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# ELECTRONIC STRUCTURES AND POTENTIAL ENERGY CURVES 

FOR THE LOW-LYING STATES OF THE CN RADICAL*
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ABSTRACT
At eleven internuclear separations $a b$ initio calculations have been carried out on those 59 molecular states of CN which dissociate to atomic limits up to ${ }^{1} D C+{ }^{2} D N$. Four electrons are held frozen in carbon and nitrogen ls Hartree-Fock atomic orbitals, and a full configuration interaction is carried out for the remaining nine electrons using optimized 2 s and $2 p$ Slatertype orbitals on each atom. The ${ }^{2} I I$ calculations, which include 486 configurations, are the most complicated. Eighteen significantly bound states ( $D_{e} \geqslant 0.84 \mathrm{eV}$ ) were obtained, nine of which have been observed spectroscopically. With the exception of the third ${ }^{2} \Pi$ state, the theoretical ordering of states agrees with experiment. Three of the states never observed experimentally, $\left({ }^{4} \Sigma^{+},{ }^{4} \Pi\right.$, and $\left.{ }^{4} \Delta\right)$ lie below all but three of the known states of $C N$. Calculated spectroscopic constants are compared with experiment. The potential curves show many interesting features, including potential maxima in the ${ }^{4} \Sigma^{-},{ }^{2} \Sigma^{-}$, $J^{2} \Delta$, and ${ }^{2} \Pi$ IV bound states. By performing natural orbital analyses, dominant molecular orbital configurations have been unambiguously assigned to the lowest 18 bound states. The second, third and fourth ${ }^{2}$ II states experience numerous avoided crossings among themselves, and naturid orbitals have been

## INTRODUCTION

The fact that there are four low-lying states of the carbon atom $\left({ }^{3} P,{ }^{1} D,{ }^{1} S,{ }^{5} S\right)$ and three low-lying states $\left({ }^{4} S,{ }^{2} D,{ }^{2} P\right)$ of the nitrogen atom guarantees the existence of a substantial number of low-lying (less than 10 eV ) statis of the $C N$ molecule. Combined with the experimental interest, l-11 particularly astrophysical, in $C N$, there would appear tc be a great deal of motivation for $a b$ initio calculations on the low-lying states of CN. Nevertheless we have been able to find only one such study ir the literature, by Guerin. ${ }^{12}$ He carried out calculations based on SCF orbitals and including no more than three configurations for the $A{ }^{2} \Pi, D^{2} \Pi, F^{2} \Delta$, and $J{ }^{2} \Delta$ states of $C N$. Although such calculations can be useful ${ }^{13}$ in the study of excitation energies, it is well known ${ }^{14}$ that diatomic molecular formation and dissociation canrot be properly described within the single configuration approximation unless one of the atoms is a closed shell species.

Over a wide range of internuclear separations, we have carried out ab initio configuration interaction (CI) calculations on all the states of $C N$ which dissociate to atomic limits up to ${ }^{1} D$ carbon plus ${ }^{2} D$ nitrogen. Perhaps the most important aspect of the present work is the prediction of the existence of nine new bound states of $\mathrm{CN} .{ }^{15}$ A second area of emphasis in the present worl involves the use of natural orbitals ${ }^{16}$ to discuss the electronic structure of the valence-excited states of CN .

BASIS SET.
Hartree-Fock atomic orbitals ${ }^{17}$ for the ground syates of $C$ and $N$ were used to describe the inner shell electrons. 2 s and 2 p siater-type orbitals on each atom complete the basis set. The orbital exponents for the latter functions were optimized in repeated calculations on the $X{ }^{2} \Sigma^{+}$ground state at the experimental internuclear separation. The resulting exponents for carbon were $\zeta(2 s)=\zeta(2 p)=1.674$ and for nitrogen $\zeta(2 s)=\zeta(2 p)=1.988$. With the exception that the $1 \sigma$ and $2 \sigma$ molecular orbitals (MO's) are always doubly occupied, full CI calculations were carried out for all symmetries of interest. The calculated atomic energies for $C$ and are combined to give molecular dissociation limits in Table $I$. The comparison with experiment in Takle I indicates that the primary deficiency in the atomic calculations is due to the fact that the ${ }^{5} S$ state of carbon lies too low relative to the ${ }^{l} D$ and. ${ }^{1} S$ states.

The basis set outlined above is the smallest with which one can reasonably expect to get meaningful results for potential surfaces. And in fact CI calculations of the same type (with molecule-optimized exponents) yielded good qualitative agreement with experiment for $\mathrm{CO},{ }^{18}$ with seven of the eight linown valence (i.e. non-Rydberg) states lying in the experimental order. Calculations of this type with atom-optimized exponents have also yielded qualititively correct potential curves for $0_{2},{ }^{19} \mathrm{NH},{ }^{20} \mathrm{~N}_{2},{ }^{21}$ and sio. ${ }^{22}$ Althourh much more accurate total energies than those reported here can be obtained using extended basis sets, the problem of treating molecular formation and dissociation is a difficult one within larger basis sets, and accurate potential curves of this type have only been reported for a few states of a few
diatomic molecules. 23 Perhaps the primary virtue of CI treatments of the type used here is that all molecular states dissociate smoothly to their exact atomic limits.

Since our all-numerical methods ${ }^{24}$ for the computation of molecular integrals allow for the use of arbitrary orbitals, the present calculation: could equally well have been done entirely in terms of accurate Hartree-Fock orbitals. ${ }^{17}$ This would have yielded much lower total energies and still retained the correct dissociation behavior for all states. However, as we have shown for $\mathrm{F}_{2}{ }^{24}$ and $\mathrm{Cl}_{2}$, ${ }^{25}$. such a basis is optimum for the separated atoms but far from optimum for the molecule, and this results in very poor calculated dissociation energies. The basis set adopted here, HFAO's for the core and STO's for the valence region, is about equally good (or bad) for both the molecule and the separated atoms and thus yields reasonable potential curves.

CALCULATIONS
The methods used in the present study for the evaluation of integrals and construction of symmetry-adapted linear combinations of determinants are described elsewhere. 24, 26 Fifty-nine molecular states dissociate to the first seven atomic limits (see Table I) of $C N$. The resulting full valence $C I$ calculations include the largest computations of this type reported to date. 18-22 The calculations are summarized in Table II, where it is seen that the largest calculation, of ${ }^{2} \Pi$ symmetry, requires the ten lowest eigenvalues of a $486 \times$ 486 matrix. Total CDC 6600 time used for all calculations was about seven hours.

