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# Electronic States of the NiCu Molecule Determined by *ab initio* Hartree–Fock and Configuration Interaction Methods

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The interaction between a Ni atom and a Cu atom in the configurations $(3d)^9(4s)^1$ and $(3d)^{10}(4s)^1$, respectively, has been calculated using *ab initio* Hartree–Fock and configuration interaction methods. The chemical bond between the two atoms is due to a bonding $4s\sigma$ molecular orbital. Equilibrium distances, dissociation energies and vibrational frequencies are predicted for the low-lying states. Finally the influence of spin–orbit coupling on the low-lying states is considered.

**Key words:** NiCu molecule, electronic states of the ~

## 1. Introduction

During the last few years homonuclear, diatomic molecules composed of transition metal atoms have been the subject of several investigations both experimentally [1, 2] and theoretically [3–5].

We have undertaken a study of the heteronuclear NiCu molecule. Presently, no experimental data are available for this molecule, but such species probably will receive more attention in the future. Thus, experimental data for other heteronuclear intermetallic molecules have been reported in the literature [6, 7] recently.

There are several reasons for our interest in the NiCu molecule. It represents the smallest possible unit containing information about the NiCu alloy, and this alloy has lately been intensively studied partly due to its characteristic magnetic and catalytic properties. Thus, both the Curie temperature and the average magnetic moment decrease linearly with the Cu content and approach zero at about 40% Ni and 60% Cu [8]. Adding Cu to a Ni catalyst not merely results in a drop in activity, it also causes an enhanced selectivity [9].

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We, of course, did not expect to explain all these phenomena during this investigation, but we expect that a detailed understanding of the interaction between the constituent atoms is necessary for further progress.

In the present work the interaction between a Ni atom and a Cu atom has been investigated using *ab initio* calculations.

Our calculations were carried out in the Hartree–Fock–Roothaan formalism [10] followed by a limited configuration interaction (CI) treatment. The integrals were computed using the program MOLECULE [11], the Hartree–Fock (HF) calculations were performed using ALCHEMY [12], and finally we carried out the CI calculations using ALCHEMY in conjunction with a program written at this laboratory [13].

## 2. Basis Sets and Atomic Configurations

The basis sets used in the calculations consisted of contracted Gaussian type functions ($14s$, $11p$, $5d/8s$, $6p$, $3d$). It was a modification of the basis sets determined by Wachters [14] for the $^3F(3d)^8(4s)^2$ term of the Ni atom, and for the $^2S(3d)^{10}(4s)^1$ term of the Cu atom. The changes of the basis set for the Ni atom have been described previously [5].

The basis set for the Cu atom has undergone similar changes; it was extended by addition of two $p$ functions with exponents 0.25 and 0.10, respectively, and the exponents of the most diffuse $s$ functions were altered from 0.113303 and 0.040791 to 0.25 and 0.08. The alterations provide an orbital appropriate for representing the $4p$ orbital and altogether a better description of the valence region of the molecule.

From the tables of Moore [15] it is known that the $^2S(3d)^{10}(4s)^1$ term of the Cu atom lies 0.0548 a.u. below the $^2D(3d)^9(4s)^2$ term. However, HF calculations performed with the above basis set place the $^2D$ term 0.0030 a.u. below the $^2S$ term.

A similar problem was analyzed in connection with our investigation of the $Ni_2$ molecule [5], and therefore we make no further comments here.

We have chosen to describe the interaction between a Ni atom in the $(3d)^9(4s)^1$ configuration and a Cu atom in the $(3d)^{10}(4s)^1$ configuration. According to our work on the $Ni_2$ molecule we expect that a chemical bond between the two atoms can only arise from the above-mentioned configurations.

## 3. Results of HF and CI Calculations

Due to the arguments presented in the Appendix we have chosen to optimize the molecular orbitals for the $^2\Pi$ state and use the resulting orbitals to describe all low-lying states of the molecule.

