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RATIP – a toolbox for studying the properties of open-shell atoms and ions

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Abstract

Recent developments and the current capabilities of the RATIP package are reviewed. During the last years, this atomic structure code has been proven useful for studying the level structures, transition probabilities, and Auger properties of atoms and ions with rather different shell structures. RATIP extends the widely applied GRASP program to calculate a variety of atomic transition and ionization properties within a relativistic framework. It not only supports large-scale applications but also facilitates the handling and interpretation of the generated data. The *object-oriented design* of RATIP, which is open to further applications, provides a new route for accurate ab-initio predictions on open-shell systems. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Atomic properties; Atomic structure calculations; MCDF method; Relativistic, relaxation and correlation effects

1. Overview to the RATIP package

The need for accurate atomic data has grown steadily over the last two decades. Today, reliable predictions about the dynamical behaviour and the properties of free atoms are required not only in astro-physics and fusion research (the traditional areas for applying atomic structure theory) but also in a variety of other, recently emerging fields. A detailed knowledge about a large number of atomic processes, for example, is needed in order to improve the diagnostics of plasmas or to develop models which can be applied over a wide range of (plasma) temperatures and densities. Several other research areas, which attracted a lot of interest recently, are

the UV- and X-ray lithographie, the generation of nanostructures, the laser-induced fusion program, as well as the search for more efficient X-ray laser schemes. Moreover, accurate structure calculations are among the basic requirements if one is to obtain a better understanding of the *fundamental* interactions in nature and of the role of *correlations* in quantum many-particle systems.

Many of the applications mentioned above include (multiple and highly-charged) ions of the medium and heavy elements. For these ions, any *accurate* description must be based on a relativistic theory in order to elucidate the underlying processes. To predict the properties of such systems, the multiconfiguration Hartree–(Dirac–)Fock (MCDF) models [1] have been found very useful in ab-initio investigations. These models not only support the incorporation of all dominant physical effects into

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the theoretical description, but can also be applied to atoms and ions with complex shell-structures which naturally occur in plasmas. In contrast to non-relativistic or semi-relativistic methods, the major relativistic contributions are inherently included when the many-particle Dirac–Coulomb (–Breit) Hamiltonian is applied.

Two implementations of the MCDF model are now widely used in studying the properties of free atoms and ions. These are a successor of Desclaux's program [2] and the Oxford structure code GRASP92 [3]. Both of these programs provide the energies and wave functions of selected atomic states which – at least in principle – can be improved systematically. In GRASP92, for example, an atomic state function with given angular momentum and parity (J^P) is approximated by a linear combination of configuration state functions (CSF) of the same symmetry

$$|\psi_\alpha(PJM)\rangle = \sum_r^{n_c} c_r(\alpha) |\gamma_r PJM\rangle, \quad (1)$$

where the number of CSF, n_c , characterizes the size of the wave function expansion. In the standard implementation of the MCDF method, each CSF is built from antisymmetrized products of a common set of *orthonormal* Dirac orbitals, represented on a numerical grid. Expansions of several ten thousand CSF in Eq. (1) are often required to describe the atomic levels for open-shell structures properly.

The RATIP package extends GRASP92 [3] to calculate a variety of (relativistic) atomic transition and ionization properties. This package has originally been developed in the early 1990s to study atomic processes with one electron in the continuum. Since then, RATIP has been maintained for almost one decade and exploited in a number of elaborate case studies. As we will explain below, it now supports a whole set of different tasks including the computation of (relaxed) transition probabilities and lifetimes, the representation of symmetry-adapted functions in a determinant basis, the generation of continuum orbitals as well as calculations on various Auger properties and photoionization cross sections. During the last 2 years, moreover, RATIP particularly helped improve the available database on Einstein coefficients, oscillator strengths, and branching ratios for multiple charged ions of the iron group.

