10. Program BSR_DMAT (version 3)

The BSR_DMAT program prepares the dipole matrix, **d.nnn**, for subsequent use in the BSR_PHOT program for photoionization calculations, or to perform the calculations of oscillator strengths between *B*-spline bound-state solutions. For completeness, BSR_DMAT also has the option to calculate oscillator strengths between MCHF solutions, and between *B*-spline bound states and MCHF solutions. Version 3 increased the output different forms of the dipole matrix elements.

10.1.Dipole transition matrix

For photoionization calculations we need the D-files, which contain the dipole matrix elements between the initial state and the *R*-matrix solutions for a given partial wave. It is convenient to represent the dipole matrix elements by using the dipole transition matrix, which consists from the dipole matrix elements between the basis states. Suppose we have two sets of solutions of the Hamiltonian matrix in different bases. In our case, it can be either the configuration basis from the MCHF calculations, or a close-coupling *B*-spline expansion (7.2) from a BSR calculation. Then the matrix element for the given solutions *a* and *b* is

$$< a \mid E^{[\lambda]} \mid b >= \sum_{i,j} a_i d_{ij} b_j = \boldsymbol{a}^T \boldsymbol{d}\, \boldsymbol{b}, \tag{10.1}$$

where $\{a_i\}$ and $\{b_i\}$ are the corresponding expansion coefficients in the respective bases. Once we generate the dipole transition matrix $\boldsymbol{d}$, the matrix elements for any other solutions is simply defined by convoluting $\boldsymbol{d}$ with the corresponding expansion vectors. The logical structure of BSR_DMAT is such that it first generates the relevant dipole transition matrix, and then, if indicated, calculates the corresponding set of oscillator strengths. This enables us to use the same code for photoionization and bound-state calculations.

Consider the structure of the transition matrix in the *B*-spline representation. This structure is very similar to the structure of the Hamiltonian matrix considered in the write-up of the BSR_MAT program in Section 7. In the present close-coupling approach, the *B*-spline bound-state solution vector, $\boldsymbol{c}$, can be written as

$$\boldsymbol{c} = [\boldsymbol{a}_1, ..., \boldsymbol{a}_{N_c}, \boldsymbol{b}]^T \tag{10.2}$$

where each $\boldsymbol{a}_i$ is a column vector of *B*-spline coefficients for the given channel functions $\overline{\Phi}_i^{\Gamma}$

$$\boldsymbol{a}_i = [a_{1i}, a_{2i}, ..., a_{n_s i}]^T \tag{10.3}$$

and $\boldsymbol{b}$ is the column vector of perturber coefficients

$$\boldsymbol{b}_j = [b_1, b_2, ..., b_{N_p}]^T , \tag{10.4}$$

where N_c is the number of channels while N_p is the number of perturbers. Then the transition matrix $\boldsymbol{d}$ has the form

$$\begin{pmatrix} D(11) & D(12) & \cdots & D(1N_c) & d(1p) \\ D(21) & D(22) & \cdots & D(2N_c) & d(2p) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ D(N_c 1) & D(N_c 2) & \cdots & D(N_c N_c) & d(N_c p) \\ d(1p)^T & d(2p)^T & \cdots & d(N_c p)^T & d(pp) \end{pmatrix} \tag{10.5}$$

where $d(pp)$ is an $N_p \times N_p$ matrix that comes from the bound-bound interaction, the $d(ip)$ are the $n_s \times N_p$ matrices, representing the interaction between the i-th channel and the bound states, and the $D(ij)$ are the $n_s \times n_s$ matrices for the channel-channel interaction. When we work with MCHF solutions, the transition matrix is reduced to the single last row, if the initial state is given in the MCHF representation, or simply to the $d(pp)$ matrix, if both solutions are MCHF configuration expansions.

