# STUDIES ON E2 TRANSITION IN THE Na-LIKE HIGHLY STRIPPED ION Fe xvi 

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#### Abstract

The spectrum of the solar corona and plasma spectra in astrophysical objects and fusion devices exhibit forbidden lines in alkali-like ions. Ions belonging to the iron group are particularly important in this respect. The electric quadrupole (E2) transitions for Fe xvi are computed using the highly correlated relativistic wave function obtained by using coupled cluster theory including all single, double, and some triple excitations from the core. Term values of the present ion obtained by our method are compared with the available experimental and theoretical data. The detailed highly accurate relativistic data for line strengths and transition probabilities are presented for a large number of transitions of low transition rates, and a few of both of them are compared with existing data as samples.


Subject heading: atomic data
On-line material: machine-readable table

## 1. INTRODUCTION

The study of atomic transition is a subject of considerable interest in many fields. The extremely hot environment of the stars (for instance, the corona of the sun and planetary nebulae) show abundances (Feldman 1992) of the highly stripped ions. With the advent of high-resolution spectrographs, observation of weak or forbidden transition lines becomes possible, and they are of great astrophysical interest. Many astrophysical phenomena such as coronal heating, the evolution of many chemical compositions in the stellar envelope, and the determination of the chemistry in planetary nebulae precursors' envelopes are believed to be explained largely by these forbidden lines.

In astrophysics, the study of transition probabilities plays an important role in the determination of atomic abundances. In controlled thermonuclear reactions, atomic radiation is one of the primary loss mechanisms. In laboratory tokamak plasmas and in various astronomical objects, suitably chosen electric quadrupole (E2) forbidden lines serve as a basis for reliable electron density and/or temperature diagnostics (Biemont \& Zeippen 1996). Accurate estimates of radiative transition probabilities between multiplet states are an important source for the successful experimental identification of the spectra of astrophysical and laboratory plasmas. Probabilities of magnetic dipole and electric quadrupole transitions, in particular, are important in plasma diagnostics, but the experimental determination of these quantities is difficult, and only an accurate theoretical calculation can provide important information.

In the present article we are interested in studying the electric quadrupole transition properties of the Na-like highly stripped ion Fe xvi. We have successfully (Ray 2002a) performed similar calculations for Co xvii (Ray 2002b) and Ni xviiI (Ray \& Das 2002) that are in very good agreement with the other relativistic and nonrelativistic calculations. Tull et al. (1972) have mentioned the additional need for both theoretical and experimental studies on such systems. The present availability of intense tunable radiation sources has made it feasible to measure transition probabilities of electric quadrupole (E2) transition. However, no
experimental E2 transition probability data on Fe xvI appear to be available in the literature.

A number of theoretical calculations on electric and magnetic multipole transition rates have been performed in recent years using various approximations (Huang 1985; Johnson, Plante, \& Sapirstein 1995; Safronova, Johnson, \& Livingston 1999; Avgoustoglou \& Beck 1998; Beck 1998; Ishikawa \& Vilkas 2001), and it has become evident that accurate, correlated wave functions must be employed to evaluate the transition rate accurately. For the electric dipole forbidden transition in high- $Z$ ions, electric quadrupole (E2) transition rates are dominant over magnetic dipole (M1) rates. High-precision calculation of transition energies as well as of wave functions is necessary because E2 transition rates involve a fifth-power dependence on transition energy. A relativistic description is required for describing the highly stripped ions such as Fe xvi where the orbital electrons probe regions of space with high potential energy near the atomic nuclei. The primary effect of this relativistic description is to include changes in spatial and momentum distributions, spin-orbit interactions, quantum electrodynamic corrections such as the Lamb shift, and vacuum polarization, whereas the secondary effect in many-electron systems is the modification of orbitals due to shielding of the other electrons in penetrating orbits.

