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Stark broadening of neutral germanium spectral lines

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Abstract. Stark broadening of the 11 Ge I transitions, within the 4p^2–4p5s transition array has been analyzed within the framework of the semiclassical perturbation method. Obtained results have been compared with available experimental and theoretical data. The importance of the electron-impact broadening in the case of the 4226.562 Å line for A star atmospheres has been tested

Key words. line: profiles – atomic data – molecular data – atomic processes – line: formation

1. Introduction

The interest in atomic data on larger numbers of emmiters/absorbers has increased considerably in the last years, since with space born spectrographs, one obtaines stellar spectra with such resolution that a large number of different spectral lines may be indentified. As an example, in the spectrum of Przybylski's star, Cowley et al. (2000) indentified lines belonging to 75 various atom/ion species. Consequently, data on the Stark broadening of neutral germanium spectral lines are of interest not only for laboratory but also for astrophysical plasma research as e.g. for germanium abundance determination and opacity calculations (Seaton 1988). Moreover, germanium is commonly associated with slow-neutron-capture nucleosynthesis in stellar interiors (see e.g. Leckrone et al. 1993). Also germanium lines are present in the Solar (see e.g. Moore et al. 1966; Grevesse 1984) spectrum and with the help of the Goddard High Resolution Spectrograph (GHRS) on the Hubble Space Telescope (HST), the presence of germanium is confirmed e.g. for the χ Lupi binary star (Leckrone et al. 1993). The primary component of this system has $T_{\rm eff} = 10\,650$ K and $\log g = 3.8$ and the secondary $T_{\rm eff} = 9200$ K and $\log g = 4.2$. Since around $T = 10\,000$ K hydrogen is mainly ionized, Stark broadening is the principal pressure broadening mechanism for such plasma conditions. It is interesting to note as well that beginning with germanium ($Z = 32$) and extending to heavier elements, there is a "dramatic increase in the magnitude of overabundances" (Leckrone et al. 1993) in chemically peculiar (CP) star spectra. An illustration of the increasing astrophysical interest for trace element spectra is also the work of Cardelli et al. (1991). With the GHRS they have for the first time detected in the interstellar medium the presence of trace elements like germanium and krypton, so that data on germanium spectral line shapes are obviously of interest for astrophysical plasma research. Moreover, Stark broadening parameters of germanium lines are of interest for the consideration of regularities and systematic trends (see e.g. Sarandaev et al. 2000) as well, and the corresponding results may be of interest in astrophysics for interpolation of new data and critical evaluation of existing data.

The first discussion on the Stark broadening of germanium lines was published in Minnhagen (1964), who considered correlation between observed wavelength shifts produced in electrodeless discharge tube and predicted Stark effect shifts in the spectrum of neutral germanium. Shifts in the wavelength of spectral lines in spark discharges have been investigated as well in the first experimental work on Ge I Stark broadening (Kondrat'eva 1970). After these pioneer works, reliable data on Ge I spectral line Stark broadening parameters have been obtained experimentally by Jones & Miller (1974) and Musiol et al. (1988). For the Ge I 4p^2 ^{1}S–5s^{1}S^0 multiplet, Dimitrijević & Konjević (1983) performed a semiclassical calculation within the framework of the theory developed by Griem et al. (1962) (see also Griem 1974). Moreover, Lakićević (1983) estimated on the basis of regularities and systematic trends the Stark broadening parameters for the Ge I 4p^2 ^{3}P–5s^{3}P^0 multiplet. The estimates based on regularities and systematic trends were performed also by Sarandaev et al. (2000) for the Ge I 4p^2 ^{1}S–5s^1P^0 and 4p^2 ^{1}S–5s^{3}P^0 multiplets. Here, we will calculate within the semiclassical perturbation approach the Stark broadening parameters of 11 Ge I transitions within the 4s^{2}4p^2–4s^{2}4p5s transition array, for conditions typical of astrophysical and laboratory plasmas. The obtained results will be compared with available experimental and theoretical values. Also, the importance of the electron-impact broadening for A type star atmospheres will be tested.

