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On the Stark Broadening of Lu III Spectral Lines

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Abstract. The electron-impact widths for 27 Lu III spectral lines have been calculated by using the modified semiempirical method. Calculations have been also performed with the published relativistic Hartree-Fock oscillator strengths and additionally, with the approximate formula of Cowley. With the obtained results, the influence of Stark broadening on Lu III lines was investigated in the spectra of A-type stars. The obtained data will be included in the STARK-B database, which is part of the Virtual Atomic and Molecular Data Center – VAMDC.

Key words. Stark broadening—atomic data—Lu III: line profiles.

1. Introduction

Stark broadening is the most important mechanism of spectral line broadening in high temperature plasma conditions. Therefore, a spectral analysis without accounting for Stark broadening in the calculation of line shape in a spectrum of a hot star could cause errors in abundance determination. This problem is for example significant in the case of chemically peculiar (CP) stars, which have abundance anomalies (elements in their atmospheres are overabundant or under abundant compared to the Sun). High overabundances of the rare-earth elements are the most typical characteristic of the upper main-sequence, magnetic, chemically peculiar (Ap) stars, so that for analysis and synthesis of their spectra data on Stark broadening, they are of significant interest, as well as for white dwarf spectra, where the conditions for Stark broadening are very favorable. It should be noted as well that rare earths form one of the peaks in abundance distribution of chemical elements.

The lines of such trace elements became astrophysically interesting with the development of space-borne astronomy. Recently, Lu II lines were observed in stellar

spectra (Roederer *et al.* 2012; Siqueira *et al.* 2013) and one can expect that Lu III lines, not yet found in stellar spectra, will be observed in the future. Taking all this in view, we have calculated Stark widths of 27 Lu III spectral lines, of interest not only for laboratory plasma research and diagnostics but also for abundance determination and spectrum analysis and synthesis of CP stars and white dwarfs. Moreover, since there is no other calculations or experimental data to compare with our results, we performed and calculated by using the relativistic Hartree-Fock oscillator strengths of Biémont *et al.* (1999) for transitions with $\Delta n = 0$. Calculations were also performed with the approximate formula of Cowley.

The obtained results are also used for an investigation of the influence of Stark broadening on Lu III spectral lines in a parameter range relevant for A-type stars.

2. Basics about the element

Lutetium (Lu) is a silvery white metal with atomic number 71, which resists corrosion in dry, but not in moist air. As a transition metal and the last element in the lanthanide series, it is traditionally counted among the rare-earth elements (REE). Lutetium was independently discovered in 1907 by French scientist Georges Urbain, Austrian mineralogist Baron Carl Auer von Welsbach, and American chemist Charles James. Because of the rarity and high price, it has very few commercial uses. However, stable lutetium can be used as a catalyst in petroleum cracking in refineries and can also be used in alkylation, hydrogenation and polymerization applications (Samsonov 1968).

Doubly ionized lutetium (Lu III) is a part of Tm I sequence with an electron configuration of ground state $4f^{14}(^1S)\ 6s\ ^2S_{1/2}$ and an ionization energy of 20.96 eV (Martin *et al.* 1978). Investigations have revealed that Lu III has its importance also in technology because double-charged ions are considered as a significant link of inverse population obtaining process in recombination lasers.

3. The method of calculations

The modified semiempirical method (MSE) has its origin in the semiempirical theory (SE) by Griem (1968) where Stark widths are calculated as a function of inelastic cross sections for the emitter collisions with perturbers, expressed with the help of empirical Gaunt factors, within the impact approximation taking into account the elastic collisions approximately, by extrapolation of Gaunt factors below the threshold for inelastic collisions. SE has been developed for singly charged ions and in fact for its application one needs the same number of atomic data as well as for more sophisticated semiclassical calculation. The MSE is valid also for two, three and more times charged ions and the number of input atomic data is minimized. In the MSE method, only the matrix elements of transitions with $\Delta n = 0$ should be calculated, while other transitions are separated and lumped together. The advantage of this method is that smaller number of atomic data is needed for calculation, so that it is applicable where no sufficient set of atomic data is needed for more sophisticated calculations, like is usually the case for rare-earth spectral lines. Accuracy of MSE results is usually within the error bars of $\pm 50\%$ (Dimitrijević & Konjević 1980), but for complex emitters like Lu III, it may be worse.