Apart from RATIP's advantages, however, also several weaknesses of the program became apparent to us with its frequent use. These drawbacks finally induced us to wish for a major revision of the program. In the earlier version of RATIP, for instance, most components could (i) not easily be applied to wave function expansions (Eq. (1)) of more than a few thousand CSF (which appeared insufficient in many cases). Also, (ii) a rather tight binding to the IBM XL Fortran standard applied for all components, similar to GRASP92, which made it difficult to port the program to other architectures and, thus, (iii) to maintain the package over a long term. The binding to the IBM standard, in particular, also complicated the development and adaptation of further components of RATIP to a sufficiently modern design. In addition, (iv) a static allocation was used for representing important arrays so that often the source code needed to be adapted to the respective problem explicitly.

Our new version of RATIP now remedies these shortcomings by using the concepts of Fortran 90/95 throughout. Below, we discuss the basic structure and features of these (new) developments. Fig. 1 displays an overview of the RATIP package as a whole. The revised program is now divided into several groups for calculating level properties, transition and ionization parameters, and many other features which are useful for the characterization of open-shell atoms and ions.

2. Basic components

In RATIP, various *groups* of program components are distinguished. Each of these groups deals with a number of well-defined tasks and is typically implemented in either one or several independent components. In the following, we briefly describe all of these components. For the sake of brevity, however, we will not provide detailed information and instructions to use these program components. For each program, a long write-up is usually available describing the theoretical background and also examples to test the code. During the discussions below, reference to these long descriptions will be made for the interested reader.

For those program components of RATIP, for which

■ RATIP

Relativistic Atomic Transition and Ionization Properties

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■ Level properties

■ Relativistic CI calculations

RELCI: Set-up and diagonalization of a relativistic CI matrix including
Breit interactions and QED estimates;
program component: xrelci

■ Radial electron densities

■ Bound-state transition

■ (Auto-) Ionization

■ Further components

■ Utilities

Fig. 1. Main structure of RATIP which is divided into several groups of programs. Details are displayed only for the calculation of level properties.

previous implementations [4,5] were available, the main difference of the present version concerns the size of the wave function expansions that are feasible. Most components now support wave function expansions of several ten thousand CSF and, thus, are comparable in its size with the best non-relativistic computations. To facilitate the further development and maintenance of RATIP, all components were *re-designed* by applying an *object-oriented* approach in Fortran 90/95. In addition, most of the revised components have got also a much more flexible user interface.

2.1. Level properties

The first group of programs deals with the calculation of level properties, i.e. those properties which only depend on a single wave function expansion. At present, this group [cf. Fig. 1] just contains the improved (relativistic) configuration interaction program RELCI and a small utility program for calculating either the radial density of some given level or, equivalently, the effective charge in dependence of the radius r . However, since the computation of level properties is not the major concern of RATIP, here we will give only a few remarks on this group. In

general, we will support only those properties which are not (yet) available in MCDF implementations like GRASP92 or whose calculation appeared somehow as *bottleneck* in previous investigations.

Just in this latter sense, RELCI has been developed to provide a more efficient set-up and diagonalization of large Hamiltonian matrices [6]. In the case of open-shell systems, the size of these matrices often increase dramatically as the number of active orbitals is increased. In such a case, RELCI is intended to *replace* the GRASP92 component Rci92 [3]. Attention has to be paid, however, to keep the interface to other components, i.e. the mixing coefficient files, the same. When compared with Rci92, the recently developed RELCI program now easily supports wave function expansions of several ten (to hundred) thousand CSF on all platforms and has become faster by approximately a factor of 5–10. Also, it typically requires less storage owing to a more efficient management of the available memory. A larger size of the Hamiltonian matrices supports, in particular, accurate calculations on transition probabilities (see below). Thereby, a large gain in the efficiency of the set-up of the Hamiltonian matrix has been obtained by exploiting a new scheme of angular integration [7,8].