In the present calculation we have used an improved methodology (Majumder et al. 2001) of generating the basis set. The Dirac-Hartree-Fock method adapted in the numerical MCDF GRASP code by Parpia (1992) is able to generate only the bound orbitals because of the boundary conditions imposed to solve the differential equation; generating higher orbitals creates a convergence problem. The Gaussian basis set expansion method is able to generate both the bound and continuum orbitals solving the Dirac-Hartree-Fock equation, but these orbitals are highly dependent on two arbitrary parameters, known in the literature as $\alpha_{0}$ and $\beta$; there is a great debate on the choice of these two parameters. In our calculation we have chosen a basis of a total of 98 orbitals with both bound and continuum; the continuum orbitals are confined within a maximum energy of 500 a.u. All
the bound orbitals in our basis are obtained by using the MCDF GRASP code (Parpia 1992), and the rest continuum orbitals are from the Gaussian code (Chaudhuri, Panda, \& Das 1999), choosing best values for $\alpha_{0}$ and $\beta$. We have taken nine $s$ orbitals up to $9 s$, eight each of the $p_{1 / 2}$ and $p_{3 / 2}$ orbitals up to $9 p_{1 / 2}$ and $9 p_{3 / 2}$, seven each of the $d_{3 / 2}$ and $d_{5 / 2}$ orbitals up to $9 d_{3 / 2}$ and $9 d_{5 / 2}$, five each of the $f_{5 / 2}$ and $f_{7 / 2}$ orbitals up to $8 f_{5 / 2}$ and $8 f_{7 / 2}$, and four each of the $g_{7 / 2}$ and $g_{9 / 2}$ orbitals up to $8 g_{7 / 2}$ and $8 g_{9 / 2}$ as bound orbitals; the rest in our basis are virtual orbitals. These two different types of orbitals, bound and continuum, are generated by two different codes, so they may not be orthogonal. We are considering that the MCDF GRASP orbitals are closer to the actual orbitals since they are obtained by imposing the proper physical boundary conditions. In our methodology, first we make the virtual orbitals orthogonal to the more accurate GRASP orbitals one by one following the Schmidt orthogonalization principle. These new orthogonal virtual orbitals are normalized using the same Fock space. We have adapted a total of $12 s$ orbitals up to $12 s ; 11$ each of the $p_{1 / 2}$, $p_{3 / 2}, d_{3 / 2}, d_{5 / 2}, f_{5 / 2}$, and $f_{7 / 2}$ orbitals up to $12 p_{1 / 2}, 12 p_{3 / 2}$, $13 d_{3 / 2}, 13 d_{5 / 2}, 14 f_{5 / 2}$, and $14 f_{7 / 2}$; and 10 each of the $g_{7 / 2}$ and $g_{9 / 2}$ orbitals up to $14 g_{7 / 2}$ and $14 g_{9 / 2}$. The motivation in choosing such an improved basis is to make the basis orbitals as close as possible to the actual physical orbitals so that it can provide more accurate data in a finite set. However, the Slater determinant formed by these orbitals to represent the atomic state function are deficient from the physical point of view because of the lack of the correlation effect that is approximated by an equivalent single-particle potential in the Dirac-Hartree-Fock theory. How the effect of correlation can be included properly in a many-electron system is a great challenge to quantum chemists and atomic and molecular physicists.

One of the most advanced methods for treating this problem is the coupled cluster method (CCM; Bishop \& Kümmel 1987). It is a quantum many-body method in which the wave function is decomposed in terms of amplitudes for exciting clusters of a finite number of particles. The development of this theory was started in the nuclear physics community by Coester and Kümmel (Coester 1958; Coester \& Kümmel 1960) and was later introduced in quantum chemistry by Cizek and coworkers (Paldus et al. 1978; Paldus 1983); it was applicable mainly to the closed shell system. Subsequent development of this theory using the idea of complete model spaces (Lindgren 1978; Ey 1978; Mukherjee 1986; Lindgren \& Mukherjee 1987) and a Hermitian formulation (Lindgren 1991) of the CCM has led to connected cluster operators and an effective Hamiltonian, also for an incomplete model space.

## 2. THEORY

### 2.1. Coupled Cluster Method

The idea of the CCM is as follows: two particles in the filled Fermi sea interact with each other and lift themselves out of the Fermi sea, so that after the interaction both particles are in orbitals that in the previous simplified picture were unoccupied. This process may be described by a quantum mechanical operator $\boldsymbol{S}_{2}$ that acts on the Fermi sea wave function (say $|\Phi\rangle$ ) to produce the wave function $\boldsymbol{S}_{2}|\Phi\rangle$, which describes two particles outside the Fermi sea and con-
sequently two holes inside it, and all remaining $N-2$ particles are in their previous orbitals, where $N$ is the total number of electrons present in the atom.