The calculated total energies for 59 states at eleven internuclear separations $(1.85,2.0,2.25,2.5,2.75,3.0,3.25,3.5,4.0,5.0,6.0)$ are not included here but can be obtained from the authors. 27

## SPECTROSCOPIC CONSTANTS: COMPARISON WITH EXPERIMENT

In Table III the ab initio spectroscopic constants are compared with available experimental data. Eight states of $C N$ have been fairly unambiguously identified and a ninth, designated $G{ }^{2} \Pi$, has been tentatively assigned by Lutz. 11 For the eight known states our predicted ordering agrees with experiment except for the $H^{2} \Pi$ state. The $H$ state is calculated to lie 0.049 eV below the $\mathrm{E}^{2} \Sigma^{+}$state and 0.072 eV below the $\mathrm{F}^{2} \Delta$ state, but Douglas and Routly's measurements ${ }^{2}$ indicate that the $\mathrm{H}^{2}$ II state in fact lies 0.156 eV above the $F^{2} \Delta$ state. Thus if our calculated $H^{2} \Pi$ state were to lie 0.073 eV higher the ab initio order would be in complete agreement with experiment for CN.

Our calculations predict a fourth ${ }^{2}$ II bound state which lies 0.95 eV above the ${ }^{2}$ II III state. $L^{\prime} \mathcal{Z}^{11}$ however tentatively assigns a fourth ${ }^{2}$ II state lying 0.04 eV below the $H^{2} \Pi$ state. However, inspection of Lutz's potential curves ${ }^{11}$ shows that, if his analysis is correct, the $G$ and $H$ states at $60,624 \mathrm{~cm}^{-1}$ and $60,939 \mathrm{~cm}^{-1}$ are not two states but two different minima in a single ${ }^{2}$ II III state.

The theoretical $r_{e}$ values are in all eight cases larger than experiment, the differences ranging from 0.064 to $0.104 \AA$. The relative differences are even better and the calculated ordering of $r_{e}$ agrees with experiment except, again, for the $H^{2}$ II state. The predicted rotational constants $B_{e}$ follow the same pattern with respect to experiment, since $B_{e}$ is proportional to $\left(1 / r_{e}\right)^{2}$.

The calculated values of $\omega_{e}$ are the following percentages of experiment $X^{2} \Sigma^{+} 94 \%, A^{2} \Pi 89 \%, B^{2} \Sigma^{+} 82 \%, D^{2} \Pi 104 \%, E^{2} \Sigma^{+} 102 \%, J^{2} \Delta 108 \%$. Except for the $B^{2} \Sigma^{+}$value; the theoretical $\omega_{e}^{\prime}$ s fall in the experimentally observed order.

The higher spectroscopic constants $w_{e} x_{e}$ and $\alpha_{e}$ are usually qualitatively similar to the experimental values. As can be seen from Table III, however, for the $E^{2} \Sigma^{+}$state, the agreement for $\omega_{e} x_{e}$ is particularly poor.

NEW BOUND STATES OF CN

Since qualitatively correct spectroscopic constants were obtained for the known bound states of $C N$, it is to be expected that useful predictions can be made concerning states not yet observed experimentally. Table III predicts the existence of nine new states of CN . It is not surprising that none of these states have been observed, since six are quartet sitates, two are ${ }^{2} \Sigma^{-}$, and the lastis a ${ }^{2} \Phi$ state. Transitions from these nine states to the ground $X^{2} \Sigma^{+}$state are electronically forbidden.

It is perhaps surprising how low-lying some of the quartet states are. For example the ${ }^{4} \Sigma^{+}$state is predicted to lie only 0.25 L eV above the very well characterized $B^{2} \Sigma^{+}$state. And both the ${ }^{4} \Pi$ and ${ }^{4} \Delta$ states lie below the fourth known state of $C N, D^{2} \Pi$. Since all nine of these new states are observably bound $\left(D_{e}>0.85 \mathrm{eV}\right)$, we hope that the present theoretical predictions will spur new experimental interest in the $C N$ spectrum.

POTENTIAL CURVES
Figures 1-10 contain the calculated potential curves for 59 states of CN. In Fig. 11 the lowest bound states are seen. Several attempts were made to plot the higher bound states but the number of curve crossings makes the resulting figure virtually inscrutable. So, in Fig. 12 we indicate the energy of each of these bound states and the $r_{e}$ value. This group of cN potential curves is the most interesting we have studied $18,19,22$ to date, since there are a large number of significantly bound states and many more potential maxima than previousiy encountered.

Among the eighteen lowest bound states the ${ }^{4} \Sigma^{-},{ }^{2} \Sigma^{-}, J^{2} \Delta$, and ${ }^{2}$ II IV all have potential maxima at about four bohrs. The heights of these maxima are, respectively, $0.43 \mathrm{eV}, 0.24 \mathrm{eV}, 0.43 \mathrm{eV}$, and 0.32 eV . All four maxima appear to be, due to avoided crossings with higher states. The curves for the two lowest ${ }^{2} \Sigma^{-}$and ${ }^{2} \Delta$ states are particularly interesting, since for both of these symmetries there are two nearly parallel bound states. Figure 6 shows that the ${ }^{4} \Pi$ II state is quasi-bound. This state has a potential well of depth 1.41 eV , but the minimum nevertheless lies 0.67 eV above the dissociation limit. Two higher states having potential maxima are ${ }^{2} \Delta$ III and ${ }^{4} \triangle$ III.

The fact that, in our calculations, the ${ }^{5}$ S state of carbon lies too low is reflected in our ${ }^{2} \Sigma^{+}$results. Figure limplies that the B state dissociates to ${ }^{5}$ S carbon plus ${ }^{4}$ S nitrogen, whereas in fact, it must disscciate to ${ }^{3} \mathrm{PC}+{ }^{2} \mathrm{DN}$. The ${ }^{2}{ }^{+}$IV curve is also affected, the maximum in its potential curve being a result of the ${ }^{5} \mathrm{~S}+{ }^{4} \mathrm{~S}$ atomic limit lying too low. If we realize this limitation of the present results, one can more sensibly predict that the ${ }^{2} \Sigma^{+}$IV state should dissociate smoothly to ${ }^{3} \mathrm{P} C+{ }^{2} \mathrm{P} N$. Thus the ${ }^{2} \Sigma^{+}$IV state
is predicted to be bound with a dissociation energy of $\div 0.5 \mathrm{eV}$. Lutz ${ }^{l l}$ has mentioned the possibility of the existence of a fourth ${ }^{2} \Sigma^{+}$state.