The energy levels used to calculate electron-impact FWHM of spectral lines have been taken from Martin *et al.* (1978). The matrix elements needed for the present calculations are obtained within the Coulomb approximation formalism of Bates & Damgaard (1949), while the line and multiplet factors are taken from Shore & Menzel (1968) whenever it is necessary. Since there is no other experimental data to compare with our results, and in order to obtain an estimate of their reliability we performed additional calculations deducing the needed matrix elements for transitions without the change of the principal quantum number n, from relativistic Hartree-Fock gf values from Biémont *et al.* (1999).

Additionally, we performed calculations of the Lu III Stark full widths (FWHM) by using the approximate formula of Cowley (1971). In spite of the fact that this is a very rough approximation, obsolete now when different and more sophisticated methods exist, due to its simplicity it is still sometimes used in astrophysics, especially when data for a large number spectral lines are needed, and they are missing in existing literature and databases. So it is useful to check this formula for a complex spectrum like that of Lu III, by comparison with more sophisticated calculations. We used this formula in the form published in Ziegler *et al.* (2012) (see equation (4) in Ziegler *et al.* (2012)).

Table 1. Parameters a, b and c needed for fitting of line widths W_{MSE} – calculated by using the MSE method (Dimitrijević & Konjević 1980) as a function of temperature using equation (1). The temperature range is 10000 K $\leq T \leq$ 300000 K. In column 5, correlation coefficients are given in per cent.

Wavelength (Å)	a	b	c	Correlation coefficient (%)
972.7	4.502	−2.269	0.210	99.929
996.4	4.073	−2.087	0.192	99.950
1001.2	6.258	−3.293	0.320	99.453
1029.8	4.506	−2.267	0.210	99.907
1030.3	6.350	−3.320	0.323	99.514
1031.5	6.350	−3.320	0.323	99.514
1056.5	4.074	−2.086	0.192	99.927
1062.0	4.559	−2.278	0.211	99.917
1854.6	5.006	−2.320	0.205	99.675
2066.0	5.061	−2.294	0.202	99.657
2071.2	4.501	−2.090	0.190	99.996
2100.1	5.051	−2.286	0.201	99.650
2236.9	3.945	−1.816	0.148	99.818
2382.3	4.384	−2.100	0.192	99.995
2564.3	3.754	−1.718	0.137	99.831
2604.1	4.160	−1.864	0.154	99.838
2773.4	3.828	−1.721	0.137	99.824
3058.8	4.005	−1.775	0.144	99.854
4491.3	6.689	−2.716	0.263	99.692
4957.8	6.918	−2.758	0.266	99.665
5047.5	6.917	−2.746	0.265	99.671
5750.3	7.834	−3.181	0.314	99.424
5788.1	7.848	−3.184	0.314	99.423
5871.3	7.849	−3.176	0.313	99.438
7536.4	8.324	−3.331	0.323	99.402
7938.7	8.395	−3.343	0.324	99.402
8010.9	8.404	−3.344	0.324	99.420

Table 2. Stark electron-impact widths (full widths at half maximum, FWHM) for Lu III spectral lines: W_{MSE}, calculated by using the modified semiempirical (MSE) method (Dimitrijević & Konjević 1980); W_{B}, calculated by using MSE but with the relativistic Hartree-Fock oscillator strengths of Biémont *et al.* (1999) for transitions with $\Delta n = 0$; W_{C}, calculated by using the approximate formula of Cowley (1971). The temperatures are from 10000 K up to 100000 K and the electron density is 10^{17} cm^{-3}.

