}$$

Here we define the observation error as the sum of squared errors (SSE) between P and R/N_{shot},

$$\mathrm{SSE}(R; N_{\mathrm{shot}}, P) = \sum_i^k (n_i/N_{\mathrm{shot}} - p_i)^2. \tag{S22}$$

The expected value for $\mathrm{SSE}(R; N_{\mathrm{shot}}, P)$ is given by definition as

$$\begin{aligned}\mathbb{E}[\mathrm{SSE}(R; N_{\mathrm{shot}}, P)] &= \sum_{n_1,\cdots,n_k} \left\{ \mathrm{PMF}(R; N_{\mathrm{shot}}, P) \sum_{i}^{k} (n_i/N_{\mathrm{shot}} - p_i)^2 \right\} &\text{(S23)}\\ &= \sum_{i}^{k} \mathbb{E}[(n_i/N_{\mathrm{shot}} - p_i)^2] &\text{(S24)}\end{aligned}$$

The following formula transformation is performed by focusing on the term with $(n_i/N_{\mathrm{shot}} - p_i)^2$ of eq. (S24),

$$\begin{aligned}&\mathbb{E}[(n_i/N_{\mathrm{shot}} - p_i)^2] &\text{(S25)}\\ =&\sum_{n_1,\cdots,n_k} \mathrm{PMF}(R; N_{\mathrm{shot}}, P)(n_i^2/N_{\mathrm{shot}}^2 - 2n_i p_i/N_{\mathrm{shot}} + p_i^2) &\text{(S26)}\\ =&\frac{\mathbb{E}[n_i^2]}{N_{\mathrm{shot}}^2} - \frac{2p_i\mathbb{E}[n_i]}{N_{\mathrm{shot}}} + p_i^2 \sum_{n_1,\cdots,n_k} \mathrm{PMF}(R; N_{\mathrm{shot}}, P) &\text{(S27)}\\ =&\frac{\mathrm{var}[n_i] + \mathbb{E}[n_i]^2}{N_{\mathrm{shot}}^2} - \frac{2p_i N_{\mathrm{shot}} p_i}{N_{\mathrm{shot}}} + p_i^2 \cdot 1 &\text{(S28)}\\ =&\frac{N_{\mathrm{shot}} p_i(1-p_i) + N_{\mathrm{shot}}^2 p_i^2}{N_{\mathrm{shot}}^2} - \frac{2p_i N_{\mathrm{shot}} p_i}{N_{\mathrm{shot}}} + p_i^2 &\text{(S29)}\\ =&\frac{p_i - p_i^2}{N_{\mathrm{shot}}}. &\text{(S30)}\end{aligned}$$

By summing over all i, the following formula is obtained,

$$\begin{aligned}\mathbb{E}[\mathrm{SSE}(R; N_{\mathrm{shot}}, P)] &= \sum_{i}^{k} \frac{p_i - p_i^2}{N_{\mathrm{shot}}}\\ &= \frac{1 - \sum_i^k p_i^2}{N_{\mathrm{shot}}} &\text{(S31)}\\ &= \frac{1 - \sum_i^k |c_i|^4}{N_{\mathrm{shot}}}. &\text{(S32)}\end{aligned}$$

From the inequality of the arithmetic mean and the geometric mean, it follows that the maximum value of $\mathbb{E}[\mathrm{SSE}(R; N_{\mathrm{shot}}, P)]$ with fixed N_{shot} and k is $(1 - \frac{1}{k})/N_{\mathrm{shot}}$, which is reached when $p_i = \frac{1}{k}$ for all i.

S5 Geometries of $\{[Cu(NH_3)_3]_2O_2\}^{2+}$ complex along the reaction coordinate

$F = 0.0$

1	O	0.00000000	0.00000000	1.14524700
2	O	0.00000000	0.00000000	-1.14524700
3	Cu	-0.16460900	1.39103100	0.00000000
4	Cu	0.16460900	-1.39103100	0.00000000
5	N	0.00000000	2.69289600	-1.50278000
6	N	0.00000000	2.69289600	1.50278000
7	N	0.00000000	-2.69289600	1.50278000
8	N	0.00000000	-2.69289600	-1.50278000
9	N	-2.62497900	1.61604600	0.00000000
10	N	2.62497900	-1.61604600	0.00000000
11	H	-3.19950700	2.46202600	0.00000000
12	H	3.19950700	-2.46202600	0.00000000
13	H	-2.93875400	1.07966600	0.81100500
14	H	2.93875400	-1.07966600	-0.81100500
15	H	-2.93875400	1.07966600	-0.81100500
16	H	2.93875400	-1.07966600	0.81100500
17	H	0.88252700	3.20934800	-1.53262500
18	H	0.88252700	3.20934800	1.53262500
19	H	-0.88252700	-3.20934800	1.53262500
20	H	-0.88252700	-3.20934800	-1.53262500
21	H	-0.76084000	3.37424500	-1.53392600
22	H	-0.76084000	3.37424500	1.53392600
23	H	0.76084000	-3.37424500	1.53392600
24	H	0.76084000	-3.37424500	-1.53392600
25	H	-0.04996700	2.13380200	-2.35872700
26	H	-0.04996700	2.13380200	2.35872700
27	H	0.04996700	-2.13380200	2.35872700
28	H	0.04996700	-2.13380200	-2.35872700