In RELCI, the default for the Hamiltonian matrix includes the Dirac–Coulomb part, H_{DC} , as well as the frequency-independent Breit interaction. This default can be overwritten interactively by choosing either the (frequency-independent) Gaunt or the full transverse interaction in the Hamiltonian; of course, any of these additional corrections to the instantaneous Coulomb repulsion can also be omitted from the computation if time is to be saved or if the influence of the relativistic contributions is to be studied in detail. Further *interactions* like the normal and specific mass shift or the effects of the vacuum polarization can be added to the Hamiltonian matrix. These corrections are implemented in RELCI very similar to RCI92 [3].

An estimate of the self-energy, finally, is obtained from RELCI by exploiting a simple hydrogenic model. In this model, the effective charge of each (spectroscopically occupied) orbital function near the origin, i.e. within a small sphere of about 40 fermi, is compared with the corresponding charge of a hydrogenic orbital (for a point nucleus) in order to scale the tabulated QED estimates by Mohr [9] and Mohr and Kim [10]. This model has been found to give better results than obtained previously for the self-energy in GRASP92. These calculations are carried out independently of the set-up of the Hamiltonian matrix.

2.2. Transition probabilities and lifetimes

Most applications of RATIP, so far, concerned the investigation and ab-initio prediction of accurate

transition probabilities along various isoelectronic sequences. Detailed case studies, in particular, have been carried out for several astro-physically relevant spectra of the iron group elements [11–14] as well as for the spectra of Ni II [15] and Cu II [16] during the last few years. Further computations have been performed even for the low-lying excitation spectrum of atomic fermium ($Z = 100$). These investigations clearly demonstrated, that large-scale wave function expansions are usually required in order to obtain precise predictions, particularly for most medium and weak transitions. If compared with other ab-initio and semiempirical computations, our investigations also showed that the effects of relativity, electron correlations, and of the rearrangement of the electron density should be treated consistently within a common framework.

Till now, this second group of programs for calculating bound-state transition parameters is basically formed by REOS99 [17]. Fig. 2 displays a short summary of this group. The revised version of REOS99 is now prepared for real large-scale computations of *relaxed-orbital* transition probabilities and lifetimes by utilizing a determinant representation of the atomic wave functions. Such a representation is obtained from CESD99 [18] as shown below in Fig. 4. Since the inclusion of relaxation effects typically improves the theoretical transition probabilities (at least, for most of the transitions), REOS99 has become of great practical importance. Rearrangement effects in the electron cloud, when the atom undergoes a transition, are naturally included if the electronic wave functions of both, the initial and final atomic

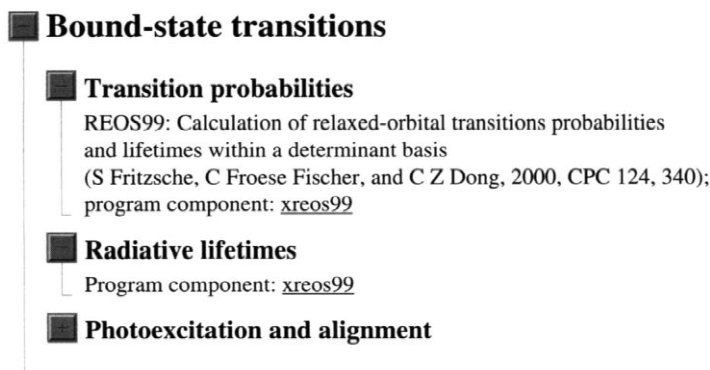


Fig. 2. Calculation of transition properties involving (localized) bound states.

levels are optimized independently. In contrast, standard computations in the GRASP92 environment neglect the *relaxation* of the electron density for the absorption and emission of photons.

Apart from its *large-scale* capabilities, REOS99 provides a more user-friendly interface. Additional features of the revised program include an *assumed orthogonality* between the two orbitals sets of the initial and final states (in order to speed up the calculations) as well as the optional use of *experimental* energies in the evaluation of the transition amplitudes. The latter choice has been found helpful in the computation of atoms and nearly neutral ions for which the fine structure of the (excited) atomic levels is often not well reproduced by ab-initio theory. By using the experimentally known energies for such systems, the energy dependence of the transition amplitudes is taken into account properly; in practice, this choice usually reduces the deviations between different gauges for the coupling of the radiation field, i.e. between the Babuskin and Coulomb gauge in the present context.