Each individual matrix element in (10.5) is expressed by the program MULT in the form

$$\sum c_i R^{\lambda}(a,b) \times O(\{nl\};\{n'l'\}) \tag{10.6}$$

where the c_i are numeric coefficients that only depend on the angular symmetry of the CSFs involved, R^{λ} stands for the corresponding one-electron dipole integrals (9.17), and $O(\{nl\},\{n'l'\})$ is the overlap factor which depends only on the orthogonality of the radial orbitals used in the construction of the basis CSFs. In general, the overlap factor is the multiplier of determinants of matrices consisting of one-electron overlaps between radial functions in the initial and final states (see eq. 7.8).

The *B*-spline orbitals can appear in the radial integrals R^{λ}, as well as in the determinant factors. To derive the final expression for the matrix elements in the *B*-spline basis, let us first simplify the overlap factors (7.8) by expanding them over those rows which contain one-electron overlaps with the *B*-spline orbitals. At most, there can be two such rows. The residual overlap determinants depend only on the known bound orbitals and they can be calculated in a standard manner. It is convenient to redefine the angular coefficients c_i by multiplying them by these residual overlap factors. As a result, the initial overlap factor $O(\{nl\},\{n'l'\})$ in expression (10.6) is reduced to one-electron or two-electron overlaps of the form

$$\langle kl \,|\, nl \rangle, \quad \langle kl \,|\, k'l \rangle \quad \text{or} \quad \langle kl \,|\, nl \rangle \langle n'l' \,|\, k'l' \rangle , \tag{10.7}$$

where $|kl\rangle$ stands for the radial function of the B-spline orbital

$$u_{kl}(r) = \sum_i a_i B_i(r) \quad . \tag{10.8}$$

Each term in (10.6) gives rise to some matrix in the spline basis. To elucidate the structure of these matrices, we introduce the following $n_s \times n_s$ matrices with elements

$$B(\bullet\bullet)_{ij} = \langle B_i \mid B_j \rangle, \qquad R(\bullet\bullet)_{ij} = \langle B_i \mid r \mid B_j \rangle \tag{10.9}$$

To describe the channel-bound interaction, we introduce the following vectors with elements

$$B(\bullet a)_i = \sum_{j=1}^{n_s} a_j B_{ij}, \qquad R(\bullet\, a)_i = \sum_{j=1}^{n_s} a_j R_{ij} \,, \tag{10.10}$$

Finally, for bound-bound interaction we have

$$R(ab) = \sum_{i,j=1}^{n_s} a_i R_{ij} b_j \,. \tag{10.11}$$

With this notation, table 10.1 represents the contributions of the different terms from the matrix element expression (10.6), which usually produces the angular integration codes, to the transition matrix (10.5), along with an indication of its structure.

Table 10.1. Contribution of different terms (without indication of angular coefficients) in the transition matrix. The symbols a,b stand for the bound orbitals, while the symbol k_i indicates the B-spline orbital in channel i.

Term	Contribution	Remarks
Channel-channel interaction		
$R(k_i, k_j)$	$R(\bullet\bullet)$	banded matrix
$\langle k_i \mid a\rangle \langle b \mid k_j\rangle R^\lambda$	$B(\bullet\, a) \bullet B(\bullet\, b) * R^\lambda$ (or L)	Full matrix, contribution due to non-orthogonality
$\langle k_i \mid k_j\rangle R^\lambda$	$B(\bullet\bullet) * R^\lambda$	Banded matrix,
$R^\lambda(k_i,a) \langle b \mid k_j\rangle$	$L(\bullet\, a) \bullet B(\bullet\, b)$	full matrix, contribution due to non-orthogonality
Channel-bound interaction		
$R^\lambda(k_i,a)$	$R^\lambda(\bullet\, a)$	vector
$\langle k_i \mid a\rangle R^\lambda$	$B(\bullet\, a) * R^\lambda$	vector, contribution due to non-orthogonality
Bound-bound interaction		
$R^\lambda(a, b)$		scalar