$F = 0.2$

1	O	0.00000000	0.00000000	1.06233000
2	O	0.00000000	0.00000000	-1.06233000
3	Cu	-0.21403300	1.47433700	0.00000000
4	Cu	0.21403300	-1.47433700	0.00000000
5	N	0.00000000	2.76085100	-1.52335400
6	N	0.00000000	2.76085100	1.52335400
7	N	0.00000000	-2.76085100	1.52335400
8	N	0.00000000	-2.76085100	-1.52335400
9	N	-2.62667900	1.62969200	0.00000000
10	N	2.62667900	-1.62969200	0.00000000
11	H	-3.19635300	2.47857100	0.00000000
12	H	3.19635300	-2.47857100	0.00000000
13	H	-2.93980200	1.09397400	0.81151900
14	H	2.93980200	-1.09397400	-0.81151900
15	H	-2.93980200	1.09397400	-0.81151900
16	H	2.93980200	-1.09397400	0.81151900
17	H	0.90469100	3.21957500	-1.56274200
18	H	0.90469100	3.21957500	1.56274200
19	H	-0.90469100	-3.21957500	1.56274200
20	H	-0.90469100	-3.21957500	-1.56274200
21	H	-0.70904000	3.48395300	-1.54782700
22	H	-0.70904000	3.48395300	1.54782700
23	H	0.70904000	-3.48395300	1.54782700
24	H	0.70904000	-3.48395300	-1.54782700
25	H	-0.09028700	2.21939400	-2.38241400
26	H	-0.09028700	2.21939400	2.38241400
27	H	0.09028700	-2.21939400	2.38241400
28	H	0.09028700	-2.21939400	-2.38241400

$F = 0.4$

1	O	0.00000000	0.00000000	0.97941300
2	O	0.00000000	0.00000000	-0.97941300
3	Cu	-0.26345700	1.55764300	0.00000000
4	Cu	0.26345700	-1.55764300	0.00000000
5	N	0.00000000	2.82880600	-1.54392700
6	N	0.00000000	2.82880600	1.54392700
7	N	0.00000000	-2.82880600	1.54392700
8	N	0.00000000	-2.82880600	-1.54392700
9	N	-2.62837900	1.64333900	0.00000000
10	N	2.62837900	-1.64333900	0.00000000
11	H	-3.19319900	2.49511600	0.00000000
12	H	3.19319900	-2.49511600	0.00000000
13	H	-2.94085000	1.10828200	0.81203400
14	H	2.94085000	-1.10828200	-0.81203400
15	H	-2.94085000	1.10828200	-0.81203400
16	H	2.94085000	-1.10828200	0.81203400
17	H	0.92685400	3.22980200	-1.59285900
18	H	0.92685400	3.22980200	1.59285900
19	H	-0.92685400	-3.22980200	1.59285900
20	H	-0.92685400	-3.22980200	-1.59285900
21	H	-0.65724000	3.59366100	-1.56172800
22	H	-0.65724000	3.59366100	1.56172800
23	H	0.65724000	-3.59366100	1.56172800
24	H	0.65724000	-3.59366100	-1.56172800
25	H	-0.13060700	2.30498500	-2.40610100
26	H	-0.13060700	2.30498500	2.40610100
27	H	0.13060700	-2.30498500	2.40610100
28	H	0.13060700	-2.30498500	-2.40610100