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2. Results and discussion

For the determination of Stark broadening parameters (the full line width at half maximum – *W* and the line shift – *d*) of neutral germanium, the semiclassical perturbation formalism has been used. This formalism, as well as the corresponding computer code (Sahal-Bréchot 1969a,b), have been updated and optimized several times (Sahal-Bréchot 1974; Fleurier et al. 1977; Dimitrijević & Sahal-Bréchot 1984; Dimitrijević et al. 1991; Dimitrijević & Sahal-Bréchot 1996). The calculation procedure, with the discussion of updatings and validity criteria, has been briefly reviewed e.g. in Dimitrijević (1996). Atomic energy levels needed for calculations have been taken from Sugar & Musgrove (1993). The oscillator strengths have been calculated within the Coulomb approximation (Bates & Damgaard 1949; and the tables of Oertel & Shomo 1968). For higher levels, the method of van Regemorter et al. (1979) has been used.

In Table 1, electron-, proton-, and Ar II-impact broadening parameters for 11 Ge I transitions for a perturber density of 10^{16} cm^{-3} and temperatures from 2500 up to 50 000 K are shown. Moreover, we present in Table 1 a parameter *C* (Dimitrijević & Sahal-Bréchot 1984) which gives an estimate of the maximum perturber density for which the line may be treated as isolated, when it is divided by the corresponding full width at half maximum. After electrons, the most important charged perturbers in hot stellar atmospheres are protons, and Stark broadening parameters due to interaction of the emitter/absorber with them are included in Table 1. Due to its importance for laboratory and technological plasma investigations, Stark broadening parameters due to collisions with argon ions are included as well. The validity of the impact approximation has been estimated for data shown in Table 1, by checking if the collision volume (*V*) multiplied by the perturber density (*N*) is much less than one (Sahal-Bréchot 1969a,b), and in all considered cases the product *NV* is less than 0.1. When the impact approximation is not valid, the ion broadening contribution may be estimated by using the quasistatic approach (Sahal-Bréchot 1991 or Griem 1974). In the region between where neither of these two approximations is valid, a unified type theory should be used. For example in Barnard et al. (1974), a simple analytical formula for such a case is given. The accuracy of the results obtained decreases when broadening by ion interactions becomes important.

Jones & Miller (1974) determined experimentally Stark widths of Ge I $4p^2\ ^1S{-}5s^1P^0$ 4685.83 Å and $4p^2\ ^1S{-}5s^3P^0$ 4226.56 Å spectral lines by using a gas-driven spectroscopic shock tube with hydrogen as a driver gas, and runs were made with various filling pressures and different compositions of GeH$_4$, Ar and Ne. They used photographic techniques and Konjević & Wiese (1990) in his critical analysis of the experimental Stark broadening data stated that “self-absorption may have been an important factor for the 4226.56 Å line” in his experiment. In Konjević et al. (1984), the error bars of their results are critically estimated to be within ±50% (accuracy denoted as C in their notation).

Musiol et al. (1988) determined experimentally Stark widths of 9 lines from Ge I $4p^2$–4p5s and $4p^2$–4p4d transition arrays by using a wall-stabilized arc operated at atmospheric pressure with various mixtures of GeH$_4$ and Ar. In Konjević & Wiese (1990), the error bars of their results are critically estimated to be within ±50% (accuracy denoted as C in their notation), except for the 4226.56 Å line where the accuracy is denoted as D$^+$ (error bars larger than ±50%).