10.2. Oscillator strengths and decay probabilities

For completeness of the description, we provide below the main formulae used in the present code for the calculation of radiative properties. The line strength for a transition between levels *i* and *j* is defined as

$$S_{ij}^{\lambda} = S_{ji}^{\lambda} = \sum_{m's} |< J_i M_i \mid D_{\mu}^{[\lambda]} \mid J_j M_j >|^2, \tag{10.12}$$

It is given in atomic units, which are $e^2 a_0^{2\lambda}$ and $\beta^2 a_0^{2(\lambda-1)}$ for electric and magnetic transitions, respectively. Here $\beta = e\hbar/2mc$ is the Bohr magneton. The $D_{\mu}^{[\lambda]}$ is either electric (9.1) or magnetic (9.2) operator with multipole index λ . The transition probability for transition $i \rightarrow j$ can be written as

$$A_{ij}^{\lambda} = \frac{2(2\lambda+1)(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \frac{1}{g_i} \frac{1}{\hbar} \left(\frac{E_j - E_i}{\hbar c} \right)^{2\lambda+1} S_{ij}^{\lambda}, \tag{10.13}$$

where g_i is the statistic factor for initial level *i*: $g = (2S+1)(2L+1)$ for LS multiplets and g=(2J+1) for fine-structure levels. The first λ-factor = 4/3, 1/15, 8/4725 for λ = 1,2 3.

The oscillator strength (unitless) is related to the transition probability by

$$f_{ij}^{\lambda} = \frac{mc^3}{2e^2} \frac{A_{ij}}{\omega^2} = \frac{2(2\lambda+1)(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \frac{1}{g_i} \frac{mc}{2e^2\hbar} \left(\frac{E_j - E_i}{\hbar c} \right)^{2\lambda-1} S_{ij}^{\lambda}, \tag{10.14}$$

independent of the nature of the radiative transition. The above definition of oscillator strength is common in literature only for dipole operator. We may rewrite dipole λ=1 case in atomic units as

$$f_{ij}^{1} = \frac{2 |< \gamma_i L_i \| rC^1(\hat{\mathbf{r}}) \| \gamma_i L_i >| \omega_{ij}}{(2\lambda+1) g_i} \tag{10.15}$$

It is convenient to extend this expression to other electric multipoles and define

$$f_{ij}^{(k)} = \frac{2 |< \gamma_i L_i \| r^k C^k(\hat{\mathbf{r}}) \| \gamma_i L_i >|^2 \omega_{ij}}{(2k+1) g_i} \tag{10.16}$$

Here we will use symbol *k* for multipole index in parentheses to differ this definition from (10.14). That will provide different numerical values for $k \geq 2$ and different relation between oscillator strengths and decay probabilities. This definition is convenient to use in calculation of polarizabilities.

The classical formula for the polarizability of a harmonic oscillator of frequency ω_0 is

$$\alpha(\omega) = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2} \tag{10.17}$$

The dipole polarizability of an atom is equal to the sum of the polarizabilities of the "atomic oscillators", in which each oscillator is represented with a weighting factor (strength) f(γJ,γ'J'):

$$\alpha(\gamma J,\omega)=\frac{e^2}{m}\sum_{\gamma' J'}\ \frac{f(\gamma J,\gamma' J')}{\omega_0^2-\omega^2};\ \ \omega_0=\omega_{\gamma J,\gamma' J'} \tag{10.18}$$

Using definition (3.9) for oscillator strengths, we may get following expansions for static multipole polarizability of state *i*