$F = 0.6$

1	O	0.00000000	0.00000000	0.89649600
2	O	0.00000000	0.00000000	-0.89649600
3	Cu	-0.31288200	1.64094800	0.00000000
4	Cu	0.31288200	-1.64094800	0.00000000
5	N	0.00000000	2.89676200	-1.56450100
6	N	0.00000000	2.89676200	1.56450100
7	N	0.00000000	-2.89676200	1.56450100
8	N	0.00000000	-2.89676200	-1.56450100
9	N	-2.63007800	1.65698500	0.00000000
10	N	2.63007800	-1.65698500	0.00000000
11	H	-3.19004600	2.51166000	0.00000000
12	H	3.19004600	-2.51166000	0.00000000
13	H	-2.94189800	1.12259100	0.81254800
14	H	2.94189800	-1.12259100	-0.81254800
15	H	-2.94189800	1.12259100	-0.81254800
16	H	2.94189800	-1.12259100	0.81254800
17	H	0.94901800	3.24002900	-1.62297600
18	H	0.94901800	3.24002900	1.62297600
19	H	-0.94901800	-3.24002900	1.62297600
20	H	-0.94901800	-3.24002900	-1.62297600
21	H	-0.60543900	3.70336800	-1.57563000
22	H	-0.60543900	3.70336800	1.57563000
23	H	0.60543900	-3.70336800	1.57563000
24	H	0.60543900	-3.70336800	-1.57563000
25	H	-0.17092700	2.39057700	-2.42978700
26	H	-0.17092700	2.39057700	2.42978700
27	H	0.17092700	-2.39057700	2.42978700
28	H	0.17092700	-2.39057700	-2.42978700

$F = 0.8$

1	O	0.00000000	0.00000000	0.81357900
2	O	0.00000000	0.00000000	-0.81357900
3	Cu	-0.36230600	1.72425400	0.00000000
4	Cu	0.36230600	-1.72425400	0.00000000
5	N	0.00000000	2.96471700	-1.58507400
6	N	0.00000000	2.96471700	1.58507400
7	N	0.00000000	-2.96471700	1.58507400
8	N	0.00000000	-2.96471700	-1.58507400
9	N	-2.63177800	1.67063200	0.00000000
10	N	2.63177800	-1.67063200	0.00000000
11	H	-3.18689200	2.52820500	0.00000000
12	H	3.18689200	-2.52820500	0.00000000
13	H	-2.94294600	1.13689900	0.81306300
14	H	2.94294600	-1.13689900	-0.81306300
15	H	-2.94294600	1.13689900	-0.81306300
16	H	2.94294600	-1.13689900	0.81306300
17	H	0.97118100	3.25025600	-1.65309300
18	H	0.97118100	3.25025600	1.65309300
19	H	-0.97118100	-3.25025600	1.65309300
20	H	-0.97118100	-3.25025600	-1.65309300
21	H	-0.55363900	3.81307600	-1.58953100
22	H	-0.55363900	3.81307600	1.58953100
23	H	0.55363900	-3.81307600	1.58953100
24	H	0.55363900	-3.81307600	-1.58953100
25	H	-0.21124700	2.47616800	-2.45347400
26	H	-0.21124700	2.47616800	2.45347400
27	H	0.21124700	-2.47616800	2.45347400
28	H	0.21124700	-2.47616800	-2.45347400

$F = 1.0$

1	O	0.00000000	0.00000000	0.73066200
2	O	0.00000000	0.00000000	-0.73066200
3	Cu	-0.41173000	1.80756000	0.00000000
4	Cu	0.41173000	-1.80756000	0.00000000
5	N	0.00000000	3.03267200	-1.60564800
6	N	0.00000000	3.03267200	1.60564800
7	N	0.00000000	-3.03267200	1.60564800
8	N	0.00000000	-3.03267200	-1.60564800
9	N	-2.63347800	1.68427800	0.00000000
10	N	2.63347800	-1.68427800	0.00000000
11	H	-3.18373800	2.54475000	0.00000000
12	H	3.18373800	-2.54475000	0.00000000
13	H	-2.94399400	1.15120700	0.81357700
14	H	2.94399400	-1.15120700	-0.81357700
15	H	-2.94399400	1.15120700	-0.81357700
16	H	2.94399400	-1.15120700	0.81357700
17	H	0.99334500	3.26048300	-1.68321000
18	H	0.99334500	3.26048300	1.68321000
19	H	-0.99334500	-3.26048300	1.68321000
20	H	-0.99334500	-3.26048300	-1.68321000
21	H	-0.50183900	3.92278400	-1.60343200
22	H	-0.50183900	3.92278400	1.60343200
23	H	0.50183900	-3.92278400	1.60343200
24	H	0.50183900	-3.92278400	-1.60343200
25	H	-0.25156700	2.56176000	-2.47716100
26	H	-0.25156700	2.56176000	2.47716100
27	H	0.25156700	-2.56176000	2.47716100
28	H	0.25156700	-2.56176000	-2.47716100