In Table 2, our results are compared with experimental results of Jones & Miller (1974) and Musiol et al. (1988). With $W_{\rm m}$ are denoted experimental full widths at half maximum in [Å], and with $W_{\rm e}$ and $W_{\rm GeII}$ our theoretical values for Stark widths due to electron- and Ge II-impacts, respectively. Since ionization potentials of H, Ar and Ge are 13.595 eV, 15.755 eV and 7.88 eV respectively, the most appropriate way to estimate the influence of ion-impact broadening for the considered experiments is to compare electron-impact widths with widths due to impacts with ions of heavy electron donors like germanium. One can see that the ion contribution is around 13−14 per cent which is well within the estimated error bars of the semiclassical perturbation approach of ±30 per cent (Griem 1974). Our results are in disagreement with experimental results of Jones & Miller (1974) for the 4226.56 Å line. This result is in disagreement with other theoretical (Dimitrijević & Konjević 1983; Sarandaev et al. 2000) and experimental (Musiol et al. 1988) results, and selfabsorption is indicated as a possible reason in Konjević & Wiese (1990). The ratio of the experimental Stark width of Jones & Miller (1974) for the 4685.83 Å line and our result is $W_{\rm m}/W_{\rm e} = 1.41$, that is within the estimated (Konjević et al. 1984) error bars of the experiment. The agreement of our values with experimental results of Musiol et al. (1988) is reasonable. The largest disagreement is for the 4226.56 Å line, where $W_{\rm m}/W_{\rm e} = 0.59$, that is however within the estimated (Konjević et al. 1984) error bars of ±50 per cent. The agreement for other lines is considerably better. However, if we analyse experimental and theoretical widths within the $4p^2\ ^3P{-}5s^3P^0$ multiplet, one can notice that the largest difference of experimental values is for 2754.59 Å $4p^2\ ^3P_2{-}5s^3P^0_1$ ($W_{\rm m}$ = 0.0509 Å) and 2651.57 Å $4p^2\ ^3P_0{-}5s^3P^0_1$ ($W_{\rm m}$ = 0.0358 Å) line. The corresponding theoretical values are $W_{\rm e}$ = 0.0502 Å and 0.0466 Å respectively. Since both lines have the same upper energy level and the lower level contribution is small, this is in contradiction with findings that if the perturbing energy level positions are regular, line widths within a multiplet should be approximately the same (Wiese & Konjević 1982). If we eliminate the influence of the wavelength differences multiplying values for the 2651.57 Å line by $(2754.59/2651.57)^2$, we will obtain for the theoretical width the value of 0.0503 Å which is practically equal to the calculated value for the 2754.59 Å line (0.0502 Å). Contrary, for experimental width the scaled value is 0.0386 Å, different to the experimental value of 0.0509 Å for the 2754.59 Å line. It is interesting to obtain new experimental results for these lines in order to see if the reason is configuration mixing.

For Ge I $4p^2\ ^1S{-}5s^1P^0$ multiplet, Dimitrijević & Konjević (1983) performed a semiclassical calculation within the framework of the theory developed by Griem et al. (1962) (see also Griem 1974). It should be noted that atomic data needed for calculations were not taken from Sugar & Musgrove (1993), not available at that time, but from Moore (1971) and

Table 1. This table shows electron-, proton- and Ar II-impact broadening parameters for Ge I for perturber density of 10^{16} cm^{-3} and temperatures from 2500 up to 50 000 K. Transitions and calculated (λ) and experimental (in the air – from NIST 2003 – λ_o) wavelengths (in Å) are also given in the table. By dividing C by the corresponding full width at half maximum (Dimitrijević et al. 1991), we obtain an estimate for the maximum perturber density for which the line may be treated as isolated and tabulated data may be used.