HF calculations were performed for the $^2\Pi$ state at internuclear distances 3.60, 4.34, 4.80, 6.00, and 8.00 a.u. The molecular orbitals determined in the HF calculations were utilized in CI calculations allowing full reorganization within the $3d$ and $4s$ shells.

**Table 1.** Mulliken population analyses of the valence orbitals of NiCu at an internuclear distance of 4.80 a.u.

| State | Orbital | Atomic population | | Overlap population |
|---|---|---|---|---|
| | | Ni | Cu | |
| $^2\Delta$, CI | $\sigma$ | 0.04 | 0.03 | −0.00 |
| | $\sigma$ | 0.54 | 0.80 | 0.60 |
| | $\sigma$ | 1.76 | 0.43 | −0.19 |
| | $\sigma$ | 0.32 | 1.65 | 0.04 |
| | $\pi$ | 3.85 | 0.14 | 0.01 |
| | $\pi$ | 0.13 | 3.85 | 0.02 |
| | $\delta$ | 2.76 | 0.24 | −0.00 |
| | $\delta$ | 0.24 | 3.76 | 0.00 |
| Total | | 27.63 | 28.89 | 0.48 |
| $^2\Pi$, CI | $\sigma$ | 0.04 | 0.03 | −0.00 |
| | $\sigma$ | 0.54 | 0.80 | 0.60 |
| | $\sigma$ | 1.42 | 0.69 | −0.01 |
| | $\sigma$ | 0.67 | 1.29 | 0.04 |
| | $\pi$ | 3.95 | 0.04 | 0.01 |
| | $\pi$ | 0.03 | 3.95 | 0.02 |
| | $\delta$ | 3.96 | 0.12 | −0.09 |
| | $\delta$ | 0.01 | 3.99 | 0.00 |
| Total | | 27.62 | 28.90 | 0.48 |
| $^2\Sigma^+$, CI | $\sigma$ | 0.04 | 0.03 | −0.00 |
| | $\sigma$ | 0.51 | 0.82 | 0.60 |
| | $\sigma$ | 1.02 | −0.06 | 0.04 |
| | $\sigma$ | 0.03 | 1.99 | −0.02 |
| | $\pi$ | 3.70 | 0.30 | 0.00 |
| | $\pi$ | 0.28 | 3.69 | 0.03 |
| | $\delta$ | 3.95 | 0.05 | −0.00 |
| | $\delta$ | 0.05 | 3.95 | 0.00 |
| Total | | 27.58 | 28.87 | 0.54 |

In Table 1 we have presented Mulliken population analyses for the valence orbitals of the three lowest-lying states resulting from CI calculations at the internuclear distance 4.80 a.u. The population analyses for the three states are very much alike, and especially it is noted that only one of the orbitals in each analysis has an appreciable overlap population. This orbital is of $\sigma$ symmetry, and a closer examination shows that it is mainly an $s$ type orbital ($\sim$42% Ni $s$ character and $\sim$54% Cu $s$ character).

The chemical bond between the two atoms is explainable in terms of a bonding $\sigma$ molecular orbital. The $4p$ and the $3d$ orbitals hardly participate in the bonding. The $3d$ orbitals remain well-localized for all internuclear distances considered, however they give rise to splittings between states originating from specific atomic configurations. This agrees with our previous results concerning the $Ni_2$ molecule [5].