It may also happen that two pairs of particles do this completely independently. This process may be described by applying this operator $\boldsymbol{S}_{2}$ twice and so on, with the proviso that we must include the proper weighting factor. By the principle of linear superposition, the total amplitude for excitation of an arbitrary number(s) $m$ (including zero) of independent pairs is

$$
\begin{equation*}
\sum_{m=0}^{\infty} \frac{1}{m!} \boldsymbol{S}_{2}^{m}|\Phi\rangle=e^{\boldsymbol{S}_{2}}|\Phi\rangle \tag{1}
\end{equation*}
$$

Simultaneous excitation of three particles can be described by a contribution $\boldsymbol{S}_{3}|\Phi\rangle$ to the exact wave function, and the simultaneous excitation of $n$ independent triplets will be $(1 / n!) S_{3}^{n}|\Phi\rangle$. We must count also the possibility of simultaneous excitation of pairs and triplets. Again by linear superposition, the amplitude for simultaneous excitation of $m$ pairs and $n$ triplets from the Fermi sea is $(1 / m!n!) \boldsymbol{S}_{2}^{m} \boldsymbol{S}_{3}^{n}|\Phi\rangle$. Here $\boldsymbol{S}_{2}$ and $\boldsymbol{S}_{3}$ are independent processes, so they commute, and we need not worry about their ordering. Summing over all possible values of $m$ and $n$ leads to the amplitude $e^{\left(\boldsymbol{S}_{2}+\boldsymbol{S}_{3}\right)}|\Phi\rangle$ for the total effect of all pair and triplet excitations. Proceeding in this way with the excitation of clusters of $4,5, \ldots, N$ particles, we arrive at a wave function

$$
\begin{equation*}
|\Psi\rangle=e^{S}|\Phi\rangle \tag{2}
\end{equation*}
$$

where

$$
\begin{equation*}
\boldsymbol{S}=\sum_{n=1}^{N} \boldsymbol{S}_{n} \tag{3}
\end{equation*}
$$

Here $\boldsymbol{S}_{n}$ indicates excitation of $n$ particles at a time. Hubbard (1957) noticed first that the operator generating the wave function of a quantum many-body system has an exponential form. This exponential representation may be regarded as an expansion of the exact wave function in a complete orthonormal basis. But we have to keep always in mind the arguments we have used. Such an interpretation of the wave function is very useful in practical application of the CCM. Because of its wide range of applicability in different fields of many-body systems of both bosons and fermions, quite regardless of the type and range of interaction, and for yielding high-precision results for the ground state as well as low-energy excited states, it is considered a universal theory for including correlation in many-body physics.

The CCM equations for the matrix elements of $\boldsymbol{S}_{n}$ are easily obtained by projecting the Schrödinger equation

$$
\begin{equation*}
e^{-\boldsymbol{S}} \boldsymbol{H} e^{\boldsymbol{S}}|\Phi\rangle=E|\Phi\rangle \tag{4}
\end{equation*}
$$

onto the complete $N$-body space spanned by the Fermi sea states and those states obtained by creating $n$ general particle-hole excitations out of it. This yields a series of coupled equations, each of which contains a finite number of terms. The excitation operators can be written as

$$
\begin{gather*}
S_{1}=\sum_{i, a} s_{i}^{a} \boldsymbol{a}^{+} \boldsymbol{i}  \tag{5}\\
S_{2}=\sum_{i, j, a, b} s_{i j}^{a b} \boldsymbol{a}^{+} \boldsymbol{i b}^{+} \boldsymbol{j} \tag{6}
\end{gather*}
$$

and so on. Here $\boldsymbol{i}$ and $\boldsymbol{j}$ are the hole annihilation, $\boldsymbol{a}^{+}$and $\boldsymbol{b}^{+}$ are the particle creation operators, and $s_{i}^{a}$ and $s_{i j}^{a b}$ are the amplitudes for single-particle and two-particle excitations, respectively.

The first equation in this series yields an expression for $E$. Because of the special form of the above Schrödinger equation, the remaining equations do not involve the energy $E$ or other macroscopic terms and represent a truly microscopic decomposition of the Schrödinger equation into a set of coupled equations that describe the dynamics of the $N$-body clusters. These equations are intrinsically nonlinear. We consider all the single $\left(S_{1}\right)$, double ( $S_{2}, S_{1} \times S_{1}$ ), and some disconnected triple $\left(S_{2} \times S_{1}\right)$ excitations (Bartlett 1995) from the core in the present calculation.