The advantages of REOS99 for providing accurate transition probabilities and lifetimes of multiple and highly charged ions are now well recognized. But apart from investigations on resonance and *forbidden* lines, this program is also appropriate to study two-electron–one-photon (TEOP) transitions where (generally) two inner-shell holes are filled simultaneously under the emission of a single photon [19]. To *describe* such a transition in perturbation theory, a (second) electron–electron interaction would be required in addition to the interaction of the atom with the radiation field. In REOS99, a non-zero amplitude

arise already in first order due to the effects of configuration mixing and relaxation. This and other *second-order processes* like the radiative Auger decay [20] are a much less studied subject in a multiconfiguration Dirac–Hartree–Fock approach although they are known to be governed by correlation effects and, in particular, the relaxation of the electron density.

2.3. Ionization and Auger parameters

A third group of programs intends to provide Auger and ionization parameters as seen from Fig. 3. In contrast to bound-state properties, these emission processes are accommodated by a change in the number of bound electrons. The AUGER component, for instance, supports the computation of Auger energies, (relative) intensities, as well as of angular distributions. So far, only this component is fully re-designed and distributed with RATIP. Another component, PHOTO, provides cross sections and angular distribution parameters for atomic photoionization spectra; this component has been part of a previous version of RATIP and will be made available, again, in the future.

The study of atomic ionization and capture processes usually requires a proper description of the *scattering states* as a whole, i.e. of the wave functions for the (ionic) bound states *plus* the outgoing electron. To construct (and apply) these states, one has to include not only the continuum spinors in the field of the ion but also information about scattering phases and the correct boundary conditions. Recent developments in high-resolution

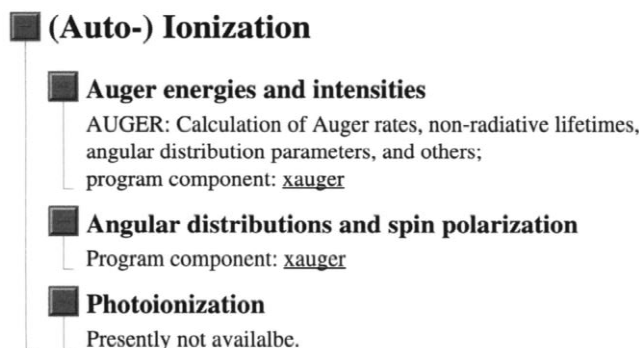


Fig. 3. Calculation of ionization and Auger properties.

Auger spectroscopy [21] clearly increased the requirements for the construction of these states. With the revised AUGER component of RATIP, we now support for the first time the calculation of Auger properties by systematically enlarged wave function expansions to include the effects of the initial and final-state configuration interaction (i.e. the ISCI and FISCI, respectively).

During the last 2 years, AUGER has been applied for analyzing the argon $L_{23}[L_{23}],MM[L_{23}]$ Auger cascade following a $1s$ inner-shell ionization [22] as well as for angular distributions and interference properties in the spectra of resonantly excited noble-gas atoms [23,24]. With some minor modification, the AUGER component might be useful also to investigate a coherence transfer through two or several steps of the excitation and/or de-excitation of such resonantly excited atoms [25].

The AUGER program is mainly built on the COWF component [see below]. In this component, the interaction of the outgoing electron with the bound-state electron density is treated within a central-field approximation which gives rise to continuum orbitals of well defined symmetry, κ . By default, all continuum spinors are generated – for given, fixed energy and by using an *optimal level procedure* in

the set-up of the one-particle equations – independently for each final state of the (auto-) ionization. In practice, COWF supports both, a homogeneous solution of these equations as well as the incorporation of the exchange of the emitted electron with the bound electrons.