Figure 1 shows the potential energy curves resulting from CI calculations. The six lowest-lying energy curves represent the interaction between a Ni atom in the $^3D(3d)^9(4s)^1$ term and a Cu atom in the $^2S(3d)^{10}(4s)^1$ term. The three highest-lying

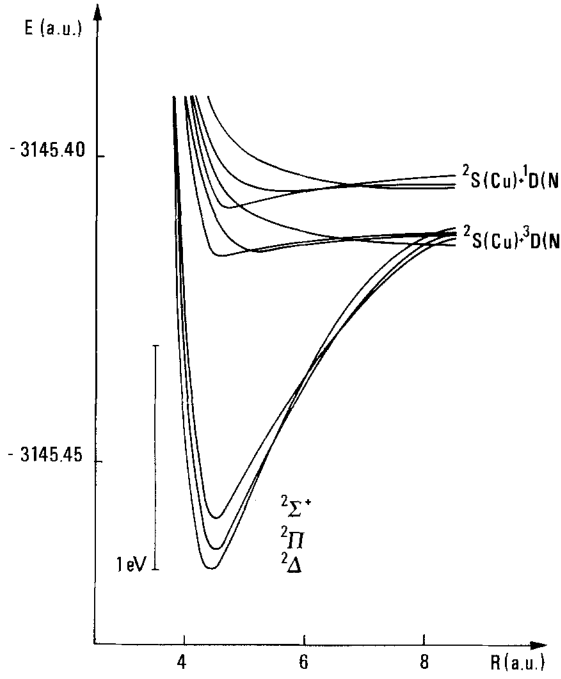

**Fig. 1.** Potential energy curves for the NiCu molecule as resulting from a limited CI treatment

curves correspondingly represent the interaction between a Ni atom in the $^1D(3d)^9(4s)^1$ term and a Cu atom in the $^2S(3d)^{10}(4s)^1$ term.

From Fig. 1 it is noted that a crossover of the potential energy curves occurs as the internuclear distance increases. At the equilibrium internuclear distance the state of lowest energy ($^2\Delta$) originates from a configuration with a hole in the $3d\delta$ subshell of Ni. At large internuclear distances, on the other hand, the lowest-lying state is due to a configuration with a hole in the $3d\sigma$ subshell of Ni.

The splittings between the low-lying states are thus mainly caused by splitting of the $3d$ orbitals of the Ni atom due to the axial symmetry, but the interaction between the atoms gives rise to an interchange of the split orbitals.

Approximating the low-lying potential energy curves from Fig. 1 with Morse curves yield equilibrium distances, dissociation energies and vibrational frequencies as reported in Table 2. This table also contains results from the HF calculations on the $^2\Pi$ state. Unfortunately we have no experimental data for comparison.

It is noted that the dissociation energy of the $^2\Pi$ state changes very little in going from the HF to the CI approximation. This is due to the fact that the lack of inversion symmetry in the molecule allows proper localization of the molecular orbitals, and therefore the HF method provides a good description of the molecule for all internuclear distances.

Table 2. Spectroscopic data for the low-lying states of the NiCu molecule as resulting from Hartree–Fock and CI treatments

| | Equilibrium distance (a.u.) | Dissociation energy at 0°K(eV) | Vibrational frequency ($cm^{-1}$) |
|---|---|---|---|
| $^2\Pi$, HF | 4.69 | 1.42 | 386 |
| $^2\Delta$, CI | 4.55 | 1.54 | 347 |
| $^2\Pi$, CI | 4.60 | 1.43 | 311 |
| $^2\Sigma^+$, CI | 4.63 | 1.29 | 300 |

## 4. Spin–Orbit Coupling

Since the states of the molecule are closely spaced, the spin–orbit coupling ought to be considered in some detail.

We have calculated the spin–orbit coupling energies for the low-lying states of the NiCu molecule using the following approximations: we have neglected overlap integrals, since the 3*d* orbitals of the two nuclei are all very well localized. Likewise, the very small hybridization between *s*, *p*, and *d* orbitals is neglected. Hereby, we have reduced the molecular problem to an atomic problem in an axial symmetric field.

Finally, we have assumed that the radial integrals arising when evaluating the matrix elements of the spin–orbit coupling operator are all equal, and the value of 603 $cm^{-1}$ for the appropriate radial integral was taken from a work by Laporte and Inglis [16].