### 2.2. Electric Quadrupole (E2) Transition

The matrix element for electric quadrupole transitions is

$$
\begin{equation*}
\hat{\boldsymbol{Q}}_{f i}=\left\langle\Psi_{f}\right| \hat{\boldsymbol{Q}}\left|\Psi_{i}\right\rangle \tag{7}
\end{equation*}
$$

where $\left|\Psi_{i}\right\rangle$ and $\left|\Psi_{f}\right\rangle$ denote the initial and final atomic state functions, respectively. Here electric quadrupole operator $\hat{\boldsymbol{Q}}$ is a rank 2 tensor and may be written as

$$
\begin{equation*}
\hat{\boldsymbol{Q}}=e r^{2} C_{q}^{2}(\hat{\boldsymbol{r}}) \tag{8}
\end{equation*}
$$

The line strength is defined as

$$
\begin{equation*}
\left.S_{f i}=\sum_{M_{f}, M_{i}}\left|\left\langle\Psi_{f}\right| \hat{\boldsymbol{Q}}\right| \Psi_{i}\right\rangle\left.\right|^{2} \tag{9}
\end{equation*}
$$

Applying the Wigner-Eckart theorem, the above expression transforms to

$$
\begin{align*}
S_{f i}= & \sum_{M_{f}, M_{i}} \sum_{q}\left(2 J_{f}+1\right) \\
& \times\left(\begin{array}{ccc}
J_{f} & 2 & J_{i} \\
-M_{f} & q & M_{i}
\end{array}\right)^{2}\left|\left\langle\Psi_{f}\|\hat{\boldsymbol{Q}}\| \Psi_{i}\right\rangle\right|^{2} . \tag{10}
\end{align*}
$$

The transition probability (per second) for the present E2 transition is related to the line strength (in atomic or $e^{2} a_{0}^{4}$ units) by the relation (Sobel'man 1972)

$$
\begin{equation*}
A=\left(1.11995 \times 10^{18} / g_{f} \lambda^{5}\right) S_{f i} \tag{11}
\end{equation*}
$$

Here $\lambda$ is the wavelength in angstroms of the associated electromagnetic radiation, $A$ is the transition probability, and $g_{f}$ is the degeneracy of the final state.

### 2.3. Computation Using CCM

The expression for the present E2 transition using the CCM is

$$
\begin{equation*}
\left\langle\Psi_{f}\right| \hat{\boldsymbol{Q}}\left|\Psi_{i}\right\rangle=\left\langle\Phi_{f}^{0}\right|\left\{e^{\boldsymbol{S}_{f}^{\dagger}}\right\} \overline{\boldsymbol{Q}}\left\{e^{\boldsymbol{S}_{i}}\right\}\left|\Phi_{i}^{0}\right\rangle \tag{12}
\end{equation*}
$$

with

$$
\begin{equation*}
\overline{\boldsymbol{Q}}=e^{T^{\dagger}} \hat{\boldsymbol{Q}}^{T} \tag{13}
\end{equation*}
$$

where $\boldsymbol{T}, \boldsymbol{S}_{i}$, and $\boldsymbol{S}_{f}$ are the cluster operators for excitations from the core and the valence orbitals in the initial and final states, respectively. The connected parts of equations (12) and (13) will contribute, and hence we compute only those parts in our quadrupole matrix element calculation. Here
$\left|\Phi_{i}^{0}\right\rangle$ and $\left|\Phi_{f}^{0}\right\rangle$ are the Slater determinants obtained by using the Dirac-Hartree-Fock single-particle orbitals.

## 3. RESULTS AND DISCUSSION

We are presenting theoretical data for the term values, E2 transition line strengths, and transition probabilities that are far more accurate. First, we have used fully relativistic Dirac-Hartree-Fock orbitals, and second, we have included the effect of Coulomb correlation through an ab initio allorder many-body coupled cluster theory. It should be noted that the present coupled cluster theory is equivalent to an all-order many-body perturbation theory. We have included all the single $\left(S_{1}\right)$, double ( $S_{2}, S_{1} \times S_{1}$ ), and some disconnected triple $\left(S_{2} \times S_{1}\right)$ excitations from the atomic core in our calculations. In Table 1, we compare our term values with the corresponding available experimental data (Feldman 1971) and theoretical data (Tull et al. 1972). In their calculation of term values, Tull et al. (1972) have included the relativistic effects through a first-order perturbation theory using nonrelativistic frozen core type Har-tree-Fock orbitals. The percentage errors with respect to the observed values are presented in the same table for both the theoretical results and for the theoretical results obtained by the simple Dirac-Hartree-Fock theory. We have used negative signs to indicate the direction of error, that is, whether it is below the corresponding observed values or above the corresponding observed values. A negative sign before the error indicates that the experimental values are lower than the theoretical values, and no negative sign indicates that the experimental values are higher than the theoretical values, in the present data set. The effect of the Coulomb correlation can be understood by comparing the columns with footnotes "a" and "b." All our theoretical results indicate the importance of correlation in such a system. The effect of correlation is greater in low-lying states and in all the $p$ orbitals. Again it is to be noted that the effect of correlations have changed all the errors to negative, which indicates that in the present improved situation, all the theoretical values are a little higher than the experimental term values. However, the low-lying $p_{3 / 2}, d_{3 / 2}$, and $d_{5 / 2}$ have a greater deviation; the percentage error is $10^{-1}$, whereas in other cases it is $10^{-2}$. In Table 2, a few of our line strength data are compared with the existing line strength data (Tull et al. 1972; Charro, Bielinska-Waz, \& Martin 2000). They are in good agreement with both the theories. Similarly, in Table 3 we have compared a few of our transition probability data with the existing relativistic transition probability data (Fuhr, Martin, \& Wiese 1988). Our transition probability data are also in agreement with theirs.