PERTURBER DENSITY IS 1.E+16 cm–3							
PERTURBERS ARE:		ELECTRONS		PROTONS		Ar II IONS	
TRANSITION	T (K)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)
	2500.	0.168	0.139	0.0439	0.0370	0.0271	0.0202
Ge I 4p^2 ^{1}S$_0$–5s^{1}P$^0_1$	5000.	0.201	0.162	0.0489	0.0429	0.0299	0.0241
	10 000.	0.235	0.190	0.0546	0.0491	0.0331	0.0279
λ = 4227.8 Å	20 000.	0.261	0.211	0.0611	0.0558	0.0367	0.0320
λ_o = 4226.562 Å	30 000.	0.272	0.213	0.0652	0.0600	0.0390	0.0345
C = 0.12E+20	50 000.	0.290	0.202	0.0709	0.0656	0.0423	0.0379
	2500.	0.172	0.145	0.0463	0.0389	0.0292	0.0214
Ge I 4p^2 ^{1}S$_0$–5s^{3}P$^0_1$	5000.	0.207	0.168	0.0515	0.0449	0.0320	0.0253
	10 000.	0.243	0.198	0.0574	0.0513	0.0352	0.0293
λ = 4687.1 Å	20 000.	0.273	0.223	0.0641	0.0583	0.0390	0.0335
λ_o = 4685.829 Å	30 000.	0.285	0.228	0.0684	0.0627	0.0414	0.0361
C = 0.18E+20	50 000.	0.306	0.217	0.0742	0.0685	0.0447	0.0396
	2500.	0.0843	0.0710	0.0221	0.0191	0.0132	0.0105
Ge I 4p^2 ^{1}D$_2$–5s^{3}P$^0_1$	5000.	0.101	0.0825	0.0247	0.0220	0.0147	0.0124
	10 000.	0.119	0.0969	0.0277	0.0252	0.0164	0.0144
λ = 3270.4 Å	20 000.	0.132	0.113	0.0310	0.0286	0.0183	0.0164
λ_o = 3269.489 Å	30 000.	0.136	0.112	0.0331	0.0307	0.0196	0.0177
C = 0.89E+19	50 000.	0.145	0.111	0.0360	0.0336	0.0212	0.0194
	2500.	0.0844	0.0721	0.0224	0.0193	0.0134	0.0106
Ge I 4p^2 ^{1}D$_2$–5s^{3}P$^0_2$	5000.	0.102	0.0838	0.0251	0.0224	0.0149	0.0126
	10 000.	0.120	0.0985	0.0281	0.0256	0.0166	0.0146
λ = 3125.7 Å	20 000.	0.135	0.111	0.0315	0.0291	0.0186	0.0167
λ_o = 3124.816 Å	30 000.	0.140	0.115	0.0337	0.0313	0.0198	0.0180
C = 0.67E+19	50 000.	0.148	0.109	0.0366	0.0342	0.0216	0.0198
	2500.	0.0873	0.0723	0.0223	0.0193	0.0133	0.0105
Ge I 4p^2 ^{1}D–5s^{1}P^0	5000.	0.104	0.0843	0.0250	0.0223	0.0148	0.0125
	10 000.	0.122	0.0986	0.0280	0.0255	0.0166	0.0145
λ = 3040.0 Å	20 000.	0.134	0.113	0.0314	0.0290	0.0185	0.0166
	30 000.	0.138	0.111	0.0336	0.0312	0.0198	0.0180
C = 0.62E+19	50 000.	0.147	0.109	0.0366	0.0341	0.0215	0.0197
	2500.	0.0557	0.0469	0.0145	0.0126	0.00855	0.00692
Ge I 4p^2 ^{3}P$_0$–5s^{3}P$^0_1$	5000.	0.0669	0.0545	0.0162	0.0146	0.00955	0.00819
	10 000.	0.0785	0.0640	0.0182	0.0166	0.0107	0.00948
λ = 2652.4 Å	20 000.	0.0869	0.0721	0.0204	0.0189	0.0120	0.0109
λ_o = 2651.568 Å	30 000.	0.0896	0.0742	0.0218	0.0203	0.0128	0.0117
C = 0.58E+19	50 000.	0.0948	0.0707	0.0237	0.0222	0.0139	0.0128
	2500.	0.0588	0.0494	0.0152	0.0133	0.00901	0.00729
Ge I 4p^2 ^{3}P$_1$–5s^{3}P$^0_0$	5000.	0.0707	0.0575	0.0171	0.0153	0.0101	0.00862
	10 000.	0.0827	0.0674	0.0191	0.0175	0.0113	0.00998
λ = 2710.4 Å	20 000.	0.0914	0.0758	0.0215	0.0199	0.0126	0.0114
λ_o = 2709.624 Å	30 000.	0.0940	0.0774	0.0230	0.0214	0.0135	0.0123
C = 0.63E+19	50 000.	0.0997	0.0767	0.0250	0.0234	0.0146	0.0135
	2500.	0.0573	0.0483	0.0149	0.0130	0.00881	0.00713
Ge I 4p^2 ^{3}P$_1$–5s^{3}P$^0_1$	5000.	0.0689	0.0561	0.0167	0.0150	0.00985	0.00843
	10 000.	0.0808	0.0659	0.0187	0.0171	0.0110	0.00977
λ = 2692.1 Å	20 000.	0.0895	0.0743	0.0210	0.0194	0.0123	0.0112
λ_o = 2691.341 Å	30 000.	0.0923	0.0764	0.0225	0.0209	0.0132	0.0121
C = 0.60E+19	50 000.	0.0977	0.0727	0.0244	0.0229	0.0143	0.0132

Table 1. continued.