The energies of the $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states were added to the appropriate diagonal elements of the $10 \times 10$ matrix representing the spin–orbit coupling, and the spin–orbit coupled states were then obtained by diagonalization of the matrix.

As reported in Table 3 the above-defined procedure was performed for three different sets (a, b, and c) of energies of the $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states at the internuclear distance 4.80 a.u. The energies of both a) and b) are results of CI calculations. In a) the CI calculations are based on molecular orbitals optimized for the $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states, separately. In b) all states are calculated using the molecular orbitals optimized for the $^2\Pi$ state. The energies used in c) are the HF results for the $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states.

From Table 3 it is recognized that the projection of the sum of the orbit and spin angular momentum onto the internuclear axis ($\Omega$) is 5/2 for the lowest-lying state, and thereafter in order of increasing energies the states have $\Omega = 3/2, 1/2, 3/2, 1/2$, respectively. This result is obtained in all three cases a), b), and c).

However, a detailed analysis shows that the results of b) differ from the results of a) and c). Considering the contributions from the original states in the spin–orbit coupled states it is evident that the states with $\Omega = 3/2$ are interchanged in b) relative to a) and c). This discrepancy is probably only of minor importance, since in all cases the original states are mixed considerably.

**Table 3.** Relative energies (in cm$^{-1}$) with and without spin–orbit coupling of low-lying states of the NiCu molecule at the internuclear distance 4.80 a.u. a) CI calculations based on molecular orbitals optimized for the $^2\Delta$, $^2\Pi$ and $^2\Sigma^+$ states separately, b) CI calculations based on molecular orbitals optimized for the $^2\Pi$ state, c) HF calculations for the $^2\Delta$, $^2\Pi$ and $^2\Sigma^+$ states

| Without spin–orbit coupling | | | | With spin–orbit coupling | | | |
|---|---|---|---|---|---|---|---|
| | | | | | Combinations in % of original states | | |
| | State | Energy | $\Omega$[a] | Energy | $^2\Delta$ | $^2\Pi$ | $^2\Sigma^+$ |
| a) | $^2\Delta$ | 0 | $\frac{5}{2}$ | −603 | 100 | 0 | 0 |
| | $^2\Delta$ | 0 | $\frac{3}{2}$ | 116 | 60 | 40 | 0 |
| | $^2\Pi$ | 1163 | $\frac{3}{2}$ | 1349 | 40 | 60 | 0 |
| | $^2\Pi$ | 1163 | $\frac{1}{2}$ | 999 | 0 | 72 | 28 |
| | $^2\Sigma^+$ | 2170 | $\frac{1}{2}$ | 2636 | 0 | 28 | 72 |
| b) | $^2\Delta$ | 0 | $\frac{5}{2}$ | −603 | 100 | 0 | 0 |
| | $^2\Delta$ | 0 | $\frac{3}{2}$ | 1066 | 63 | 37 | 0 |
| | $^2\Pi$ | 581 | $\frac{3}{2}$ | −183 | 37 | 63 | 0 |
| | $^2\Pi$ | 581 | $\frac{1}{2}$ | 433 | 0 | 73 | 27 |
| | $^2\Sigma^+$ | 1648 | $\frac{1}{2}$ | 2097 | 0 | 27 | 73 |
| c) | $^2\Delta$ | 0 | $\frac{5}{2}$ | −603 | 100 | 0 | 0 |
| | $^2\Delta$ | 0 | $\frac{3}{2}$ | 72 | 56 | 44 | 0 |
| | $^2\Pi$ | 1058 | $\frac{3}{2}$ | 1288 | 44 | 56 | 0 |
| | $^2\Pi$ | 1058 | $\frac{1}{2}$ | 850 | 0 | 68 | 32 |
| | $^2\Sigma^+$ | 1921 | $\frac{1}{2}$ | 2430 | 0 | 32 | 68 |

[a] $\Omega$ is the projection of the sum of the orbit and the spin angular momentum onto the internuclear axis.