$$\alpha_k=\sum_n\frac{f_{in}^{(k)}}{(\Delta E_{in})^2} \tag{10.19}$$

nonadiabatic polarizabilities

$$\beta_k=\sum_n\frac{f_{in}^{(k)}}{2(\Delta E_{in})^3} \tag{10.20}$$

and higher-order nonadiabatic terms

$$\gamma_k=\sum_n\frac{f_{in}^{(k)}}{4(\Delta E_{in})^4} \tag{10.21}$$

10.3. Structure and data flow

The block diagram of the program BSR_DMAT, along with the data flow, is given in Fig. 10.1. Since BSR_DMAT requires only a small number of input parameters, all of them must be defined in the command line as arguments. The input parameters for the BSR_DMAT program are the names of the *c*-files with a list of configuration state functions for the initial and final states involved, and the mode of calculation, **ctype** (see Section 10.4.) The input *c*-files may be the ordinary *c*-files from MCHF calculations, or **cfg.nnn** files generated in BSR calculations. The mode of calculation defines whether this is the generation of the transition matrix for subsequent photoionization calculations or the calculation of oscillator strengths between bound states. The **ctype** parameter also defines the representation format for the initial and final states, which can be in the *LS* or *LSJ* coupling schemes. BSR_DMAT reads a set of other input data files. All of them have default names, or names which are directly connected to the names of the input *c*-files.

First, the program read all input data related to the given case. It includes input parameters from the command line, subroutine **read_arg**, the list of configurations, **read_conf**, the list of LS terms involved, **read_terms**, the target states and channel information, routines **read_target** and **read_channels**, B-spline basis, **define_splines**, and the list of one-electron orbitals involved in description of the initial and final states, routine **read_bsw**. The orbitals in the initial and final sets are supposed to be non-orthogonal. All one-electron radial functions should be in the *B*-spline representation. They can be either the user-prepared **name1.bsw** files, or the **bound.nnn** files generated by the BSR_HD program (only in this case the program requires the **target** file with a description of the relevant close-coupling expansions). The above programs also generate all needed working arrays to keep the input information. These arrays are automatically allocated in accordance with the input data.

The **read_conf** routine also analyses the information contained in the databank **mult_bnk**, and determines whether the data bank contains all angular coefficients needed for the given case. If not, the program stops, suggesting to rerun MULT program. Note that the multipole index and the type of transition under consideration are defined in **mult_bnk.** As the next, step the program prepare DJ- or DJM-arrays connected the LS matrix elements with the fine-structure transitions, see Eq.(9.10).