Several other points of interest can be seen in Figs. 1-12. The second ${ }^{4} \Sigma^{+}$state has a very unusual shape, much like that of a bathtub. The lowest ${ }^{6} \Sigma^{+}$state is slightly bound ( $D_{e} \approx 0.3 \mathrm{eV}$ ) with a minimum at $r=3.25$ bohrs. Furthermore, since this state dissociates to ground state carbon and nitrogen atoms, it is very low-lying ( $\mathrm{T}_{\mathrm{e}}<6.0 \mathrm{eV}$ ).

A particularly interesting series of crossing occurs for the ${ }^{2}{ }^{2}-$ states, where the $3 \mathrm{rd}, 4 \mathrm{th}, 5 \mathrm{th}$, and 6 th potential curves avoid crossing a curve which dissociates to a higher atomic limit than those considered here.

Mention should be made concerning the possibility of molecular Rydberg states causing serious deviations from the predictions given here, since our basis set is incapable of describing such Rydberg states. Iable I shows that the lowest Rydberg dissociation limit occurs 3.3 l eV above the highest dissociation limit we have considered. However, since some of the CN Rydberg states are no doubt more bound than our higher predicted states, there is still a possibility of some interaction. The dissociation erergies of these Rydberg states should be close to those of the lowest states of $\mathrm{CN}^{+}$. However the ground state dissociation energy of $\mathrm{CN}^{+}$is only $4.7 \pm 0.4 \mathrm{eV}^{6}$ which implies (see Table I) that the lowest Rydberg state of CN lies 2.7 eV above ground state carbon plus ground s.tate nitrogen. Our highest rejorted bound state,, ${ }^{2}$ II IV, lies $\sim 2.6 \mathrm{eV}$ above the ground state atoms, so if Rydberg states affect our predicted bound states at all, it is likely that on $y$ the very highest potential curves are altered.

## ELECTRONIC STRUCTURES

Molecular orbital configurations for the low-lying states of CN have been discussed in several experimental papers. 2,3,11 In this work, we hav? directly investigated this problem by computing natural orbitals (NO's) ${ }^{16}$ for the lowest state of each symetry. The natural orbitals have a highly des irable non-arbitrary form in these calculations, since our full CI calculations assume no foreknowledge of the form of the orbitals.

## A. Molecular Orbital Configurations

For the lowest state of each symmetry except ${ }^{2} \pi$ which yielded at least one of the 18 significantly bound states, natural orbital occupaticn numbers are given in Table IV. The fact that almost all the numbers in Table IV are nearly integral implies that most of these states are well represented by a single configuration. For the ground state, No analyses have been carried out at five different internuclear separations. It is seen that es $r$ becomes larger the $2 \pi$ NO becomes more important. This is a manifestation of the fact ${ }^{14}$ that for diatomic molecules made up of two open-shell atoms, as $r \rightarrow \infty$, the single configuration MO approximation becomes increasingly poover.

Using the natural orbitals thus obtained for each symmetry, the fill CI wave functions were recomputed to determine the dominant configurations il each wave function. These dominant configurations are reported in Table $V$ and give quantitative information on the electronic structure of CN. For eight of the fourteen bound states in Table $V$, there is only one configuration with coefficient greater than 0.25 , corresponding to $\sim 6.25 \%$ of the total wave function. For only one state, ${ }^{4} \Sigma^{+}$II, is it not possible to clearly identify a single dominant configuration. Table $V$ shows that for all eight doublet states
excluding ${ }^{2} \Pi$, the predicted electron configurations of Douglas and Routly ${ }^{2}$ and Lutz ${ }^{11}$ are correct. For the quartet states, electron configurations have not been predicted.
B. Avoided Crossings Among the ${ }^{2} \Pi$ States

The ${ }^{2} \Pi$ wave functions were recomputed at five $r$ values using $X^{2} \Sigma^{+}$ natural orbitals. This was done in order to "follow", in terms of MO configurations, the avoided crossings which occur among the second, third, and fourth $2_{\Pi}$ states. As can be seen in Table $V I$, three configurations $-5 \sigma^{2} 1 \pi^{3}, 5 \sigma^{2} 1 \pi^{2} 2 \pi$, and $1 \pi^{4} 2 \pi$--dominate these four states. By simultaneously looking at Fig. 5 and Table VI it can be seen that each avoiding crossing is accompanied by a change in the dominant electron configuration.

At its minimum, the $D^{2} \Pi$ state is dominated by the $5 \sigma^{2} 1 \pi^{2} 2 \pi$ configuration (actually two ${ }^{2} \Pi$ il configurations arise from this orbital occupancy ${ }^{26}$ ). However, between $r=2.75$ and $r=2.50$, the $D^{2} \Pi$ states shifts to the $1 \pi^{4} 2 \pi$ configuration.

The third calculated ${ }^{2}$ II state (which we assume is the $H$ state) experiences two avoided crossings. At $r=2.25$ and $r=2.50,{ }^{2}$ II III is dominated by $5 s^{2} 1 \pi^{2} 2 \pi$. However, at the lowest calculated energy, $r=2.75$, the $H$ state i:: dominated by the $1 \pi^{4} 2 \pi$ configuration. At $r=3$ bohrs both the $5 \sigma^{2} 1 \pi^{2} 2 \pi$ and $1 \pi^{4} 2 \pi$ orbital occupancies are important, indicating that this is near another avoided crossing. Finally, at $R=3.25$, the $5 \sigma^{2} 1 \pi^{2} 2 \pi$ configuration again becomes dominant.

The lowest calculated energy for the fourth ${ }^{2}$ II state is found at $R=\equiv .0$ bohrs, but the calculated energy is less than 0.1 eV higher at $\mathrm{R}=2.75$.

Thus the minimum of the ${ }^{2} \Pi$ IV state occurs very near an avoided crossing between the third and fourth ${ }^{2} \Pi$ states. For smaller $r$ tlan $3.0,{ }^{2} \Pi$ IV is dominated by $5 \sigma^{2} 1 \pi^{2} 2 \pi$, and for larger $r, 1 \pi^{4} 2 \pi$ is the dominant configuration. Our MO conflguration assignments for the four ${ }^{2} I$ states at their equilibrium internuclear separations are the same as the se of Lutz, ll except for the ${ }^{2} \Pi$ IV state (which he calls $G$ ), for which we car not specify a single configuration. A final interesting point is that, at cifferent $r$ values the $1 \pi^{4} 2 \pi$ configuration dominates the second, third, and fourth ${ }^{2} \Pi$ states.