2.4. Further components

The modular structure of RATIP is one of the key features for providing a user-friendly environment for large-scale computations. Such a structure, however, also leads rather automatically to a number of independent program components. Although these components often remain *hidden* to many users, they form the backbone (and still another *group*) of the RATIP package. In the future, several of these components might also become part of further applications. Fig. 4 displays five of these components; many of them have been developed in collaboration with different coworkers whose help in developing RATIP is gratefully acknowledged.

The first two components from Fig. 4, RCFP [26] and ANCO [8] deal with the definition of (reduced) coefficients of fractional parentage and the angular integration for (scalar) two-particle operators. They

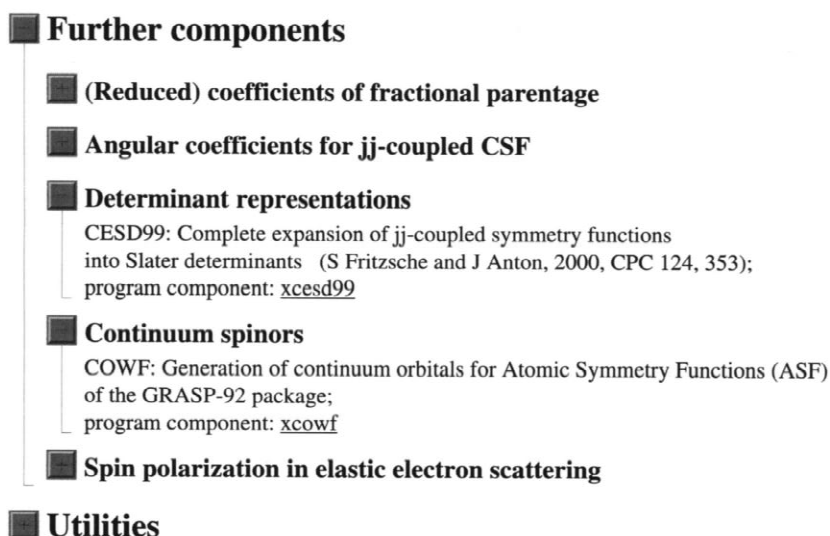


Fig. 4. Further components of the RATIP package which are utilized by other parts of the program but which can be applied also independently.

are presently utilized in RELCI and AUGER but may become part also of other programs. As mentioned before, a new implementation of the angular coefficients became necessary to allow for large-scale wave function expansions and a more time-efficient set-up of the Hamiltonian, respectively, the Auger transition matrices. Our new implementation is based on second quantization which is applied to both, the angular momentum and quasi-spin space [7]. When compared with the former GRASP92 component MCP, ANCO now supports open subshells with $j = 9/2$ and is faster by about a factor of five.

Two other components of this group are CESD99 [18] for a complete expansion of symmetry-adapted functions into Slater determinants as well as COWF for generating the continuum spinors. The CESD99 component was first developed several years ago in order to support an evaluation of transition matrices also for not quite orthogonal orbital sets of the initial and final atomic states, based on Löwdin's expressions [27]. Since then, such *relaxation* effects of the electron density has been taken into account in several case studies of radiative transition probabilities [28,29]; they can also be utilized, however, for many other ionization and decay properties as demonstrated earlier for the Auger effect [30,31] or in atomic photoionization [32]. The other component, COWF, is currently exploited in the computation

of Auger properties and will be used, again, for photoionization properties. COWF usually generates continuum spinors in the static field of a given (final-ionic) state. As described in Subsection 2.3, it is currently tested for calculating coherence and interference properties in Auger spectra and will soon be prepared for publication.

Finally, a last component of this group concerns the spin polarization in the elastic scattering of electrons [33]; this component is currently under development and will need more time to become part of the distributed version.

2.5. Utilities

Although systematically enlarged wave functions enables one to monitor the (convergence) behaviour of properties (as the size of the expansions is increased), they often also result in a large amount of intermediate and output data. In order to facilitate the handling of these data, we presently develop a UTILITY program whose *functionality* will be briefly summarized in this section. Fig. 5 shows the main menu of this interactive tool which appears at the top-level of the execution. By typing the appropriate integer (1–10), special submenus will follow and guide the user through the particular task. Here, we need not provide a detailed description of these

- 1 - Energy levels and level splittings (simple).
- 2 - Energy levels and level splittings (extended).
- 3 - Weights of major CSF to atomic levels.