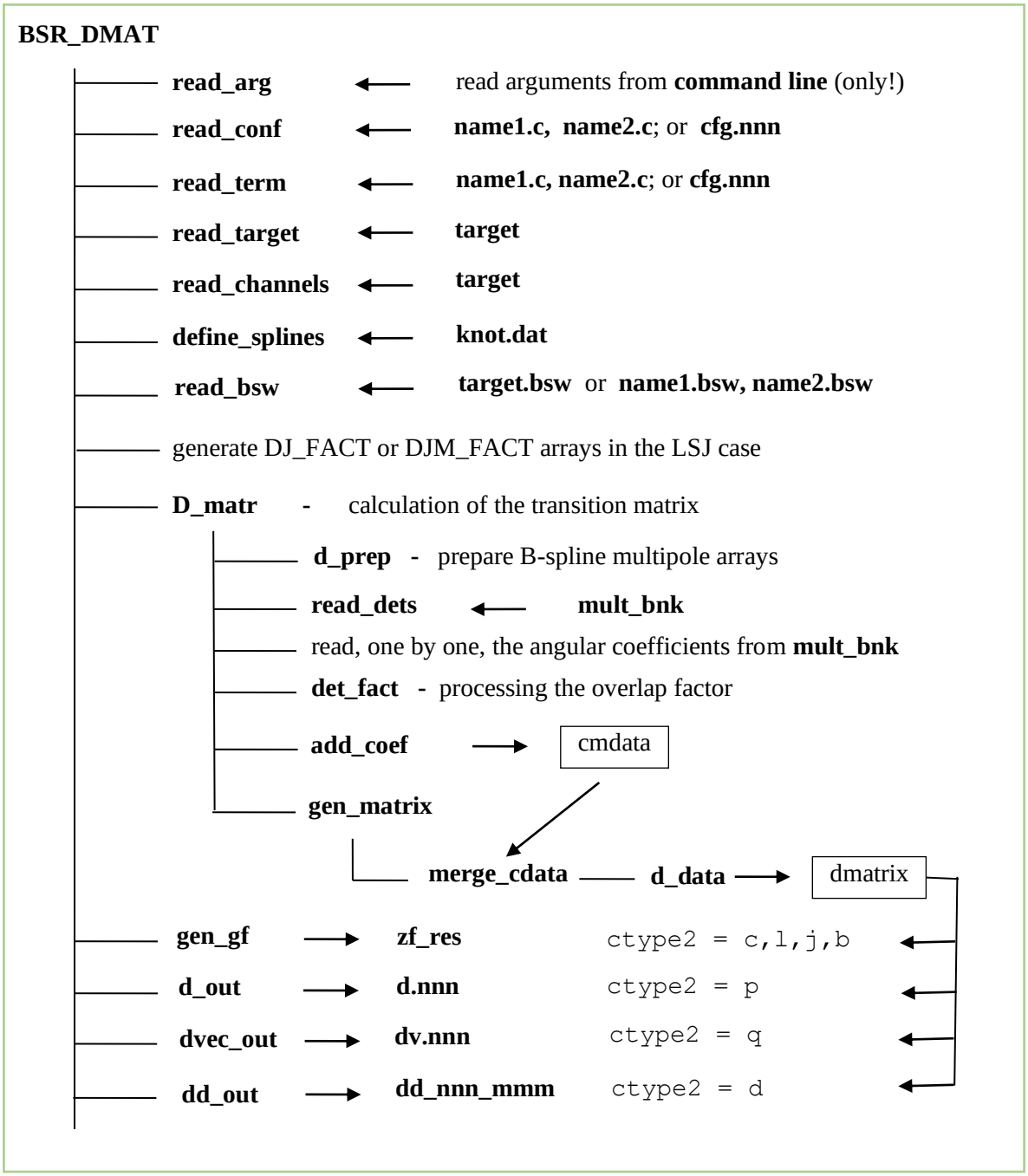

Fig. 10.1. Block diagram for the program BSR_DMAT3 and data flow (see text).

The routine **D_matr** controls the calculation of the transition matrix (10.5). First, the routine prepare all needed B-spline multipole arrays, which are related to the individual B-splines. Then the program reads all overlap factors $O(\{nl\},\{n'l'\})$ from data bank in routine **read_dets.** These overlap factors are presented in the symbolic form, without indication of the specific one-electron orbitals involves. Then the program reads and processes all one-configurational matrix elements presented in the **mult_bnk**. First, it

is determined if the given matrix elements is relevant to the given transition. If so, the overlap factor $O(\{nl\},\{n'l'\})$ in expression (10.6) is reduced to one-electron or two-electron overlaps of the form (10.8) by the routine **det_fact** for specific one-electron orbitals. The integrals are then sorted according to their structure (see table 10.1) and stored in the module **cmdata** in different ordered blocks, routine **add_coef.** When all coefficients from **mult_bnk** are exhausted, or when all blocks are full, they are processed by **gen_matrix** to get the *B*-spline representation for specific integrals, routine **d_data** (this may require preliminary merging different blocks in the large-scale case, routine **merge_cdata**). The corresponding contributions are then added to the transition matrix (10.5), located in module **dmatrix**.

The next step of the calculation depends on the input mode. In photoionization calculations, the dipole matrix (10.1) is calculated on the base of the *R*-matrix solutions placed in the file **rsol.nnn**, and then is recorded in the file **d.nnn**. For calculations of oscillator strengths, however, the program calls the routine **gen_gf** for processing transitions between *LS* or *LSJ* states. The resulting line strengths, oscillator strengths, transition energies, and transition probabilities are recorded in the file **zf_res** (see section 10.6 below). The present version 3 also contain two additional output options **ctype2=q** and **ctype2=d** (see below section 10.5)