## C. The Question of $g$ and $u$ Symmetry

Douglas and Routly, ${ }^{2}$ on the basis of the observance and non-observance of certain transitions, have suggested that the $C N$ radical is nearly enough homonuclear that the symbols $g$ and $u$ have some meaning. Carroll ${ }^{3}$ and Lutz ${ }^{7.1}$ have also discussed this matter. In particular, both Dcuglas and Routly ${ }^{2}$ and Lutz ${ }^{l l}$ state that the ground state can be approximately labeled as ${ }_{\Sigma_{g}}{ }^{+}$, and thus that the $5 \sigma$ orbital is more appropriately termed $3 \sigma$ g as in the $N_{\text {, }}$, molecule.

Our 50 natural orbital from the $X^{2} \Sigma^{+} r=2.25$ calculation has the form

$$
\begin{aligned}
5 \sigma= & 0.60922 \mathrm{~s}(\mathrm{c})+0.18882 \mathrm{~s}(\mathrm{~N}) \\
& -0.63752 \mathrm{p}(\mathrm{C})-0.49582 \mathrm{p}(\mathrm{~N})
\end{aligned}
$$

in terms of the normalized STO's used to describe the valence region. This; orbital does not appear to approximate $g$ character. However, the $1 \pi$ natural orbital from the same calculation has the form

$$
1 \pi=0.59352 \mathrm{p}(\mathrm{C})+0.66172 \mathrm{p}(\mathrm{~N})
$$

and thus approximates a $1 \pi_{u}$ orbital rather closely. Sinilar results to the above were also found for $r=2.5$ bohrs, and we conclude that the $g$ and $u$ labels are more appropriate for the $\pi$ than the $\sigma$ orbitals.

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*Work performed under the auspices of the U. S. Atomic lnergy Commission.

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Table I. Calculated and experimental dissociation limits for CN radical

| Atomic States C N | Calculated total energy (hartrees) | Energy relative to $3 \mathrm{PC}+{ }^{4} \mathrm{SN}$ (in eV) |  |
| :---: | :---: | :---: | :---: |
| $3_{P_{g}}+{ }^{4} S_{u}$ | -91.90734 | 0 | 0 |
| ${ }_{D}{ }_{g}+{ }^{4} S_{u}$ | -91.83672 | 1.92 | 1.26 |
| ${ }^{5} S_{u}+{ }^{4} S_{u}$ | -91.79773 | 2.98 | 4.17 |
| ${ }^{1} S_{g}+{ }^{4} S_{u}$ | -91.78503 | 3.33 | 2.68 |
| ${ }^{3} \mathrm{P}_{\mathrm{g}}+{ }^{2} \mathrm{D}_{u}$ | -91.78154 | 3.42 | 2.38 |
| $3_{P_{g}}+{ }^{2} P_{u}$ | -91.73809 | 4.61 | 3.58 |
| $I_{D}+{ }^{2} D_{u}$ | -91.71092 | 5.34 | 3.65 |
| Rydberg ${ }^{\text {b }}+{ }^{4} \mathrm{~S}$ | - | - | 7.48 |

${ }^{\text {a }}$ C. E. Moore, Atomic Energy Levels, Nat. Bur. Sta. (U. S.) Circ. No. 467 (1949).
${ }^{b}$ First Rydberg state of the carbon atom, $1 s^{2} 2 s^{2} 2 p 3 s{ }^{3} p$ state.
Table II. Summary of configuration interaction calculations on the CN radical. CDC 6600 times refer to a

| symetry | $\begin{gathered} \text { Pertinent } \\ \text { Eigenvalues } \end{gathered}$ | $\begin{gathered} \text { Orbital } \\ \text { Occupancies } \end{gathered}$ | Configurations | Distinct Contributing Determinants | Computation Time (sec. |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ${ }_{2}{ }^{+}$ | 7 | 144 | 320 | 952 | 434 |
| ${ }^{2} \varepsilon^{-}$ | 6 | 108 | 264 | 912 | 358 |
| ${ }_{48}{ }^{2}$ | 5 | 84 | 164 | 376 | 92 |
| ${ }^{4}{ }_{2}$ | 5 | 108 | 196 | 392 | 117 |
| ${ }_{2}{ }_{2}+$ | 2 | ${ }^{28}$ | 40 | 64 | 9 |
| ${ }_{2}{ }^{+}$ | 1 | 4 | 4 | 4 | 3 |
| ${ }^{2} \pi$ | 10 | 138 | 486 | 832 | $\sim 500^{\text {a }}$ |
| $4 \pi$ | 7 | 103 | 292 | 346 | 238 |
| ${ }^{6}$ | 1 | 40 | 52 | 54 | 。 |
| ${ }^{2}$ | 6 | 108 | 276 | 448 | 231 |
| ${ }^{4} \Delta$ | 4 | 76 | 152 | 172 | 50 |
| ${ }^{2}$ | 3 | 58 | 102 | 148 | ${ }_{27}$ |
| 40 | 1 | 36 | 44 | 46 | 8 |
| ${ }^{2}$ | 1 | 16 | 20 | 24 | 5 |