In Fig. 2 we present potential energy curves for the low-lying spin–orbit coupled states of the NiCu molecule. It is seen that the crossings of the potential energy curves are not removed by the spin–orbit interaction.

Finally, in Table 4 we report spectroscopic data for the five low-lying states. It is noted that the spectroscopic data for the lowest-lying state are unchanged by the spin–orbit coupling. This is to be expected, since the spin–orbit interaction in our description is purely atomic in nature, and since the lowest-lying state is a pure $^2\Delta_{5/2}$ state. The spectroscopic data of the higher-lying states on the other hand undergo small changes; this is of course due to mixing of the original states.

**Table 4.** Spectroscopic data for the low-lying states of the NiCu molecule as resulting from CI treatments, when the spin–orbit interaction is taken into account

| $\Omega$ | Equilibrium distance (a.u.) | Dissociation energy at 0°K(eV) | Vibrational frequency (cm$^{-1}$) |
|---|---|---|---|
| $\frac{5}{2}$ | 4.55 | 1.54 | 347 |
| $\frac{3}{2}$ | 4.58 | 1.47 | 322 |
| $\frac{3}{2}$ | 4.57 | 1.31 | 337 |
| $\frac{1}{2}$ | 4.61 | 1.37 | 307 |
| $\frac{1}{2}$ | 4.62 | 1.15 | 304 |

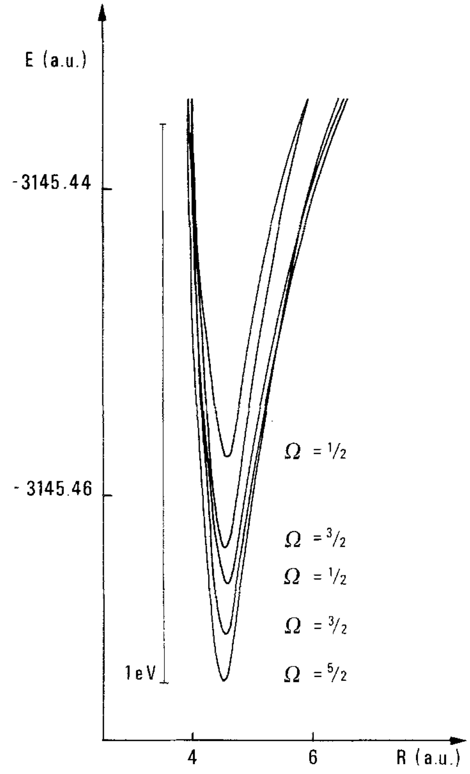

**Fig. 2.** The low-lying potential energy curves for the NiCu molecule, when spin–orbit interaction is taken into account

In general we expect that spin–orbit coupling effects are important for molecules containing transition metal atoms. Such molecules always have closely spaced electronic states, which might mix due to the spin–orbit interaction.

## 5. Conclusion

The interaction between a Ni and a Cu atom has been described using *ab initio* methods. Both HF and CI calculations have been performed for the low-lying states of the NiCu molecule for five different internuclear distances ranging from 3.6 to 8.0 a.u.

The chemical bond between the two atoms is mainly due to a bonding $4s\sigma$ molecular orbital, while the $3d$ orbitals cause small splittings between the potential energy curves.

The low-lying states of the molecule at the equilibrium distance are in order of increasing energy $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$. These three states arise from configurations with a hole in the $3d\delta$, $3d\pi$, and $3d\sigma$ subshells of the Ni atom, respectively.

We have carried out approximate calculations of the spin–orbit coupling for the three lowest-lying states of the molecule. It is shown that the spin–orbit coupling causes a considerable mixing of the states.

Spectroscopic data, that is equilibrium distances, dissociation energies and vibrational frequencies are presented for the low-lying states both with and without consideration of spin–orbit coupling effects.