PERTURBER DENSITY IS 1.E+16 cm–3							
PERTURBERS ARE:		ELECTRONS		PROTONS		Ar II IONS	
TRANSITION	T (K)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)	WIDTH (10^{-1} Å)	SHIFT (10^{-1} Å)
	2500.	0.0583	0.0498	0.0154	0.0134	0.00907	0.00731
Ge I $4p^2\ ^3P_1$–$5s^3P^0_2$	5000.	0.0701	0.0579	0.0172	0.0155	0.0101	0.00868
	10 000.	0.0831	0.0680	0.0193	0.0177	0.0114	0.0101
λ = 2593.3 Å	20 000.	0.0928	0.0769	0.0217	0.0201	0.0127	0.0115
λ_o = 2592.534 Å	30 000.	0.0962	0.0797	0.0232	0.0216	0.0136	0.0124
C = 0.46E+19	50 000.	0.101	0.0759	0.0253	0.0236	0.0148	0.0137
	2500.	0.0600	0.0505	0.0156	0.0136	0.00924	0.00746
Ge I $4p^2\ ^3P_2$–$5s^3P^0_1$	5000.	0.0721	0.0588	0.0175	0.0157	0.0103	0.00883
	10 000.	0.0846	0.0690	0.0196	0.0179	0.0115	0.0102
λ = 2755.4 Å	20 000.	0.0937	0.0777	0.0220	0.0204	0.0129	0.0117
λ_o = 2754.588 Å	30 000.	0.0965	0.0798	0.0235	0.0219	0.0138	0.0126
C = 0.63E+19	50 000.	0.102	0.0760	0.0256	0.0239	0.0150	0.0138
	2500.	0.0609	0.0521	0.0161	0.0140	0.00950	0.00764
Ge I $4p^2\ ^3P_2$–$5s^3P^0_2$	5000.	0.0733	0.0605	0.0180	0.0162	0.0106	0.00907
	10 000.	0.0868	0.0711	0.0202	0.0185	0.0119	0.0105
λ = 2652.0 Å	20 000.	0.0970	0.0804	0.0227	0.0210	0.0133	0.0121
λ_o = 2651.172 Å	30 000.	0.100	0.0832	0.0243	0.0226	0.0142	0.0130
C = 0.48E+19	50 000.	0.106	0.0793	0.0264	0.0247	0.0155	0.0143

Table 2. Comparison of our theoretical results for Stark broadening of Ge I lines with experimental results. With W_m are denoted experimental full widths at half maximum in [Å] and with W_e and W_{GeII} our theoretical values for Stark widths due to electron- and Ge II-impacts, respectively. Accuracy is denoted as in Konjević et al. (1984) and Konjević & Wiese (1990), C means that error bars are within ±50% and D+ that they are larger than ±50%. Under Ref., 1 is for Musiol et al. (1988) and 2. for Jones & Miller (1974).

Transition	λ(Å)	T(K)	N_e 10^{17} cm^{-3}	W_m (Å)	W_e (Å)	W_{GeII} (Å)	Acc.	Ref.
$4p^2\ ^3P$–$5s^3P^0$	2754.59	12 450	0.57	0.0509	0.0502	0.00644	C	1
	2709.62	12 450	0.57	0.0434	0.0490	0.00628	C	1
	2651.57	12 450	0.57	0.0358	0.0466	0.00596	C	1
	2651.17	12 450	0.57	0.0427	0.0517	0.00662	C	1
	2592.53	12 450	0.57	0.0452	0.0494	0.00633	C	1
$4p^2\ ^1S$–$5s^3P^0$	4685.83	11 000	1	0.35	0.248	0.0339	C	2
$4p^2\ ^1D$–$5s^3P^0$	3124.82	12 450	0.57	0.0628	0.0715	0.00928	C	1
$4p^2\ ^1D$–$5s^1P^0$	3039.07	12 450	0.57	0.0622	0.0721	0.00924	C	1
$4p^2\ ^1S$–$5s^1P^0$	4226.56	11 000	1	3.18	0.239	0.0318	C	2
		12 450	0.57	0.0815	0.139	0.0185	D+	1