Transition	T (K)	W_{MSE} (Å)	W_{B} (Å)	W_{C} (Å)
Lu III λ = 1001.2 Å	10000	0.0157	0.0131	0.0787
$4f^{14}(^1S)\,5d\,^2D_{3/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{5/2}$	20000	0.0111	0.0100	0.0556
	50000	0.00702	0.0076	0.0352
	100000	0.00600	0.0068	0.0249
Lu III λ = 1031.5 Å	10000	0.0167	0.0140	0.0835
$4f^{14}(^1S)\,5d\,^2D_{5/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{5/2}$	20000	0.0118	0.0106	0.0591
	50000	0.00747	0.0081	0.0374
	100000	0.00638	0.0072	0.0264
Lu III λ = 1030.3 Å	10000	0.0167	0.0140	0.0836
$4f^{14}(^1S)\,5d\,^2D_{5/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{7/2}$	20000	0.0118	0.0106	0.0591
	50000	0.00748	0.0081	0.0374
	100000	0.00640	0.0072	0.0264
Lu III λ = 3058.8 Å	10000	0.157	0.0707	0.173
$4f^{14}(^1S)\,5d\,^2D_{3/2} - 4f^{14}(^1S)\,6p\,^2P^{o}_{1/2}$	20000	0.111	0.0513	0.122
	50000	0.0703	0.0348	0.0775
	100000	0.0514	0.0274	0.0548
Lu III λ = 2564.3 Å	10000	0.114	0.0506	0.134
$4f^{14}(^1S)\,5d\,^2D_{3/2} - 4f^{14}(^1S)\,6p\,^2P^{o}_{3/2}$	20000	0.0809	0.0367	0.0951
	50000	0.0512	0.0249	0.0601
	100000	0.0368	0.0195	0.0425
Lu III λ = 2773.4 Å	10000	0.134	0.0596	0.157
$4f^{14}(^1S)\,5d\,^2D_{5/2} - 4f^{14}(^1S)\,6p\,^2P^{o}_{1/2}$	20000	0.0949	0.0432	0.111
	50000	0.0600	0.0293	0.0703
	100000	0.0431	0.0230	0.0497
Lu III λ = 1056.5 Å	10000	0.0644	0.0229	0.0748
$4f^{14}(^1S)\,5d\,^2D_{3/2} - 4f^{14}(^1S)\,7p\,^2P^{o}_{1/2}$	20000	0.0456	0.0172	0.0529
	50000	0.0324	0.0128	0.0334
	100000	0.0287	0.0111	0.0236
Lu III λ = 1029.8 Å	10000	0.0626	0.0219	0.0764
$4f^{14}(^1S)\,5d\,^2D_{3/2} - 4f^{14}(^1S)\,7p\,^2P^{o}_{3/2}$	20000	0.0443	0.0164	0.0540
	50000	0.0302	0.0121	0.0342
	100000	0.0266	0.0104	0.0242
Lu III λ = 1062.0 Å	10000	0.0666	0.0233	0.0813
$4f^{14}(^1S)\,5d\,^2D_{5/2} - 4f^{14}(^1S)\,7p\,^2P^{o}_{3/2}$	20000	0.0471	0.0175	0.0575
	50000	0.0321	0.0128	0.0363
	100000	0.0283	0.0110	0.0257
Lu III λ = 5871.3 Å	10000	1.42	1.42	5.06
$4f^{14}(^1S)\,5f\,^2F^{o}_{5/2} - 4f^{14}(^1S)\,7d\,^2D_{3/2}$	20000	1.00	1.09	3.58
	50000	0.669	0.842	2.26
	100000	0.630	0.764	1.60

Table 2. (*Continued*).