In Table 4, which appears in full in the electronic version of this article, our detailed present data for line strengths and transition probabilities are reported. All our line strength data are very close to the results of Charro et al. (2000) and Tull et al. (1972); to compare with them one has to multiply our line strength data in Table 4 by a constant factor of $1 / \sqrt{2}$. This factor arises simply because of the use of a different formulation. We have used the formulation prescribed by Sobel'man (1972). All our transition probability data are also in good agreement with Fuhr et al. (1988). The relativistic quantum defect orbital method adapted by them (Charro et al. 2000) is quasi-relativistic in nature, while Tull et al. have adapted a nonrelativistic approach where the relativistic correction to the term values is

TABLE 1
Term Values of Fe xvi

| Levels | $J$-Values | $\begin{aligned} & \mathrm{DHF}^{\mathrm{a}} \\ & \left(\mathrm{~cm}^{-1}\right) \end{aligned}$ | $\begin{aligned} & \mathrm{CCM}^{\mathrm{b}} \\ & \left(\mathrm{~cm}^{-1}\right) \end{aligned}$ | $\begin{aligned} & \text { Tull et al. } .^{\text {c }} \\ & \left(\mathrm{cm}^{-1}\right) \end{aligned}$ | Observed ( $\mathrm{cm}^{-1}$ ) | Error ${ }^{\text {a }}$ (percent) | Error ${ }^{\text {b }}$ (percent) | Error ${ }^{\text {c }}$ (percent) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $3 s . . . . . .$. | 1/2 | 0 | 0 | 0 | 0 |  |  |  |
| $3 p . . . . . .$. | 1/2 | 278216 | 277333 | 277340 | 277160 | -0.381 | -0.062 | -0.065 |
|  | 3/2 | 299611 | 298840 | 296800 | 298140 | -0.493 | -0.234 | 0.449 |
| $3 d \ldots \ldots \ldots$ | 3/2 | 678114 | 676809 | 676760 | 675480 | -0.390 | -0.197 | -0.189 |
|  | 5/2 | 681258 | 680037 | 680070 | 678410 | -0.420 | -0.240 | -0.245 |
| 4s ......... | $1 / 2$ | 1865257 | 1868505 | 1866250 | 1867530 | 0.122 | -0.052 | 0.068 |
| $4 p \ldots \ldots .$. | 1/2 | 1975523 | 1978467 | 1976200 | 1978040 | 0.127 | -0.022 | 0.093 |
|  | 3/2 | 1983944 | 1986861 | 1983860 | 1986100 | 0.108 | -0.038 | 0.113 |
| $4 d \ldots \ldots .$. | 3/2 | 2122800 | 2125890 | 2123290 | 2124070 | 0.060 | -0.086 | 0.037 |
|  | 5/2 | 2124235 | 2127355 | 2124720 | 2125360 | 0.053 | -0.094 | 0.030 |
| $4 f$........ | 5/2 | 2182244 | 2186321 | 2183720 | 2184620 | 0.109 | -0.078 | 0.041 |
|  | 7/2 | 2182741 | 2186824 | 2184220 | 2185160 | 0.111 | $-0.076$ | 0.043 |
| 5s ........ | 1/2 | 2630439 | 2664389 | 2661370 | ... | ... | ... |  |
| 5p........ | 1/2 | 2688406 | 2718587 | 2715570 | 2717170 | 1.059 | $-0.052$ | 0.059 |
|  | 3/2 | 2718588 | 2722720 | 2719360 | 2721160 | 0.094 | -0.057 | 0.066 |
| 5d........ | 3/2 | 2785573 | 2789835 | 2786630 | 2788020 | 0.088 | -0.065 | 0.050 |
|  | 5/2 | 2786324 | 2790600 | 2787360 | 2788680 | 0.084 | -0.069 | 0.047 |
| $5 f \ldots$ | 5/2 | 2815591 | 2820246 | 2817100 | 2818600 | 0.107 | -0.058 | 0.053 |