10.4 Input parameters

Input parameters must be provided in the command line. First four parameter are the mandatory position parameters. All other key-words parameters are optional.

name1.c or **cfg.nnn**	name of *c*-file for the initial state
name2.c or **cfg.nnn**	name of *c*-file for the final state
ctype1	character, denotes the representation mode for the initial state: **c** – initial state is defined by *c*-file from MCHF calculations **l** - initial state is defined by *l*-file from MCHF calculations **j** - initial state is defined by *j*-file from MCHF calculations **b** - initial state is defined by **bound.nnn** file from BSR calculations
ctype2	character, the same as **ctype1,** but for the final state. Thesemodes assume the calculation of oscillator strengths, with the output put in the file **zf_res**. An additional modes: **p -** the dipole transition vector for given initial state will be generated in the output file **d.nnn** for subsequent photoionization calculations, BSR_PHOT. **q -** the dipole transition vector for given initial state will be generated in the output file **dv.nnn** for subsequent BSR_POL calculations. **d -** the dipole transition matrix (10.5) will be generated in the output file **dd.nnn_mmm** for subsequent TRM calculations..
gf (g|f)	defines output of gf- or f-values in **zf_res** file
mstates1 [0] **mstates2** [0]	if /= 0, restricts the number of initial/final states from the input files in calculations of oscillator strengths
istate1 [0] **istate2** [0]	if /=0, indicate specific initial/final state to be considered
ialfa [0]	if /=0, for dipole transitions, **zf_res** will contain additional information: dipole matrix element, contribution of the given transition in the polarizability of the initial state, and the sum of all contribution for the initial state defined by **istate1** parameter.
debug [0]	if \= 0, provides additional information in the **bsr_dmat.log** file.

name1.c or **cfg.nnn**
name2.c or **cfg.nnn**
File type: formatted sequential input.
Created by MCHF or BSR_CONF programs.
Read by routine **read_conf**.
Description: contains the configuration expansion for the initial and final states after MCHF or BSR calculations**.**

name1.bsw or **bound.nnn**
name2.bsw or **bound.nnn**
File type: unformatted sequential input.
Created by MCHF(plus w_bsw utility) or BSR_HD programs.
Read by routine **read_bsw.**
Description: one-electron orbitals in the *B*-spline basis for the initial state after MCHF or BSR calculations.

mult_bnk
File type: unformatted sequential input.
Written by program MULT**.**
Read by routines **read_conf, d_matr**.
Description: databank for the angular coefficients of the multipole operator.

target
File type: formatted sequential input.
Written by user and modified by BSR_PREP and BSR_CONF programs.
Read by routine **read_target.**
Description: contains description of the target states and scattering channels, optional.

knot.dat
File type: formatted sequential input.
Written by user.
Read by routine **define_grid** from BSPLINE library.
Description: input parameters that define the *B*-spline grid.

target.bsw
File type: unformatted sequential input.
Created by program BSR_PREP**.**
Read by routine **read_bsw.**
Description: target one-electron orbitals in the *B*-spline basis, optional.

pert_nnn.bsw
File type: unformatted sequential input.
Created by program BDR_PREP**.**
Read by routine **read_bsw.**
Description: perturber one-electron orbitals in the *B*-spline basis, optional.

rsol.nnn
File type: unformatted sequential input.
Created by program BSR_HD**.**
Used for **ctype2=p,q,d**
Description: R-matrix solutions for the partial wave nnn.

bsr_dmat.log
File type: formatted sequential output.
Written by program BSR_DMAT**.**
Read by user.
Description: running information.

zf_res
File type: formatted sequential output.
Written by program BSR_DMAT**.**
Read by user.
Description: oscillator strengths for the multipole operator given in **mult_bnk**.

d.nnn	File type: formatted sequential output. Written by program BSR_DMAT**.** Read by BSR_PHOT. Description: dipole vector for the given initial state and R-matrix solutions in the partial wave nnn.
dv.nnn	File type: formatted sequential output. Written by program BSR_DMAT**.** Read by BSR_POL. Description: dipole vector for the given initial state (no convolutions for the final states).
dd.nnn_mmm	File type: formatted sequential output. Written by program BSR_DMAT**.** Read by BSR_POL. Description: dipole matrix between two partial waves.