Transition	T (K)	W_{MSE} (Å)	W_{B} (Å)	W_{C} (Å)
Lu III λ = 5750.3 Å	10000	1.35	1.36	4.93
$4f^{14}(^1S)\,5f\,^2F^o_{5/2} - 4f^{14}(^1S)\,7d\,^2D_{5/2}$	20000	0.953	1.05	3.48
	50000	0.636	0.811	2.20
	100000	0.601	0.737	1.56
Lu III λ = 5788.1Å	10000	1.37	1.38	4.99
$4f^{14}(^1S)\,5f\,^2F^o_{7/2} - 4f^{14}(^1S)\,7d\,^2D_{5/2}$	20000	0.966	1.06	3.53
	50000	0.645	0.822	2.23
	100000	0.609	0.747	1.58
Lu III λ = 2604.1 Å	10000	0.144	0.0563	0.126
$4f^{14}(^1S)\,6s\,^2S_{1/2} - 4f^{14}(^1S)\,6p\,^2P^o_{1/2}$	20000	0.102	0.0409	0.0888
	50000	0.0643	0.0280	0.0562
	100000	0.0471	0.0222	0.0397
Lu III λ = 2236.9 Å	10000	0.109	0.0423	0.102
$4f^{14}(^1S)\,6s\,^2S_{1/2} - 4f^{14}(^1S)\,6p\,^2P^o_{3/2}$	20000	0.0771	0.0307	0.0723
	50000	0.0488	0.0210	0.0458
	100000	0.0352	0.0166	0.0324
Lu III λ = 996.4 Å	10000	0.0620	0.0178	0.0665
$4f^{14}(^1S)\,6s\,^2S_{1/2} - 4f^{14}(^1S)\,7p\,^2P^o_{1/2}$	20000	0.0438	0.0134	0.0470
	50000	0.0310	0.0099	0.0297
	100000	0.0271	0.0088	0.0210
Lu III λ = 972.7 Å	10000	0.0600	0.0172	0.0682
$4f^{14}(^1S)\,6s\,^2S_{1/2} - 4f^{14}(^1S)\,7p\,^2P^o_{3/2}$	20000	0.0424	0.0130	0.0482
	50000	0.0288	0.0095	0.0305
	100000	0.0251	0.0083	0.0216
Lu III λ = 1854.6 Å	10000	0.0986	0.0644	0.185
$4f^{14}(^1S)\,6p\,^2P^o_{1/2} - 4f^{14}(^1S)\,6d\,^2D_{3/2}$	20000	0.0698	0.0475	0.131
	50000	0.0441	0.0337	0.0826
	100000	0.0325	0.0280	0.0584
Lu III λ = 2100.1 Å	10000	0.0129	0.0932	0.237
$4f^{14}(^1S)\,6p\,^2P^o_{3/2} - 4f^{14}(^1S)\,6d\,^2D_{3/2}$	20000	0.0912	0.0683	0.167
	50000	0.0577	0.0476	0.106
	100000	0.0421	0.0387	0.0749
Lu III λ = 2066.0 Å	10000	0.127	0.0897	0.234
$4f^{14}(^1S)\,6p\,^2P^o_{3/2} - 4f^{14}(^1S)\,6d\,^2D_{5/2}$	20000	0.0897	0.0658	0.165
	50000	0.0567	0.0459	0.105
	100000	0.0415	0.0373	0.0740
Lu III λ = 2071.2 Å	10000	0.112	0.0506	0.200
$4f^{14}(^1S)\,6p\,^2P^o_{1/2} - 4f^{14}(^1S)\,7s\,^2S_{1/2}$	20000	0.0790	0.0373	0.141
	50000	0.0554	0.0264	0.0894
	100000	0.0472	0.0219	0.0632
Lu III λ = 2382.3 Å	10000	0.152	0.0679	0.264
$4f^{14}(^1S)\,6p\,^2P^o_{3/2} - 4f^{14}(^1S)\,7s\,^2S_{1/2}$	20000	0.107	0.0501	0.187
	50000	0.0750	0.0356	0.118
	100000	0.0635	0.0296	0.0836

Table 2. (*Continued*).

Transition	T (K)	W_{MSE} (Å)	W_{B} (Å)	W_{C} (Å)
Lu III λ = 7536.4 Å	10000	1.40	0.981	4.46
$4f^{14}(^1S)\,6d\,^2D_{3/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{5/2}$	20000	0.988	0.748	3.15
	50000	0.625	0.573	1.99
	100000	0.512	0.518	1.41
Lu III λ = 8010.9 Å	10000	1.58	1.27	5.04
$4f^{14}(^1S)\,6d\,^2D_{5/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{5/2}$	20000	1.11	0.963	3.56
	50000	0.705	0.733	2.25
	100000	0.579	0.658	1.59
Lu III λ = 7938.7 Å	10000	1.55	1.34	4.96
$4f^{14}(^1S)\,6d\,^2D_{5/2} - 4f^{14}(^1S)\,5f\,^2F^{o}_{7/2}$	20000	1.10	1.02	3.51
	50000	0.693	0.769	2.22
	100000	0.570	0.685	1.57
Lu III λ = 4491.3 Å	10000	1.05	1.27	2.96
$4f^{14}(^1S)\,7p\,^2P^{o}_{1/2} - 4f^{14}(^1S)\,7d\,^2D_{3/2}$	20000	0.744	0.954	2.09
	50000	0.511	0.710	1.32
	100000	0.471	0.619	0.936
Lu III λ = 5047.5 Å	10000	1.48	1.61	3.74
$4f^{14}(^1S)\,7p\,^2P^{o}_{3/2} - 4f^{14}(^1S)\,7d\,^2D_{3/2}$	20000	1.05	1.22	2.64
	50000	0.711	0.912	1.67
	100000	0.654	0.800	1.18
Lu III λ = 4957.8 Å	10000	1.41	1.56	3.66
$4f^{14}(^1S)\,7p\,^2P^{o}_{3/2} - 4f^{14}(^1S)\,7d\,^2D_{5/2}$	20000	0.994	1.18	2.59
	50000	0.674	0.882	1.64
	100000	0.621	0.774	1.16