|  | 7/2 | 2815847 | 2820505 | 2817360 | 2819000 | 0.112 | $-0.053$ | 0.058 |
| $5 \mathrm{~g} \ldots \ldots \ldots$ | 7/2 | 2818429 | 2823650 | ... | ... | ... | ... | ... |
|  | 9/2 | 2818583 | 2823804 | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| $6 s . . . . . .$. | 1/2 | 2849097 | 3077036 | 3073690 | ... | $\ldots$ | . $\cdot$. | $\ldots$ |
| $6 p \ldots \ldots .$. | 1/2 | 2943971 | 3107609 | 3104270 | 3106360 | 5.228 | -0.040 | 0.067 |
|  | 3/2 | 3105293 | 3109944 | 3106410 | 3108870 | 0.115 | -0.034 | 0.079 |
| 6d........ | 3/2 | 3142805 | 3147537 | 3144080 | 3146020 | 0.102 | -0.048 | 0.062 |
|  | 5/2 | 3143243 | 3147983 | 3144510 | 3146660 | 0.108 | -0.042 | 0.068 |
| $6 f \ldots \ldots$ | 5/2 | 3160009 | 3164938 | 3161540 | 3163100 | 0.098 | $-0.058$ | 0.049 |
|  | 7/2 | 3160158 | 3165089 | 3161690 | 3163190 | 0.096 | $-0.060$ | 0.047 |
| $6 \mathrm{~g} . . . . . .$. | 7/2 | 3161866 | 3167124 | ... | ... | . . . | ... | ... |
|  | 9/2 | 3161955 | 3167213 | ... | ... | ... | ... | $\ldots$ |
| $7 s . . . . . .$. | 1/2 | 3117343 | 3318384 | 3134870 | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| $7 p \ldots \ldots .$. | 1/2 | 3196172 | 3337287 | 3333780 | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
|  | 3/2 | 3333824 | 3338733 | 3335110 |  |  |  |  |
| 7d........ | 3/2 | 3356962 | 3361923 | 3358350 | 3360440 | 0.103 | -0.044 | 0.062 |
|  | 5/2 | 3357239 | 3362205 | 3358620 | 3360740 | 0.104 | -0.043 | 0.063 |
| $7 f$........ | 5/2 | 3367725 | 3372798 | 3369270 | 3371190 | 0.103 | -0.048 | 0.057 |
|  | 7/2 | 3367819 | 3372894 | 3369360 | 3371070 | 0.096 | -0.054 | 0.051 |
| 7g........ | 7/2 | 3368971 | 3374253 | ... | ... | . . . | ... | ... |
|  | 9/2 | 3369027 | 3374309 | $\ldots$ | $\ldots$ | ... | ... | $\ldots$ |
| 8s ........ | 1/2 | 3290726 | 3471676 | 3468060 | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| $8 p \ldots \ldots .$. | 1/2 | 3358510 | 3484166 | 3480560 | $\ldots$ | ... | $\ldots$ | $\ldots$ |
|  | 3/2 | 3480070 | 3485123 | 3481440 |  | . | . |  |
| $8 d \ldots \ldots$. | 3/2 | 3495353 | 3500440 | 3496790 | 3498710 | 0.096 | -0.049 | 0.055 |
|  | 5/2 | 3495538 | 3500629 | 3496970 | 3498960 | 0.098 | -0.048 | 0.057 |
| $8 f . . . . . .$. | 5/2 | 3502529 | 3507687 | 3504080 | 3505700 | 0.090 | -0.057 | $0.046$ |
|  | 7/2 | 3502592 | 3507751 | 3504140 | 3505830 | 0.092 | -0.055 | 0.048 |
| 9s ........ | 1/2 | 3408424 | 3575083 | 3571410 | ... | ... | ... | ... |
| $9 p \ldots \ldots .$. | 1/2 | 3470457 | 3583762 | 3580090 | ... | ... | ... | ... |
|  | 3/2 | 3579284 | 3584428 | 3580700 | ... | ... | ... | ... |
| 9d........ | 3/2 | 3589909 | 3595075 | 3591380 | ... | ... | ... | $\ldots$ |
|  | 5/2 | 3590039 | 3595208 | 3591500 |  |  |  |  |

${ }^{\text {a }}$ Results of Dirac-Hartree-Fock theory.
${ }^{\mathrm{b}}$ Present results of CCM.
${ }^{c}$ Results of Tull et al. 1972.