[^0]Table III. Spectroscopic parameters for bound states of $C N$ molecule

| State | $\mathrm{T}_{\mathrm{e}}(\mathrm{eV})$ | $D_{e}(e \mathrm{~V})$ | $\mathrm{r}_{\mathrm{e}}(\AA)$ | $\omega_{\mathrm{e}}\left(\mathrm{cm}^{-1}\right)$ | $\omega_{e} e^{x} e^{\left(c m^{-1}\right)}$ | $\mathrm{B}_{\mathrm{e}}\left(\mathrm{cm}^{-1}\right)$ | $\alpha_{e}\left(\mathrm{~cm}^{-1}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{X}^{2} \Sigma^{+} \mathrm{I}$ calc. | 0 0 | $\begin{gathered} 6.178 \\ 7.75 \pm 0.2^{\mathrm{b}} \end{gathered}$ | $\begin{aligned} & 1.236 \\ & 1.172^{a} \end{aligned}$ | $\begin{aligned} & 1939.2 \\ & 2068.7^{a} \end{aligned}$ | $\begin{aligned} & 14.54 \\ & 13.14^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1.610 \\ & 1.900^{a} \end{aligned}$ | $\begin{aligned} & 0.0151 \\ & 0.0173^{a} \end{aligned}$ |
| $\mathrm{A}^{2}$ III calc. | $\begin{aligned} & 1.883 \\ & 1.146 \end{aligned}$ | 4.295 | $\begin{aligned} & 1.324 \\ & 1.233^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1621.4 \\ & 1814.4 \end{aligned}$ | $\begin{aligned} & 16.74 \\ & 12.88^{a} \end{aligned}$ | $\begin{aligned} & 1.403 \\ & 1.717 \end{aligned}$ | $\begin{aligned} & 0.0149 \mathrm{a} \\ & 0.0175 \end{aligned}$ |
| $B^{2} \Sigma^{+}$II ${ }_{\text {ealc. }}^{\text {exp. }}$ | $\begin{aligned} & 3.765 \\ & 3.193^{a} \end{aligned}$ | 4.335 | $\begin{aligned} & 1.226 \\ & 1.151^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1765.2 \\ & 2164.1^{a} \end{aligned}$ | $\begin{aligned} & 32.53 \\ & 20.25 \end{aligned}$ | $\begin{aligned} & 1.636 \\ & 1.970^{a} \end{aligned}$ | $\begin{aligned} & 0.0262 \\ & 0.0222^{a} \end{aligned}$ |
| ${ }^{4} \Sigma^{+}$I calc. | 4.016 | 2.162 | 1. 4448 | 1249.4 | 14.82 | 1.174 | 0.0152 |
| 4 III calc. | 5.326 | . 853 | 1.629 | 873.0 | 13.15 | 0.927 | 0.0154 |
| ${ }^{4} \Delta I \quad$ calc. | 5.913 | 2.187 | 1.441 | 1274.4 | 14.42 | 1.184 | 0.0147 |
| $D^{2} \Pi$ II $\begin{gathered}\text { calc. } \\ \text { exp. }\end{gathered}$ | $\begin{aligned} \sim & 6.593 \\ & 6.755 \end{aligned}$ | 3.008 | $\begin{aligned} & 1.590 \\ & 1.499^{c} \end{aligned}$ | $\begin{aligned} & 1041.6 \\ & 1004.7^{c} \end{aligned}$ | $\begin{aligned} & 6.38 \\ & 8.78^{c} \end{aligned}$ | $\begin{aligned} & 0.972 \\ & 1.162^{c} \end{aligned}$ | $\begin{aligned} & 0.010 \\ & 0.013^{c}\left(=\alpha_{0}\right) \end{aligned}$ |
| ${ }^{4} \Sigma^{-} \mathrm{I}$ calc. | 6.666 | $\sim 1.42$ | 1.446 | 1286.0 | 15.36 | 1.177 | 0.0138 |
| $2_{\text {¢ }}$ calc c | 7.742 | 1.860 | 1.621 | 950.7 | 12.63 | 0.936 | 0.0123 |
| $H^{2} \Pi I I I I_{\exp .}$ | $\begin{aligned} & 7.807 \\ & 7.556^{c}\left(=\mathrm{T}_{0}\right) \end{aligned}$ | ) 1.794 | $\begin{aligned} & 1.414 \\ & 1.310\left(=r_{o}\right)^{c} \end{aligned}$ | 1651.3 | 43.84 | $\begin{aligned} & 1.229 \\ & 1.520\left(=B_{0}\right)^{c} \end{aligned}$ | 0.0021 |
| $E^{2} \Sigma^{+} I I I_{\text {exp. }}^{\text {calc. }}$ | $\begin{aligned} & 7.856 \mathrm{a} \\ & 7.334 \end{aligned}$ | 1.745 | $\begin{aligned} & 1.364 \mathrm{a} \\ & 1.320 \end{aligned}$ | $\begin{aligned} & 1717.1 \\ & 1681.4 \end{aligned}$ | $\begin{gathered} 30.57 \mathrm{~d} \\ 3.60 \end{gathered}$ | $\begin{aligned} & 1.322 \\ & 1.487 \end{aligned}$ | $\begin{aligned} & 0.0151 \\ & 0.0064 \end{aligned}$ |
| $\mathrm{F}^{2} \Delta \mathrm{I} \quad \text { exp. }$ | $\begin{aligned} & 7.879 \\ & 7.400\left(=\mathrm{T}_{\mathrm{o}}\right)^{\mathrm{c}} \end{aligned}$ | c 1.722 | $\begin{aligned} & 1.461 \\ & 1.378^{\mathrm{c}}\left(=r_{0}\right) \end{aligned}$ | 1253.7 | 15.35 | $\begin{aligned} & 1.152 \\ & 1.374^{c}\left(=B_{0}\right) \end{aligned}$ | 0.0138 |
| ${ }^{4} \Sigma^{+}$II calc. | 7.898 . | 1.263 | 1.749 | - | $\square$ | - | 込 |

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Table III. (continued)

| State | $T e^{(e V)}$ | $D_{e}(\mathrm{eV})$ | $r e^{(\AA)}$ | $\omega_{e}\left(\mathrm{~cm}^{-1}\right)$ | $\omega_{e} x_{e}\left(\mathrm{~cm}^{-1}\right)$ | $B_{e}\left(\mathrm{~cm}^{-1}\right)$ | $\alpha_{e}\left(\mathrm{~cm}^{-1}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ${ }^{2}-1$ calc. | 7.988 | 1.613 | 1.453 | 1225.5 | 14.92 | 1.165 | 0.0155 |
| $J^{2} \Delta I I \quad \begin{aligned} & \text { calc. } \\ & \text { exp. }\end{aligned}$. | $\begin{aligned} & 8.432 \\ & 8.090^{c} \end{aligned}$ | 1.169 | $\begin{aligned} & 1.457 \\ & 1.414^{c} \end{aligned}$ | $\begin{aligned} & 1211.7^{c} \\ & 1121.6^{c} \end{aligned}$ | $\begin{aligned} & 17.58 \\ & 13.93^{c} \end{aligned}$ | $\begin{aligned} & 1.159 \\ & 1.305^{c} \end{aligned}$ | $\begin{aligned} & 0.0159 \\ & 0.0207\left(=\alpha_{0}\right)^{0} \end{aligned}$ |
| ${ }^{4} \Delta I I$ calc. | 8.619 | . 982 | 1.787 | 651.5 | 2.75 | 0.770 | 0.0057 |
| ${ }^{2} \Sigma^{-}$II calc. | 8.704 | 2.080 | 1.468 | 1183.2 | 14.04 | 1.142 | 0.0157 |
| ${ }^{1} \mathrm{IIV}$ calc. | $\sim 8.76$ | $\sim 0.84$ | 1.532 | 1446.4 | 15.60 | 1.047 | 0.0005 |
| ${ }^{\text {a }}$ Reference 1. |  |  |  |  |  |  |  |
| $\mathrm{b}_{\text {Reference }} 6$. |  |  |  |  |  |  |  |
| ${ }^{\text {c Reference }} 3$. |  |  |  |  |  |  |  |
| deference 11. |  |  |  |  |  |  |  |