4. Results and discussion

We evaluated the Stark widths using the MSE approach for 27 Lu III spectral lines. The Stark widths are calculated for an electron density of 10^{17} cm^{-3}, which is usually used in tables for ion emitters, and for different temperature values. To make the usage of obtained results for modelisation of stellar atmospheres and spectra easier, as well as for radiative transfer calculations, and to prepare our results for the implementation in the STARK-B database, we used the formula from Sahal-Bréchot *et al.* (2011) for fitting calculated data within the range 10000 K $\leq T \leq$ 300000 K with temperature:

$$\log W(T) = a + b \log T + c \log^2 T. \tag{1}$$

Here, $W(T)$ is Stark width in Å, T is the temperature in Kelvin and a, b and c are the fitting parameters. Parameters a, b and c are obtained for electron density of 10^{17} cm^{-3} and tabulated in Table 1.

Stark width (FWHM) values for temperatures 10000, 20000, 50000 and 100000 K are given in Table 2, since this temperature interval is of particular interest, for

example for plasma diagnostic atmospheres of white dwarfs and laser produced plasmas. In this table are also Stark widths calculated with matrix elements ($R^2_{jj'}$) for transitions without the change of the principal quantum number n, deduced from relativistic Hartree-Fock gf values from Biémont *et al.* (1999), using the expression

$$R^2_{jj'} = \frac{gf_{jj'}}{2\ell+1}\frac{3E_{\rm H}}{|E_j - E_{j'}|}\frac{1}{R^2_{\rm line}}\frac{1}{R^2_{\rm mult}}. \tag{2}$$

Here, ℓ is the angular momentum quantum number, $E_{\rm H}$ is the ionization energy of hydrogen atom, E_j and $E_{j'}$ are energies of levels j and j', and $R^2_{\rm line}$, $R^2_{\rm mult}$ are the squares of line and multiplet factors. We can see that the agreement is mostly correct for all d-f and for 6p-6d and 7p-7d transitions, but in the case of s-p, 5d-6p and 5d-7p transitions differences are up to a factor of two. Namely, in the formulation of the MSE method was assumed that for the set of included transitions, sum rules for oscillator strengths are satisfied, and summation of matrix elements for transitions with $\Delta n \neq 0$ has been made under this condition. Inclusion of matrix elements for transitions with $\Delta n = 0$ from other sources may violate such sum rules. However, the agreement of the MSE results with the larger part of these calculations is an indication of the reliability of MSE approach in the present case. In Table 2, results of our Stark width calculation using the approximate formula of Cowley (1971) are