TABLE 2
Comparison of Present Line Strengths with Available Theoretical Data of Fe xvi

| Transition ( $n^{\prime} l^{\prime} \rightarrow n l$ ) | Present Calculation Line Strength |  |  | Charro et al. 2000 Line Strength |  |  | Tullet al. 1972 <br> Line Strength <br> (Nonrelativistic) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $l-1 / 2$ | $l+1 / 2$ | Sum | $l-1 / 2$ | $l+1 / 2$ | Sum |  |
| $3 s \rightarrow 3 d$..................... | 0.118 | 0.177 | 0.295 | 0.118 | 0.177 | 0.295 | 0.284 |
| $3 s \rightarrow 4 d \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.079 | 0.119 | 0.198 | 0.072 | 0.108 | 0.180 | 0.199 |
| $3 s \rightarrow 5 d \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.011 | 0.017 | 0.028 | 0.010 | 0.015 | 0.026 | 0.027 |
| $4 s \rightarrow 4 d$...................... | 1.829 | 2.750 | 4.579 | 1.77 | 2.66 | 4.43 | 4.40 |
| $4 s \rightarrow 5 d$. | 0.538 | 0.801 | 1.339 | 0.495 | 0.738 | 1.23 | 1.35 |
| $3 p_{1 / 2} \rightarrow 4 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.308 | ... | ... | 0.316 | ... | ... | ... |
| $3 p_{3 / 2} \rightarrow 4 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.090 | 0.543 | 0.941 | 0.923 | 0.554 | 0.962 | 0.908 |
| $3 p_{1 / 2} \rightarrow 4 p \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | ... | 0.060 | ... | ... | 0.059 | ... | ... |
| $3 p_{3 / 2} \rightarrow 4 p \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.064 | 0.062 | 0.186 | 0.063 | 0.061 | 0.183 | 0.180 |
| $3 d_{3 / 2} \rightarrow 4 d \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.061 | 0.026 | ... | 0.061 | 0.026 | ... | ... |
| $3 d_{5 / 2} \rightarrow 4 d \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.026 | 0.104 | 0.217 | 0.026 | 0.105 | 0.218 | 0.209 |
| $4 f_{5 / 2} \rightarrow 5 f^{\ldots} \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.812 | 0.136 | ... | 0.774 | 0.129 | ... | ... |
| $4 f_{7 / 2} \rightarrow 5 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 0.136 | 1.128 | 2.212 | 0.129 | 1.080 | 2.110 | 2.100 |

Note.-All values are in atomic units.

TABLE 3
Comparison of Present Transition Probabilities with Available Theoretical Data for Fe xvi

| Transition ( $n^{\prime} l^{\prime} \rightarrow n l$ ) | Present E2 Transition Probabilities |  |  | Fuhr et al. 1988 E2 Transition Probabilities |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $l-1 / 2$ | $l+1 / 2$ | Sum | $l-1 / 2$ | $l+1 / 2$ | Sum |
|  | $6.62 \mathrm{E}-3$ | $6.82 \mathrm{E}-3$ | $1.34 \mathrm{E}-2$ | $6.7 \mathrm{E}-3$ | $6.8 \mathrm{E}-3$ | $1.35 \mathrm{E}-2$ |
| $3 s \rightarrow 4 d . \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . .$. | 1.37 E 0 | 1.36 E 0 | 2.73 E 0 | 1.5 E 0 | 1.44 E 0 | 2.95 E 0 |
| $3 s \rightarrow 5 d . \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | $7.45 \mathrm{E}-1$ | $7.44 \mathrm{E}-1$ | 1.49 E 0 | $7.8 \mathrm{E}-1$ | 7.6E-1 | 1.54 E 0 |
| $4 s \rightarrow 4 d . \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 8.18E-4 | $8.44 \mathrm{E}-4$ | $1.66 \mathrm{E}-3$ | $8.2 \mathrm{E}-4$ | $8.4 \mathrm{E}-4$ | $1.66 \mathrm{E}-3$ |
| $4 s \rightarrow 5 d . \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | $1.41 \mathrm{E}-1$ | $1.41 \mathrm{E}-1$ | $2.82 \mathrm{E}-1$ | $1.5 \mathrm{E}-1$ | $1.5 \mathrm{E}-1$ | $3.00 \mathrm{E}-1$ |
| $3 p_{1 / 2} \rightarrow 4 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 2.06 E 0 |  |  | 2.14 E 0 |  | ... |
| $3 p_{3 / 2} \rightarrow 4 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | $5.72 \mathrm{E}-1$ | 2.58 E 0 | 5.21 E 0 | $5.8 \mathrm{E}-1$ | 2.6 E 0 | 5.32 E 0 |
| $3 p_{1 / 2} \rightarrow 4 p \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ |  | $3.45 \mathrm{E}-1$ | ... | ... | $3.7 \mathrm{E}-1$ | ... |
| $3 p_{3 / 2} \rightarrow 4 p \ldots \ldots \ldots \ldots \ldots \ldots$ | $6.84 \mathrm{E}-1$ | $3.39 \mathrm{E}-1$ | 1.37 E 0 | $6.7 \mathrm{E}-1$ | $3.4 \mathrm{E}-1$ | 1.38 E 0 |
| $3 d_{3 / 2} \rightarrow 4 d \ldots \ldots \ldots \ldots \ldots \ldots$ | $1.54 \mathrm{E}-1$ | $4.43 \mathrm{E}-2$ | ... | $1.6 \mathrm{E}-1$ | $4.5 \mathrm{E}-2$ | ... |
| $3 d_{5 / 2} \rightarrow 4 d \ldots \ldots \ldots \ldots \ldots \ldots$. | $6.62 \mathrm{E}-2$ | $1.75 \mathrm{E}-1$ | $4.39 \mathrm{E}-1$ | $6.6 \mathrm{E}-2$ | $1.78 \mathrm{E}-1$ | $4.49 \mathrm{E}-1$ |
| $4 f_{5 / 2} \rightarrow 5 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | $2.19 \mathrm{E}-2$ | $2.76 \mathrm{E}-3$ | ... | $2.20 \mathrm{E}-2$ | $2.78 \mathrm{E}-3$ | ... |
| $4 f_{7 / 2} \rightarrow 5 f \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | $3.67 \mathrm{E}-3$ | $2.28 \mathrm{E}-2$ | $5.11 \mathrm{E}-2$ | $3.68 \mathrm{E}-3$ | $2.30 \mathrm{E}-2$ | $5.14 \mathrm{E}-2$ |