Table V. Dominant configurations for bound states of CN. The coefficients given arise from a re-computation of each wave function in terms of the natural orbitals for the lowest state of that symmetry. Each coefficient incorporates the effects of all diatomic symmetry eigenfunctions arising from the given orbital occupancy. Only configurations with coefficient greater than 0.25 are included here.

| State | $R$ (bohrs) | Configurations | Coefficient |
| :---: | :---: | :---: | :---: |
| $\mathrm{X}^{2} \Sigma^{+}$ | 2.25 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{4}$ | 0.9304 |
| $\mathrm{B}^{2} \Sigma^{+}$ | 2.25 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma 5 \sigma^{2} 1 \pi^{4}$ | 0.8587 |
|  |  | 2. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.3682 |
| $E^{2} \Sigma^{+}$ | 2.25 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.8976 |
|  |  | 2. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma 5 \sigma^{2} 1 \pi^{4}$ | 0.2803 |
| ${ }^{5}{ }^{-}$ | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9528 |
| ${ }^{2} \Sigma^{-}$II | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9324 |
| ${ }^{4} \Sigma^{+}$ | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9173 |
|  |  | 2. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi 2 \pi^{3}$ | 0.2819 |
| ${ }^{4} \Sigma^{+}$II | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma 5 \sigma^{2} 1 \pi^{3} 2 \pi$ | 0.7365 |
|  |  | 2. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{2} 2 \pi^{2}$ | $0.5168$ |
| ${ }^{4} \Sigma^{-}$ | 2.75 | I. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9348 |
| ${ }^{4} \pi$ | 3.0 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma^{2} 1 \pi^{2} 2 \pi$ | 0.9624 |
| $F^{2} \Delta$ | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9320 |
| $J^{2} \Delta$ | 2.75 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9378 |
| ${ }^{4} \Delta$ | 3.0 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{3} 2 \pi$ | 0.9292 |
| ${ }^{4} \triangle I I$ | 3.0 | I. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma 1 \pi^{2} 2 \pi^{2}$ | 0.9142 |
|  |  | 2. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma 5 \sigma^{2} 1 \pi^{3} 2 \pi$ | 0.2879 |
| ${ }^{2}$ ¢ | 3.0 | 1. $1 \sigma^{2} 2 \sigma^{2} 3 \sigma^{2} 4 \sigma^{2} 5 \sigma^{2} 1 \pi^{2} 2 \pi$ | 0.9680 |

Table VI. Dominant configurations for the 4 lowest ${ }^{2} \pi$ state of CN. These results arise from 486 configuration calculations carried out using the $X 2^{+}$ ground state natural orbitals.

|  |  | $50^{2} 1 \pi^{3}$ | $50^{2} 1 \pi^{2} 2 \pi$ | $1 \pi^{4} 2 \pi$ |
| :---: | :---: | :---: | :---: | :---: |
| $A^{2} \mathrm{I}$ | $R=2.25$ | 0.9475 | 0.1395 | 0.0555 |
|  | $R=2.50$ | 0.9320 | 0.1530 | 0.0485 |
|  | $R=2.75$ | 0.9083 | 0.1826 | 0.0421 |
|  | $R=3.00$ | 0.8704 | 0.2360 | 0.0360 |
|  | $R=3.25$ | 0.8083 | 0.3122 | 0.0286 |
| $D^{2} \pi$ | $\mathrm{R}=2.25$ | 0.0280 | 0.0608 | 0.8198 |
|  | $R=2.50$ | 0.0425 | 0.1810 | 0.8255 |
|  | $R=2.75$ | 0.1595 | 0.9107 | 0.1050 |
|  | $R=3.00$ | 0.2354 | 0.8831 | 0.0489 |
|  | $\mathrm{R}=3.25$ | 0.3372 | 0.8346 | 0.0347 |
| ${ }^{3} \pi$ III | $R=2.25$ | 0.0727 | 0.9450 | 0.0197 |
|  | $R=2.50$ | 0.1001 | 0.9247 | 0.1128 |
|  | $R=2.75$ | 0.0114 | 0.2664 | 0.8052 |
|  | $R=3.00$ | 0.0480 | 0.7175 | 0.5249 |
|  | $R=3.25$ | 0.0804 | 0.8435 | 0.2575 |
| 3 II IV | $R=2.25$ | 0.0162 | 0.1208 | 0.1001 |
|  | $R=2.50$ | 0.0339 | 0.9091 | 0.0071 |
|  | $R=2.75$ | 0.0427 | 0.8790 | 0.1659 |
|  | $R=3.00$ | 0.0407 | 0.5458 | 0.6111 |
|  | $R=3.25$ | 0.0419 | 0.2704 | 0.7082 |

## FIGURE CAPTIONS

Fig. 1. Calculated potential energy curves for ${ }^{2}{ }_{2}^{+}$states of $C N$. The arrows near the right margin indicate dissociation limits.
Fig. 2. ${ }^{2} \Sigma^{-}$states.
Fig. 3. ${ }^{4} \Sigma^{+}$states.
Fig. 4. ${ }^{4} \Sigma^{-}$states.
Fig. 5. ${ }^{2} I I$ states.
Fig. 6. ${ }^{4} I I$ states.
Fig. 7. ${ }^{2} \Delta$ states.
Fig. 8. ${ }^{4} \Delta$ states.
Fig. 9. ${ }^{6} \Sigma^{+},{ }^{6} \Pi$, and ${ }^{8} \Sigma^{+}$states.
Fig. 10. ${ }^{2} \Phi,{ }^{2} \Gamma$, and ${ }^{4} \Phi$ states.
Fig. ll. Potential curves for the eight lowest bound states of CN.
Fig. 12. Positions of the ninth through eighteenth lowest bound states of $C N$.