10.6. Output of radiative data in **zf_res.**

The output format in **zf_res** is the same as in the MCHF Atomic Structure Package [52]. An example of output is given in Fig.10.2. Each transition is represented by a block, which consists of two empty lines as a delimiter, two lines with a description of the initial and final atomic states, one line with the transition energy in cm^{-1} and Angstroms, and finally a line with the line strength, the oscillator strength, and the transition probability in the length form. For E1 transitions, there is an additional line with the results in the velocity form.

Each atomic state is represented by its spectroscopic label, its absolute energy in a.u., and the value of 2*J*, in case of a transition between *LSJ* states. The f-values are always for transitions from the lower to the higher state, whereas the transition probabilities are always reported from the higher to the lower state. The default output is the gf-values which does not depends on order of initial and final states (see parameter **gf**).

The file **zf_res** is opened in the BSR_DMAT program with access mode *append*. Hence, the results from different calculations can be accumulated.

```
 -1  -37.77853956  1s(2).2s(2).2p(2)3P2_3P
 -1  -37.48150929  1s(2).2s_2S.2p(3)2D3_3D
  65187.63 CM-1      1534.03 ANGS(VAC)      1534.03 ANGS(AIR)
E1  S =  4.85375D+00   GF =  9.61141D-01   AKI =  1.81637D+08
         6.44181D+00         1.27561D+00          2.41066D+08


 -1  -37.48150929  1s(2).2s_2S.2p(3)2D3_3D
 -1  -37.45433756  1s(2).2s(2).2p_2P.3p_3P
   5963.23 CM-1     16769.43 ANGS(VAC)     16764.85 ANGS(AIR)
E1  S =  6.26544D+00   GF =  1.13495D-01   AKI =  2.99142D+05
         1.17451D+00         2.12756D-02          5.60767D+04

  2 -940.13842975   2p(2)3P2
  2 -932.54958058   2p(4)3P2
1665544.77 CM-1        60.04 ANGS(VAC)        60.04 ANGS(AIR)
E2  S =  3.55924D-05   GF =  2.76118D-08   AKI =  1.70307D+04

  0 -940.46450303   2p(2)3P2
  2 -940.13842975   2p(2)3P2
  71564.16 CM-1      1397.35 ANGS(VAC)      1397.35 ANGS(AIR)
M1  S =  1.80864D+00   GF =  5.23415D-06   AKI =  5.96024D+03
```

Fig. 10.2. Example of the output zf_res file with gf=g mode.

10.7. Output of dipole vector for R-matrix solutions - the **d.nnn** files.

Summary of the output records:

1.	`LT1,ST1,IP1,E1`	– term and energy of the initial state.
2.	`LT2,ST2,IP2,nstate2`	– term and number of final states.
3.	`(dl(i),dv(i),i=1,nstate2)`	– dipole matrix in length and velocity form.

10.8. Output of radiative data in **dv.nnn.**

Summary of the output records:

1.	`kpol,ktype`	– type of transition
2.	`E1,J1,IP1,Label1`	– energy, J(L)-values, parity, and label of the initial state.
3.	`kdm2, nch2,npert2`	– basis dimension, number of channels and number of perturbers for final states..
4.	`(dl(i),i=1,kdm2)`	– dipole vector in length form.
5.	`(dv(i),i=1,kdm2)`	– dipole vector in velocity form.

The dipole vectors are obtained by convolution of total transition matrix (10.5) over the expansion coefficients of the initial states.

10.9. Output of the dipole matrix - the **d.nnn_mmm** files.

Has complicated records structure described in the RMATRIX1 manual (Berrington et al 1996)