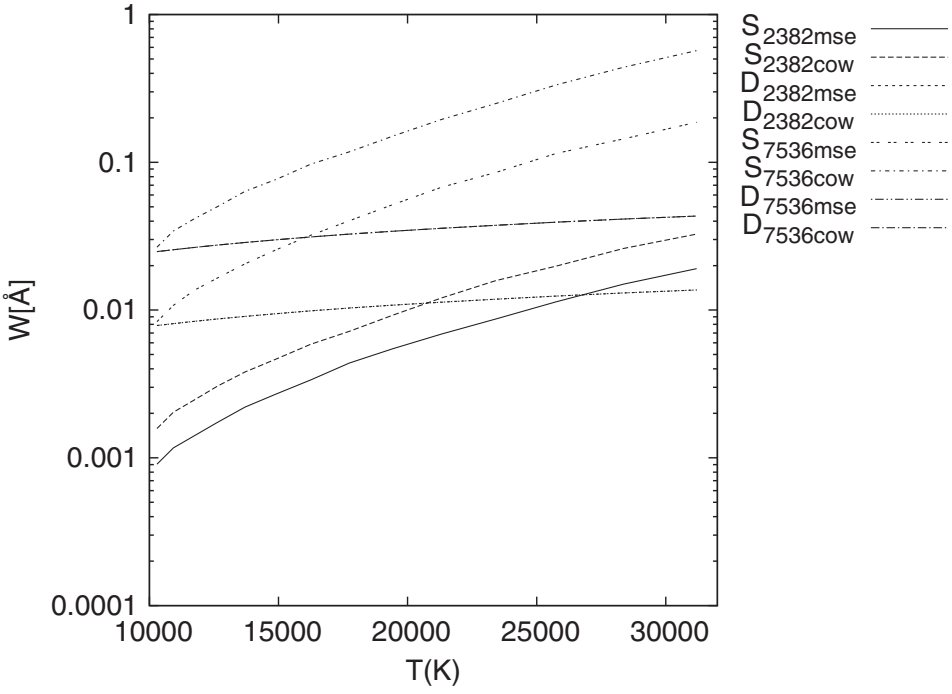

Figure 1. Stark and Doppler widths for Lu III 6p $^2P^{\rm o}_{3/2}$–7s $^2S_{1/2}$ ($\lambda = 2382.3$ Å) and 6d $^2D_{3/2}$–5f $^2F^{\rm o}_{5/2}$ ($\lambda = 7536.4$ Å) spectral lines as a function of atmospheric layer temperatures. Stark and Doppler widths are shown for an atmospheric model (Kurucz 1979) of an A-type star with a surface gravity of $\log g = 4.5$ and an effective temperature of $T_{\rm eff} = 10000$ K.

given. This rough and now obsolete approximation is still sometimes used in astrophysics. In some cases, the obtained results are in agreement with our calculations but in other cases the disagreement is five times for some of the transitions indicating the error introduced by its usage.

Finally, with the results obtained here from Table 1, we investigated, as just one example of the possible application of Stark widths obtained here in astrophysics, how Stark and Doppler width for two spectral lines of Lu III change with the atmospheric layer temperature (Fig. 1) within the atmosphere of an A-type star. The distribution of widths within the atmospheric layers is calculated for $\log g = 4.5$ (cm/s^2) and $T_{\rm eff}$ =10000 K using the distribution of temperature and electron density within the stellar atmosphere from the model atmosphere by Kurucz (1979). One line with smaller Stark width and one with larger Stark width were chosen in order to demonstrate that it is not advisable to neglect *a priori* for all lines Stark broadening contribution, since the influence of Stark broadening may be very different, especially in complex spectra where different irregularities in the position of energy levels exist. From Fig. 1, it is evident that Lu III lines exist for which Stark width may be significantly larger than Doppler width. We note that Stark broadening is even more important for white dwarfs than for A-type stars.

5. Conclusions

New Stark widths for 27 Lu III lines were calculated in this work and there is no other experimental or theoretical Stark broadening data for this emitter. These data are of interest for stellar plasma, as well as for laboratory plasma diagnosis, analysis and modeling, and also for laser produced plasma. As an example of potential astrophysical interest in our results, it was shown that Lu III lines exist whose Stark widths dominate the Doppler widths in some atmospheric layers of A-type stars. To provide and complete atomic data needed for the inclusion of Stark broadening mechanism in modeling of CP star and white dwarf atmospheres and synthesis of their spectra, as well as for laboratory and laser-produced plasma investigations, obtained Stark width results for Lu III spectral lines will enter in the STARK-B database (http://stark-b.obspm.fr/ – Sahal-Bréchot *et al.* (2015a, b)), which is a part of Virtual Atomic and Molecular Data Center (VAMDC – http://vamdc.org/) (Dubernet *et al.* 2010; Rixon *et al.* 2011) and also has a link in Serbian Virtual Observatory (SerVO – http://servo.aob.rs/ – Jevremović *et al.* 2009).

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