Conversions between A, f, and S

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One can write the transition probability A_κ^E of an electric multipole transition of type Eκ in terms of reduced matrix elements as follows (γJ is the upper level, $\gamma' J'$ is the lower level):

$$(2J+1)\lambda^{2\kappa+1}A_\kappa^E(\gamma J;\gamma' J') = \frac{2(2\kappa+1)(\kappa+1)(2\pi)^{2\kappa+2}}{[(2\kappa+1)!!]^2\kappa h}|(\gamma J\|Q_\kappa\|\gamma' J')|^2.$$

The expression for a magnetic multipole transition of type Mκ is very similar:

$$(2J+1)\lambda^{2\kappa+1}A_\kappa^M(\gamma J;\gamma' J') = \frac{2(2\kappa+1)(\kappa+1)(2\pi)^{2\kappa+2}}{[(2\kappa+1)!!]^2\kappa h}|(\gamma J\|\mathfrak{M}_\kappa\|\gamma' J')|^2.$$

These formulae can be used to derive a conversion between the transition probability A_κ and the line strength S_κ. The line strength is normally reported in atomic units. These units differ for each transition type, and therefore the unit will be indicated explicitly in each case below. Also, different definitions of S_κ have been in use (and sometimes still are in use!) for E2, M2, and E3 transitions. The reader should verify that the same definition is used when comparing line strengths from this line list with data in the literature! In modern literature the line strength S_κ^E for electric multipole transitions is defined as

$$S_\kappa^E(\gamma J;\gamma' J') = |(\gamma J\|Q_\kappa\|\gamma' J')|^2,$$

and is expressed in units $\mathrm{e}^2a_0^{2\kappa}$, while the line strength S_κ^M for magnetic multipole transitions is defined as

$$S_\kappa^M(\gamma J;\gamma' J') = |(\gamma J\|\mathfrak{M}_\kappa\|\gamma' J')|^2,$$

and is expressed in units $\mu_B^2a_0^{2\kappa-2}$, where $\mu_B = e\hbar/(2m_\mathrm{e}c)$ is the Bohr magneton. If one denotes the statistical weight of the upper level γJ as $g_k \equiv 2J+1$, and omits the designations for the lower and upper level, one can rewrite the conversion formulae as:

$$S_\kappa^E/(\mathrm{e}^2a_0^{2\kappa}) = \frac{[(2\kappa+1)!!]^2\kappa h}{2(2\kappa+1)(\kappa+1)(2\pi)^{2\kappa+2}\mathrm{e}^2a_0^{2\kappa}}g_k\lambda^{2\kappa+1}A_\kappa^E,$$

and

$$S_\kappa^M/(\mu_B^2a_0^{2\kappa-2}) = \frac{[(2\kappa+1)!!]^2\kappa h}{2(2\kappa+1)(\kappa+1)(2\pi)^{2\kappa+2}\mu_B^2a_0^{2\kappa-2}}g_k\lambda^{2\kappa+1}A_\kappa^M.$$

With these definitions it is possible to derive numeric versions for the conversion formulae. Some useful constants in electrostatic units are:

$$\mathrm{e}^2 \approx 2.30708\times10^{-19}, \mu_B^2 \approx 8.60072\times10^{-41}, a_0 \approx 5.29177\times10^{-9}, h \approx 6.62607\times10^{-27}.$$

This then gives the following conversions:

$$S_1^E/(\mathrm{e}^2a_0^2) = \frac{3h}{64\pi^4\mathrm{e}^2a_0^2}g_k\lambda^3A_1^E \approx 4.9355\times10^{-19}g_k\,(\lambda/\,\text{Å})^3A_1^E,$$

$$S_1^M/\mu_B^2 = \frac{3h}{64\pi^4\mu_B^2}g_k\lambda^3A_1^M \approx 3.7073\times10^{-14}g_k\,(\lambda/\,\text{Å})^3A_1^M,$$

$$S_2^E/(\mathrm{e}^2a_0^4) = \frac{15h}{64\pi^6\mathrm{e}^2a_0^4}g_k\lambda^5A_2^E \approx 8.9290\times10^{-19}g_k\,(\lambda/\,\text{Å})^5A_2^E,$$

$$S_2^M/(\mu_B^2a_0^2) = \frac{15h}{64\pi^6\mu_B^2a_0^2}g_k\lambda^5A_2^M \approx 6.7070\times10^{-14}g_k\,(\lambda/\,\text{Å})^5A_2^M,$$

$$S_3^E/(\mathrm{e}^2a_0^6) = \frac{4725h}{2048\pi^8\mathrm{e}^2a_0^6}g_k\lambda^7A_3^E \approx 3.1802\times10^{-18}g_k\,(\lambda/\,\text{Å})^7A_3^E.$$

The conversion between the transition probability A_κ and the oscillator strength f_κ is given by:

$$f_\kappa(\gamma' J'; \gamma J) = \frac{m_\mathrm{e} c}{8\pi^2 \mathrm{e}^2} \frac{g_k}{g_i} \lambda^2 A_\kappa(\gamma J; \gamma' J') \approx 1.4992 \times 10^{-16} \frac{g_k}{g_i} (\lambda / \,\text{Å})^2 A_\kappa,$$

where $g_i \equiv 2J' + 1$ is the statistical weight of the lower level. This conversion formula is valid for all transition types (i.e., E1, M1, E2, etc.). Note that in the formula above, the oscillator strength f has the lower level as the initial level, i.e., it is written as an absorption line, even for forbidden transitions. For emission lines the oscillator strength has negative sign, and the following relation holds:

$$(2J + 1) f_\kappa(\gamma J; \gamma' J') = -(2J' + 1) f_\kappa(\gamma' J'; \gamma J).$$

The latter form is rarely used however.