- 4 - Merge two .csl lists from GRASP92.
- 5 - Format .mix and .out files from GRASP92.
- 6 - Unformat .mix and .out files from GRASP92.

- 7 - Overlaps between two not quite orthogonal orbital sets.
- 8 - Radial charge density of an ASF.
- 9 - Display of some radial orbital.
- 10 - Display names in LS coupling (inactive).

- q - Quit.

Fig. 5. Main menu of the xutility program.

submenus since they are rather self-explanatory. No additional output files are typically generated by this UTILITY component. We intent to *add* further tasks to this menu as requests will arise from the side of the users.

As seen from Fig. 5, three different sections are currently supported. In the first section, tasks 1 and 2 collect and print the total energies and level splittings by analyzing the .mix Mixing Coefficient Files from one or several independent *runs* of the GRASP92 program (or of RELCI, respectively). Different output formats are supported by these subtasks. They have been found useful, in particular, in order to gather all necessary information from a *series* of computations if different groups of levels have been considered independently (for example, in the calculation of transition arrays). Task 3, finally, provides a similar compilation for the weights of the leading CSF in the wave function expansions. This task may later be combined with No. 10 for providing also the spectroscopic *LSJ* notation of the selected levels in cases of large wave function expansion; a request which has often been raised in recent applications.

The second section (tasks 4–6) deals with the file handling and transfer to increase the portability of the wave functions among different architectures. Since different operating systems and hardware often use different *unformatted* file formats, a transfer of the wave functions usually requires to use a *formatted* ACSII interface in between. Several components of RATIP now also support directly the use of either *formatted* or *unformatted* file input and output, as appropriate, in order to facilitate this transfer; these specifications can be selected in the source code by global flags in the header of the corresponding modules.

A third section (cf. 7–10 in Fig. 5) provides additional information which can directly be extracted from the wave functions. The ‘overlap integrals’ among two not quite orthogonal sets of (initial and final-state) orbitals, for instance, indicate the importance of relaxation effects and, thus, may provide an estimate of the *shake probabilities* in the interpretation of Auger spectra within a simple model. Other tasks concern the radial charge density (given on the internal grid) or the display of atomic orbitals for the discussion of different physical effects.

3. Program organization

Our overview in the previous section shows that, in a program environment of RATIP’s size, the *same standard* cannot always be guaranteed for all components at the *same time*. Therefore, the major concern in the present development of this package is to make use of an object-oriented design in order to ensure a *long-term maintenance*. For this purpose, we make elaborate use of the new concepts of Fortran 90/95 in the development of RATIP. Here, we briefly summarize a few of the basic features which have been taken into account; further information about the program design can be found in the long write-ups of various components [8,17,18].

When compared with previous standards, Fortran 90/95 represents rather a new language that has benefitted from Fortran’s long tradition and from the experience in language design over more than three decades [34]. Among many others, in particular two new features of Fortran 90/95, the *use of modules* for generating protected and re-usable code as well as the *derived types* have brought the language up-to-date with its alternatives. Derived types – along with pointer arrays in the current standard – enables the set up of very flexible data structures. In the present design of RATIP, the application of these features finally lead to a entirely new implementation of the code.

3.1. Use of derived types

Pointers and a partially dynamic storage management have been applied already in an intermediate version of RATIP [4,5]. In Fortran 90/95, however, these concepts are now supported much clearer and enable one to write programs which are very flexible with respect to the size of the actual investigation. In our new design of RATIP, all arrays related to the representation of the atomic states, grid sizes, Hamiltonian and transition matrices, and many others are now allocated dynamically at run time. Therefore, there are virtually no other limitations than by the resources themselves.