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## Appendix

### *Choice of orbitals for CI calculations*

Since we decided to investigate the interaction between a Ni atom in the $(3d)^9(4s)^1$ configuration and a Cu atom in the $(3d)^{10}(4s)^1$ configuration there are only three possibilities for the lowest-lying state of the molecule. This state could either be a $^2\Delta$, a $^2\Pi$ or a $^2\Sigma^+$ state, depending on the nature of the hole in the *d* shell of the Ni atom.

We wished to determine a unique set of molecular orbitals, which could be utilized in limited CI calculations describing all low-lying states of the molecule.

**Table 5.** Mulliken population analyses of the valence orbitals of NiCu at an internuclear distance of 4.80 a.u.

| State | Orbital | Atomic population | | Overlap population | Orbital analyses Ni | | | Orbital analyses Cu | | | Occupation number |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Ni | Cu | | s | p | d | s | p | d | |
| $^2\Delta$, HF | $\sigma$ | 0.61 | 0.77 | 0.62 | 0.89 | 0.03 | 0.00 | 1.04 | 0.04 | 0.00 | 2.00 |
| | $\sigma$ | 1.97 | 0.25 | −0.22 | 0.01 | −0.01 | 1.85 | 0.05 | 0.02 | 0.07 | 2.00 |
| | $\sigma$ | 0.09 | 1.89 | 0.02 | 0.01 | 0.01 | 0.08 | −0.00 | −0.00 | 1.90 | 2.00 |
| | $\pi$ | 3.89 | 0.11 | 0.00 | 0.00 | 0.00 | 3.89 | 0.00 | 0.02 | 0.09 | 4.00 |
| | $\pi$ | 0.09 | 3.89 | 0.02 | 0.00 | 0.01 | 0.09 | 0.00 | −0.00 | 3.90 | 4.00 |
| | $\delta$ | 3.00 | 0.00 | 0.00 | 0.00 | 0.00 | 3.00 | 0.00 | 0.00 | 0.00 | 3.00 |
| | $\delta$ | 0.00 | 4.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4.00 | 4.00 |
| Total | | 27.64 | 28.91 | 0.43 | 6.92 | 12.05 | 8.91 | 7.06 | 12.09 | 9.97 | |
| $^2\Delta$, CI | $\sigma$ | 0.04 | 0.03 | −0.00 | 0.02 | 0.01 | 0.00 | 0.02 | 0.01 | 0.00 | 0.07 |
| | $\sigma$ | 0.56 | 0.76 | 0.61 | 0.85 | 0.02 | 0.00 | 1.02 | 0.05 | 0.00 | 1.93 |
| | $\sigma$ | 1.87 | 0.37 | −0.24 | 0.05 | 0.00 | 1.69 | 0.02 | 0.01 | 0.22 | 2.00 |
| | $\sigma$ | 0.23 | 1.74 | 0.03 | 0.00 | 0.00 | 0.24 | 0.00 | 0.00 | 1.75 | 2.00 |
| | $\pi$ | 3.86 | 0.13 | 0.01 | 0.00 | 0.00 | 3.86 | 0.00 | 0.02 | 0.11 | 4.00 |
| | $\pi$ | 0.11 | 3.86 | 0.02 | 0.00 | 0.00 | 0.12 | 0.00 | −0.00 | 3.88 | 4.00 |
| | $\delta$ | 2.62 | 0.38 | −0.00 | 0.00 | 0.00 | 2.62 | 0.00 | 0.00 | 0.38 | 3.00 |
| | $\delta$ | 0.38 | 3.62 | 0.00 | 0.00 | 0.00 | 0.38 | 0.00 | 0.00 | 3.62 | 4.00 |
| Total | | 27.67 | 28.90 | 0.43 | 6.92 | 12.05 | 8.91 | 7.06 | 12.09 | 9.97 | |

First HF calculations were carried out for the three above-mentioned states separately at an internuclear distance of 4.80 a.u. The $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states resulting from the HF calculations were all bound relative to a Ni atom in the $^3D(3d)^9(4s)^1$ term and a Cu atom in the $^2S(3d)^{10}(4s)^1$ term by 1.24, 1.11, and 1.01 eV, respectively.