Kaufman & Edlén (1974). The comparison of semiclassical method of Griem et al. (1962) (see also Griem 1974), used in Dimitrijević & Konjević (1983) and the semiclassical perturbation method (Sahal-Bréchot 1969a,b) used here, as well as an explanation of the differences, is given in Dimitrijević & Sahal-Bréchot (1996). The present results are considerably smaller. For example at $T = 10\,000$ K and $N_e = 10^{17}$ cm^{-3}, Dimitrijević & Konjević obtain a Stark width of 0.408 Å while the present results are 0.235 Å.

Lakićević (1983) estimated Stark broadening parameters for Ge I $4p^2\ ^3P$–$5s^3P^0$ multiplet on the basis of regularities and systematic trends, and he obtained that W is 0.1 Å and the absolute value of the shift is 0.055 Å for an electron density of 10^{17} cm^{-3} and $T = 20\,000$ K. The distance between energy levels within the $5s^3P^0$ term is not negligible in comparison with the distance to the nearest perturbing levels. Consequently, the particular line widths within the corresponding multiplet differ. Our width values vary between 0.087 and 0.097 Å and shift values between 0.072 and 0.080 Å not taking into account the influence of wavelength differences. If one takes into account the simplicity of this method, the agreement is good for the width and within the error bars for the shift.

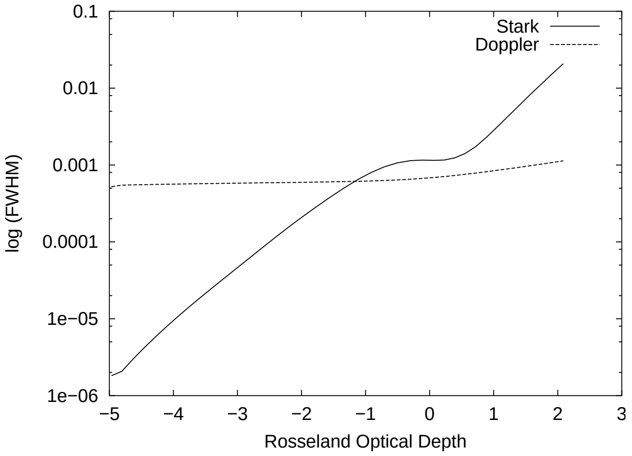

Fig. 1. Thermal Doppler (dotted line) and Stark widths (full line) for Ge I (λ = 4226.562 Å) spectral line as functions of Rosseland optical depth.

On the basis of examination of systematic trends (Purić et al. 1985, 1987, 1991, 1993; Purić 1996), dependencies enabling the estimation of the Stark widths of spectral lines due to s–p and p–s transitions of neutral atoms have been found by Sarandaev et al. (2000). These simple relations, based on the known ionization potential of the lower/upper level of the corresponding transitions and on the regularities and systematic trends, have been used to determine Stark widths for Ge I 4p^2 ^{1}S–5s^{1}P^0 and 4p^2 ^{1}S–5s^{3}P^0 transitions. For example at $T = 20\,000$ K and $N_e = 10^{17}$ cm^{-3} they obtain for Ge I 4p^2 ^{1}S–5s^{1}P^0 a Stark width of 0.33 Å while the present value is 0.261 Å.

In order to see the influence of the Stark broadening mechanism for Ge I spectral lines in stellar plasma conditions, we have calculated the Stark widths for the Ge I 4226.562 Å spectral line for a Kurucz's (1979) A type star atmosphere model with $T_{\rm eff} = 10\,000$ K and log $g = 4$. From Fig. 1 one can see the existence of atmospheric layers where Doppler and Stark widths are comparable and where the Stark width is dominant, and that the Stark broadening effect should be taken into account in abundance determination, spectra synthesis and modeling of stellar plasmas.

New experimental determination of Stark broadening of neutral germanium spectral lines will be obviously useful for comparison with experimental and theoretical data as well as for astrophysical plasma investigation and modeling.

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