A proper choice of derived data types certainly facilitates the maintenance and further development of the code. In RATIP, derived types are defined at various levels of complexity. Globally defined low-

level types are used to construct data types at some higher level in the hierarchy. Two such derived types at a rather low level, for example, concern a *determinant* and a *cs_function*, i.e. a symmetry-adapted CSF. While these data types may be declared like structured variables on their own, they may also form components of other (derived) types at some higher level. Just in this sense, an allocatable array of `type(determinant)` forms for instance a component of a variable of `type(asf_det_basis)` which keeps together all information about a whole set of determinants as well as about the internal representation of the atomic states within this basis. To these data structures, memory is allocated only according to the actual number of CSF. Another high-level derived data structure, `type(reos_transition)`, has been explained recently in Ref. [17].

3.2. Distribution and installation of the program

In Fortran 90/95, an efficient *use* of modules supports a rather simple directory structure by which the code is distributed. As mentioned before already, each module provides a means of keeping the definition of all required (global) variables, data, derived types and operations which are associated with a particular task closely together. In the course of re-designing RATIP, the advantage of modules has been exploited very carefully. In the present version, the root directory *ratip* currently contains about 20 of such modules and a set of (main) programs as found in Figs. 1–3 above. For each component, a main program like *xcesd99.f* or *xreos99.f* is available and contains (along with various *used* modules) the full source of the corresponding executables. Moreover, all main programs and executables start with the prefix *x* in order to distinguish them from other files of the package. Users may download a tar-file of the entire program *ratip2000.tar* from our home page at the University of Kassel (<http://www.physik.uni-kassel.de/fritzsche/programs.html>).

The *ratip* root directory also includes several makefiles for generating the executables as well as test suites for the different components. For example, the command `make -f make-relci` will generate the executable *xrelci* in the same directory. To

increase the portability of the program, we created the file *make-environment* in which the name of the (Fortran 90/95) compiler as well as additional compiler flags must be defined. This file is not an ordinary makefile, however; it needs first to be sourced to make these (global) definitions known to the operating system. No additional libraries nor the special adaptation of dimensions is then required. Till now, the revised version of the RATIP package has been tested mainly under Linux and, in a few case studies also under AIX. Owing to the compliance of the Fortran 90/95 standard and the simple design of the file *make-environment*, however, no serious difficulties should arise to port the code to other architectures.

The file structure of the *ratip* root also facilitates the extension of the package by further components. In fact, this is simply achieved by appending modules, (main) programs, and corresponding makefiles in order to generate the executables. Since several coworkers contributed to different parts of the package, this structure ensures that further code developments can be made independently while the maintenance on both, users and developers side, still remains straightforward.

4. Summary and outlook

The current status in developing and applying the RATIP package has been reviewed. The variety of properties, which can be investigated by means of this package, makes RATIP attractive to a broad user community. Owing to its capabilities in supporting *systematic* investigations, RATIP may be found useful also for the design and interpretation of new experiments or for analyzing trends along various isoelectronic sequences. In basic research on electron structure and spectroscopy, this includes particularly the present *hop topic* of coherence and interference effects as observed in the excitation/de-excitation of resonantly excited noble gases [21].

By taking advantage of the new ANSI Fortran 90/95 standard, the flexibility of the RATIP package has considerably been enhanced during the last years. In the future, this should facilitate the maintenance of the program to ensure a long *life-cycle*. Together with the steadily increasing computer re-

sources, the improved efficiency of RATIP now even supports investigations for atoms with open d and f shells. Since, for such shell structures, there are no many-body perturbation approaches are yet available, RATIP currently provides the only ab-initio access to the low-lying excitation spectra and the properties of many transition metals or of the actinide and transactinide elements.

Finally, RATIP has been designed as an *open* environment from the very beginning. This can be utilized in further developments by exploiting the large number of predefined data structures and procedures in order to *create* further components. A few closely related topics are the cross sections and angular distributions of photoelectron spectra, electron-impact excitation and ionization, and many other properties. Of course, the large number of desirable extensions of RATIP cannot be developed just by our group in Kassel. Any support of co-workers or even independent developments on RATIP will therefore be always gratefully acknowledged.

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