The HF orbitals from the three states were all utilized in limited CI calculations, which allowed full reorganization within the 3*d* and 4*s* shells.

Table 5 shows Mulliken population analyses for the $^2\Delta$ state as calculated in the HF and the CI approximations. It is obvious from the population analyses that very little hybridization occurs and also that the *d* orbitals are very well localized. The chemical bond can be attributed to a single orbital mainly composed of the 4*s* orbitals.

We do not present population analyses of the $^2\Pi$ and the $^2\Sigma^+$ states since they are very similar to those in Table 5.

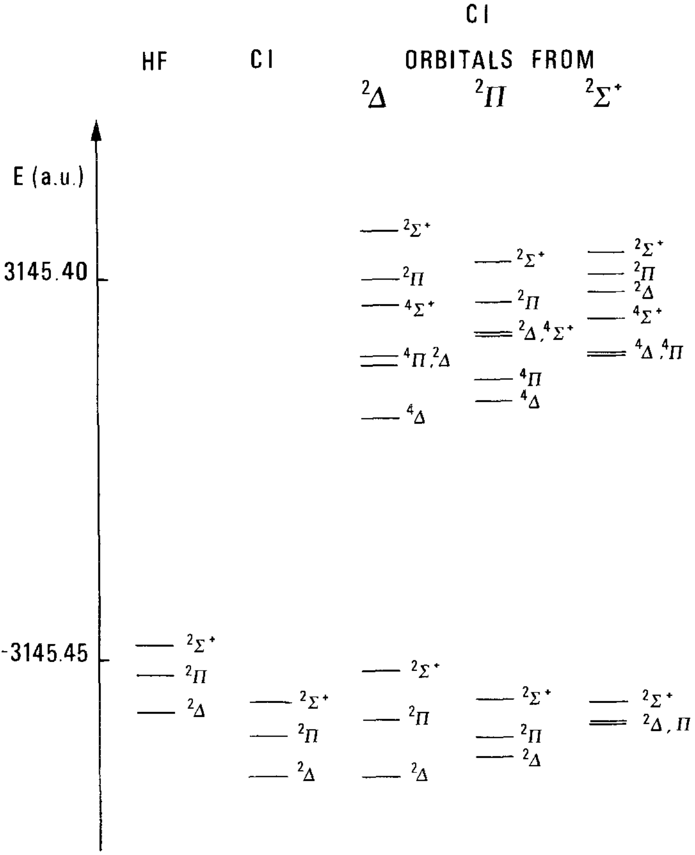

**Fig. 3.** Energies of the low-lying states of the NiCu molecule at an internuclear distance of 4.80 a.u. The energies are results of HF and several CI calculations

In Fig. 3 we have shown energies of low-lying states as resulting from HF and CI calculations.

The first column in Fig. 3 marked HF of course shows the HF results of the states indicated. The second column shows CI results based on HF orbitals for each of the three states. Each of the remaining three columns shows all low-lying states of the molecule determined in CI calculations based on a single set of molecular orbitals originating from the $^2\Delta$, $^2\Pi$, and $^2\Sigma^+$ states, respectively.

Based upon the CI calculations chosen the second column in Fig. 3 represents the most accurate results obtainable.

From Fig. 3 it is noted that describing all states in CI calculations based on molecular orbitals optimized for the lowest-lying state causes too large splittings between the three low-lying states.

On the other hand if orbitals optimized for the highest-lying state are utilized in CI calculations determining all states, the splittings between the three states get too small.

In order to obtain a fair description of the splittings between the low-lying states we decided to use orbitals optimized for the $^2\Pi$ state in CI calculations determining all states.

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