Fig. 1


Fig. 2


Fig. 3


Fig. 4


Fig. 5


Fig. 6


Fig. 7


Fig. 8


Fig. 9


Fig. 10


Fig. 11


Fig. 12

## APPENDIX

APPENDIX (continued)

| $r_{a b}$ | ${ }^{2} \Sigma^{-} \mathrm{I}$ | ${ }^{2} \Sigma^{-}$II | ${ }^{2}{ }^{-}$III | ${ }^{2} \Sigma^{-}$IV | ${ }^{2} \Sigma^{-} \mathrm{V}$ | ${ }^{2} \Sigma^{-} \mathrm{VI}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.0 | -91:57862 | -91.53993 | -91.43682 | -91.34720 | -91.12357 | -91.05129 |
| 2.25 | -91.75560 | -91.72227 | -91.60215 | -91. 51552 | -91.39669 | -91.26205 |
| 2.5 | -91.82498 | -91.79562 | -91.66382 | -91.59580 | -91.53002 | -91.42115 |
| 2.75 | -91.84082 | -91.81442 | -91.67612 | -91.65017 | -91.57631 | -91.51859 |
| 3.0 | -91.83157 | -91.80740 | -91.68592 | -91.66667 | -91.61103 | -91.56996 |
| 3.25 | -91.81272 | -91.78984 | -91.70135 | -91.66843 | -91.64606 | -91.62154 |
| 3.5 | -91.79345 | -91.77002 | -91.70982 | -91.68737 | -91.66364 | -91.65472 |
| 4.0 | -91.77282 | -91.74137 | -91.72214 | -91.70725 | -91.70083 | -91.68304 |
| 5.0 | -91.77831 | -91.73776 | -91.73440 | -91.71264 | -91.71017 | -91.70615 |
| 6.0 | -91.78120 | -91.73812 | -91.73775 | -91.71117 | -91.71088 | -91.71041 |
| $\infty$ | -91.78154 | -91.73809 | -91.73809 | -91.71092 | -91.71092 | -91.71092 |

APPENDIX (continued)

| $\mathrm{r}_{\mathrm{ab}}$ | ${ }^{4} \Sigma^{+}$I | ${ }^{4} \Sigma^{+}$II | ${ }^{4} \Sigma^{+}$III | ${ }^{4} \Sigma^{+}$IV | ${ }^{4} \Sigma^{+}$V | $\Sigma^{-}$ | $\Sigma^{-}$II | ${ }^{4} \Sigma^{-}$III | ${ }^{4} \Sigma^{-}$IV | ${ }^{4} \Sigma^{-} \mathrm{V}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.0 | -91.72694 | -91.58613 | -91.22147 | -91.05762 | -91.01565 | -91.63047 | -91.50844 | -91.25074 | -91.22522 | -91.07808 |
| 2.25 | -91.90340 | -91.75110 | -91.49980: | -91.33458 | -91. 27905 | -91.80656 | -91.67303 | -91.49953 | -91.41395 | -91.31096 |
| 2.5 | -91.97195 | -91.81604 | -91.64483 | -91.49795 | -91.42491 | -91.87468 | -91.73664 | -91.63820 | -91.48694 | -91.45478 |
| 2.75 | -91.98675 | -91.83680 | -91.71443 | -91.60222 | -91.50453 | -91.88908 | -91.75939 | -91.69640 | -91.57135 | -91.55834 |
| 3.0 | -91.97646 | -91.84259 | -91.74330 | -91.66881 | -91.54902 | -91.87848 | -91.77305 | -91.70814 | -91.65560 | -91.61358 |
| 3.25 | -91.95664 | -91.84447 | -91.75531 | -91.70972 | -91.59628 | -91.85852 | -91.77946 | -91.71574 | -91.70803 | -91.63272 |
| 3.5 | -91.93647 | -91.84371 | -91.76258 | -91.73509 | -91.64996 | -91.83861 | -91.78040 | -91.73953 | -91.72881 | -91.63875 |
| 4.0 | -91.91332 | -91.82982 | -91.77189 | -91.76353 | -91.70777 | -91.82113 | -91.77736 | -91.76802 | -91.74332 | -91.70721 |
| 5.0 | -91.90777 | -91.80166 | -91.78216 | -91.77903 | -91.73530 | -91.83257 | -91.78319 | -91.77954 | -91.73973 | -91.73551 |
| 6.0 | -91.90747 | -91.79806 | -91.78185 | -91.78130 | -91.73788 | -91.83628 | -91.78489 | -91.78135 | -91.73833 | -91.73789 |
| $\infty$ | -91.90734 | -91.79773 | -91.78154 | -91.78154 | -91.73809 | -91.83672 | -91.78503 | -91.78154 | -91.73809 | -91.73809 |

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APPENDIX (continued)

| ${ }^{\text {ab }}$ | ${ }^{6} \Sigma^{+}{ }_{I}$ | ${ }^{6} \Sigma^{+}{ }^{\text {II }}$ | ${ }^{8}$ | ${ }^{2} \Pi 1$ | ${ }^{2} \pi$ II | ${ }^{2}$ II III | 2 II IV | $\pi$ | ${ }^{2}$ II VI | I VI | 2 II VIII |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1.85 |  |  |  | -91.75829 | -91.53796 | -91.40212 | -91.30663 | -91.26002 | -91.19410 | -91.09881 | -91.05082 |
| 2.0 | -91.39728 | -91.18854 | -90.37320 | -91.91453 | -91.69880 | -91.55479 | -91.50524 | -91.46385 | -91.39586 | -91.28871 | -91.27736 |
| 2.25 | -91.67082 | -91.45330 | -90.87504 | -92.03645 | -91.82588 | -91.72580 | -91.67125 | -91.65687 | -91.55285 | -91.48610 | -91.47190 |
| 2.5 | -91.81253 | -91.59731 | -91.19654 | -92.06470 | -91.85761 | -91.83333 | -91.76018 | -91.70181 | -91.60773 | -91.60285 | -91.56034 |
| 2.75 | -91.88120 | -91 | -91.40340 | -92.05023 | -91.88033 | -91.84566 | -91.80438 | -91.7064 | -91.67950 | -91.61415 | -91.60309 |
| 3.0 | -91.90996 | -91.72514 | -91.53809 | -92.01942 | -91.89208 | -91.82882 | -91.80796 | -91.72039 | -91.70593 | -91.66222 | -91.61889 |
| $3.25{ }^{\text { }}$ | -91.91817 | -91.75485 | -91.62696 | -91.98620 | -91.88529 | -91.82057 | -91.78752 | -91.74077 | -91.70714 | -91.68839 | -91.65165 |
| 3.5 | -91.91741 | -91.77361 | -91.68609 | -91.95794 | -91.86844 | -91.80869 | -91.77420 | -91.74762 | -91.71463 | -91.69727 | -91.68453 |
| 4.0 | -91.91153 | -91.79022 | -91.75159 | -91.92452 | -91.82752 | -91.78778 | -91.76583 | -91.74595 | -91.74082 | -91.71740 | -91.70608 |
| 5.0 | -91.90811 | -91.7965 | -91.79115 | -91.90926 | -91.78782 | -91.7825 | -91.77553 | -91.74332 | -91.73975 | -91.71333 | -91.71093 |
| 6.0 | -91.90753 | -91.79760 | -91.7969 | -91.90764 | -91.78227 | $-91.78176$ | -91.78088 | -91.7387 | -91.73840 | -91.71129 | -91.71093 |
| $\infty$ | -91.90734 | -91.79773 | -91.79773 | -91.90734 | -91.78154 | -91.78154 | -91.78154 | -91.73809 | -91.73809 | -91.71092 | -91.71092 |