Note.-All values are in units of $10^{8} \mathrm{~s}^{-1}$.
performed by using a first-order perturbation theory. They both have supplied the E2 transition line strength data. However, detailed relativistic E2 transition probability data
are compiled by Fuhr et al. (1988). In our calculation there are some new results both for E2 line strength and E2 transition probabilities that are reported for the first time.

TABLE 4
Line Strengths and Transition Probabilities of Fe xvi

| Transition $(f \rightarrow i)$ | Line Strength (a.u.) | Transition Probability $\left(\mathrm{s}^{-1}\right)$ |
| :---: | :---: | :---: |
| $3 s_{1 / 2} \rightarrow 3 d_{3 / 2}$. | 0.16638 E 0 | 0.662 E 6 |
| $3 s_{1 / 2} \rightarrow 4 d_{3 / 2}$. | 0.11254 E 0 | 0.137 E 9 |
| $3 s_{1 / 2} \rightarrow 5 d_{3 / 2}$. | $0.15749 \mathrm{E}-1$ | 0.745 E 8 |
| $3 s_{1 / 2} \rightarrow 6 d_{3 / 2}$. | $0.48443 \mathrm{E}-2$ | 0.419 E 8 |
| $3 s_{1 / 2} \rightarrow 7 d_{3 / 2}$. | $0.21085 \mathrm{E}-2$ | 0.254 E 8 |
| $3 s_{1 / 2} \rightarrow 8 d_{3 / 2}$. | $0.10808 \mathrm{E}-2$ | 0.159 E 8 |
| $3 s_{1 / 2} \rightarrow 9 d_{3 / 2}$. | $0.41210 \mathrm{E}-3$ | 0.693 E 7 |
| $3 s_{1 / 2} \rightarrow 3 d_{5 / 2} \ldots$ | 0.25121 E 0 | 0.682 E 6 |
| $3 s_{1 / 2} \rightarrow 4 d_{5 / 2} \ldots \ldots$ | 0.16763 E 0 | 0.136 E 9 |
| $3 s_{1 / 2} \rightarrow 5 d_{5 / 2} \ldots \ldots \ldots$ | $0.23547 \mathrm{E}-1$ | 0.744 E 8 |

[^0]
## 4. CONCLUSIONS

The continuing developments in astrophysical and astronomical observations demand accurate theoretical transition data to determine stellar chemical composition. Our theoretical data obtained from the highly correlated manybody coupled cluster method using fully relativistic Dirac-Hartree-Fock orbitals generated by an improved methodology of forming a basis set are definitely very accurate for the highly stripped Na-like ion Fe xvi and can partially meet the present requirement.

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[^0]:    Note.-Table 4 is published in its entirety in the electronic edition of the Astrophysical Journal. A portion is shown here for guidance regarding its form and content.