APPENDIX (continued)

APPENDIX (continued)

| $r_{\text {ab }}$ | ${ }^{4} \mathrm{HI}$ | ${ }^{4}$ II II | ${ }^{4} \mathrm{II}$ III | ${ }^{4} \pi$ IV | $4 \pi \mathrm{~V}$ | ${ }^{4} \pi \mathrm{IVI}$ | ${ }^{4} \pi \mathrm{VIII}$ | $6_{\Pi}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.0 | -91.69635 | -91.53935 | -91.33330 | -91.29387 | -91. 20198 | -91.16801 | -91. 10254 | -91.41609 |
| 2.25 | -91.80031 | -91.76551 | -91.55409 | -91.49620 | -91.40891 | -91.37955 | -91.35021 | -91.61531 |
| 2.5 | -91.87533 | -91.81204 | -91.65587 | -91.58188 | -91.53377 | -91.50274 | -91.48433 | -91.69732 |
| 2.75 | -91.92309 | -91.78780 | -91.69521 | -91.64459 | -91.61032 | -91.58806 | -91.52768 | -91.71934 |
| 3.0 | -91.93800 | -91.76188 | -91.71588 | -91.69330 | -91.66853 | -91.60452 | -91.56207 | -91.71323 |
| 3.25 | -91.93628 | -91.76016 | -91.74018 | -91.72218 | -91.68095 | -91.63486 | -91.61589 | -91.73414 |
| 3.5 | -91.92754 | -91.77681 | $-91.76287$ | -91.73891 | -91.68477 | -91.67510 | -91.66363 | -91.79150 |
| 4.0 | -91.91057 | -91.81162 | -91.78518 | -91.74896 | -91.74095 | -91.73329 | -91.69054 | -91.85848 |
| 5.0 | -91.90623 | -91.83351 | -91.78348 | -91.77927 | -91.77448 | - -91.73984 | -91.73096 | -91.90032 |
| 6.0 | - -91.90725 | -91.83640 | -91.78187 | -91.78144 | -91.78076 | -91.73843 | -91.73731 | -91.90659 |
| $\infty$ | -91.90734 | -91.83672 | -91.78154 | -91.78154 | -91.78154 | -91.73809 | -91.73809 | -91.90734 |

APPENDIX (continued)

| $r_{\text {ab }}$ | ${ }^{2} \Delta I$ | ${ }^{2} \Delta$ II | ${ }^{2} \triangle$ III | ${ }^{2} \Delta \mathrm{IV}$ | ${ }^{2} \Delta \mathrm{~V}$ | ${ }^{2} \Delta$ VI |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.0 | -91.57277 | -91.56301 | -91:42872 | -91.38321 | -91.15822 | -91.13665 |
| 2.25 | -91.75361 | -91.73960 | -91.59408 | -91.55281 | -91.42923 | -91.36685 |
| 2.5 | -91.82646 | -91.80822 | -91.66047 | -91.63606 | -91.55051 | -91.51734 |
| 2.75 | -91.84452 | -91.82.423 | -91.70369 | -91.66161 | -91.59726 | -91.58921 |
| 3.0 | -91.83632 | -91.81629 | -91.73281 | -91.65770 | -91.63559 | -91.62200 |
| 3.25 | -91.81767 | -91.79959 | -91.74629 | -91.65917 | -91.65549 | -91.65335 |
| 3.5 | -91.79857 | -91.78267 | -91.75056 | -91.68368 | -91.67495 | -91.66505 |
| 4.0 | -91.78102 | -91.76977 | -91.73659 | -91.71124 | -91.70116 | -91.68404 |
| 5.0 | -91.78121 | -91.77839 | -91.73452 | -91.71394 | -91.70913 | -91.70625 |
| 6.0 | -91.78159 | -91.78120 | -91.73775 | -91.71130 | -91.71075 | -91.71042 |
| $\infty$ | -91.78154 | -91.78154 | -91.73809 | -91.71092 | -91.71092 | -91.71092 |

APPENDIX (continued)

| ${ }^{\mathrm{r}} \mathrm{ab}$ | ${ }^{4} \Delta I$ | ${ }^{4} \Delta I I$ | ${ }^{4} \triangle \mathrm{III}$ | ${ }^{4} \Delta \mathrm{IV}$ | $2_{\text {¢ }}$ I | ${ }^{\text {¢ }}$ II | $2_{\text {¢ III }}$ | ${ }^{4}$ Ф | ${ }^{2} \Gamma$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.0 | -91.66119 | -91.53012 | -91.27085 | -91.06518 | -91.44658 | -91.23860 | -91.12894 | -91.22189 | -91.14117 |
| 2.25 | -91.83624 | -91.69378 | -91.54576 | -91.33310 | -91.67464 | -91.46522 | -91.33548 | -91.42560 | -91.42221 |
| 2.5 | -91.90342 | -91.75687 | -91.68519 | -91.48303 | -91.78574 | -91.57472 | -91.45036 | -91.51102 | -91.57105 |
| 2.75 | -91.91695 | -91.78575 | -91.73559 | -91.57531 | -91.83424 | -91.62544 | -91.56300 | -91.53507 | -91.64690 |
| 3.0 | -91.90546 | -91.80779 | -91.73419 | -91.63582 | -91.84922 | -91.65310 | -91.62585 | -91.53105 | -91.68310 |
| 3.25 | -91.88442 | -91.81669 | -91.73039 | -91.66775 | -91.84668 | -91.68031 | -91.64969 | -91.59900 | -91.69892 |
| 3.5 | -91.86305 | -91.81686 | -91.74051 | -91.67988 | -91.83592 | -91.69959 | -91.65968 | -91.65966 | -91.70533 |
| 4.0 | -91.84074 | -91.80224 | -91.76257 | -91.70832 | -91.81011 | -91.71350 | -91.67342 | -91.72985 | -91.70944 |
| 5.0 | -91.83714 | -91.78372 | -91.77869 | -91.73534 | -91.78580 | -91.71258 | -91.70672 | -91.77401 | -91.71112 |
| 6.0 | -91.83685 | -91.78182 | -91.78127 | -91.73787 | -91.78210 | -91.71121 | -91.71057 | -91.78071 | -91.71103 |
| $\infty$ | -91.83672 | -91.78154 | -91.78154 | -91.73809 | -91.78154 | -91.71092 | -91.71092 | -91.78154 | -91.71092 |

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[^0]:    ${ }^{8}$ CDC 7600 time.

