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ATOMIC DATA FOR OPACITY CALCULATIONS : THE H, He AND Li SEQUENCES, Fe VIII AND Fe VII

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Résumé - Pour le calcul des opacités stellaires on a besoin des données atomiques pour toutes les transitions dipolaires permises des éléments d'abondance significative dans l'atmosphère stellaire. Les erreurs sur ces données atomiques devraient être moins de 10%. Ce critère pouvait être atteint par des méthodes théoriques qui tiennent compte explicitement des corrélations électroniques, par l'exploitation de techniques numériques efficaces, par l'optimisation des programmes d'ordinateur, et par une collaboration internationale des physiciens motivés. Les données pour les séquences isoélectroniques de H, He et Li ont été publiées et cet article discute leurs mérites. Les données fiables pour les ions du fer sont particulièrement rares car difficilement calculables. Cet article discute les premiers résultats pour Fe VIII et pour Fe VII obtenu par la méthode du 'close-coupling' en incluant les configurations qui contribuent d'une manière significative à la description des corrélations électroniques. Quelques résultats sont donnés pour y illustrer.

ABSTRACT - The calculation of stellar opacities requires atomic data for all dipole allowed transitions in elements of significant stellar abundance. Errors associated with these atomic data should be less than 10%. This goal could be achieved by the use of theoretical methods that account explicitly for electron correlation, by the exploitation of efficient numerical techniques, by optimisation of computer codes, and by an international collaboration of dedicated scientists. Data for the H-, He- and Li- isoelectronic sequences have been published and this paper discusses their merits. Reliable data for iron ions are particularly scarce as they are very difficult to calculate. This paper discusses the first close-coupling calculations for Fe VIII and Fe VII that include the configurations and terms that contribute most to electron correlation. Some illustrative results are given.

1 - INTRODUCTION

Oscillator strengths and photoionisation cross sections for ground states and excited states for all elements of significant stellar abundance are required for opacity calculations. Such data are produced in an international collaboration under the umbrella of The Opacity Project [1]. The approach is thorough but confined within well defined limits. Dipole allowed transitions only are considered. Relativistic effects are neglected. The atomic species treated include those with nuclear charge $Z = 1$ to 26, neutral to fully ionised. Throughout, the wave function for the N electron target is obtained from an optimised configuration interaction (ci) expansion. Wave functions for the $(N + 1)$ electron system are obtained in the close coupling approximation (cc), allowing not more than one electron

in a highly excited or a free state. The calculations are carried out with the structure codes CIV3 /2/ and SUPERSTRUCTURE /3/ and with the R-matrix programs combined with the new optimised asymptotic package /4/. Bound state solutions are calculated for all energies E_i such that the excited electron has principal quantum number $n < 11$ which means $E_i < -z^2/120$, where z is the residual charge of the ion, and E_i is the energy in Rydberg relative to the lowest target term i that forms a collision channel. For certain angular momenta this term may not be the ground state. Continuum state solutions are obtained from threshold to an energy such that asymptotic forms can be fitted to the photoionisation cross sections. The mesh in energy is variable and fine enough to delineate resonances up to effective quantum number $\nu = 8$ relative to the nearest new threshold. Close to threshold the average photoionisation cross section is obtained. The orbital angular momentum of the incident electron is restricted to $l \leq 4$ in all channels.

All isoelectronic sequences up to Al are included in the compilation, and the iron ions are treated individually. This report discusses results for the first three sequences and two iron ions.

2 - THE HYDROGEN SEQUENCE

Menzel and Peckeris /5/ give analytic expressions for all radiative transitions in hydrogenic ions. To make use of these formulae one has to evaluate the hypergeometric function, and this is non-trivial for high principal quantum numbers. Kramers /6/ derived approximate formulae from classical theory that are valid for high quantum numbers. In modified form, formulae applicable to hydrogenic ions are still widely used for any atomic species for which detailed calculations are not available. In the simplest modifications, the principal quantum number n is replaced by an effective quantum number $\nu = n - \mu$ where μ is the quantum defect. For valence electron states that are well removed from the core electrons these approximate formulae have been quite successful and they are also used in the opacity project for states with principal quantum number n greater than ten.

3 - THE HELIUM SEQUENCE

Although data for the He sequence have been previously calculated by many authors, by simple and also by highly sophisticated techniques, none of these authors attempted to obtain a comprehensive set of data as is required for the opacity calculations. One of the first papers in the series 'ATOMIC DATA FOR OPACITY CALCULATIONS' gives such comprehensive results for the He sequence. /7/. Three physical target states (1s, 2s, 2p) and two pseudo states ($\bar{3}p$ and $\bar{1}d$) have been used to describe the hydrogenic target. Results are given for $Z = 2$ to 14 and 16, 18, 19, 20, 24, 25, 26, 28, and 36. Because of the ready availability of data calculated by highly specialised and sophisticated techniques, or obtained by experiment (for references see /7/), the results for the He sequence also provide a test case for the programs and the theoretical approach employed by the opacity project. The authors find that energies for bound states of configuration $1snl$ agree with the best data within 0.5%, and oscillator strengths within 6%. The photoionisation cross section for the ground state of He is within the 5% experimental error bars and energies for resonances of configurations $2snp$ and $2pns$ are within 0.5% of the calculations /8/. However, the resonance widths agree only within 10% and 25% with these calculations.

Due to the limitations of the target description the calculations by Bell and Kingston /9/ should be more accurate at high energies. For neutral helium, detailed experimental and theoretical results that investigate the resonance structure in the photoionisation cross section below the $n = 3$ and 4 thresholds are also available /10,11/. These investigations

go beyond the immediate requirements of the opacity project.

4 - THE LITHIUM SEQUENCE

This sequence has a helium like target, and the first excited states, of configuration $1s2l$, lie about $0.25(Z-1)^2$ Rydberg above the ground state. If one is chiefly concerned with near threshold processes, electron correlation with excited orbitals can be neglected in favour of core polarisation effects. Such effects can be simulated by a model potential or by a close-coupling expansion that includes pseudo states. In the paper on the Li sequence /12/ the authors show that both methods yield the same results, and that these results are in good agreement with observations and more sophisticated calculations where available, except of course for such processes that involve excited core orbitals. Calculations that include excited configurations explicitly are available for Li /13/, and Li-like C, O, and Ne /14,15/. These authors only calculate the photoionisation from the ground state. Calculations for heavier ions of the Li - sequence that include core excited terms are in progress, /16/.

5 - IRON DATA, GENERAL REMARKS

Iron is astrophysically important because of its abundance. The availability of data for radiative transitions in iron ions is a function of the stage of ionisation. There is a wealth of experimental data for neutral and up to twice ionised iron, and there are detailed calculations for H- to Ne- like iron. For less than 15 times ionised iron the most sophisticated calculations hitherto tried to model the complexity of the electron shells by a suitable ci expansion supplemented by the adjustment of a few Slater parameters so that the calculated wavelengths would agree with observations (/17/ and references therein). These approaches require the availability of experimental data and give only a limited range of energy levels and oscillator strengths, and these tend to be quite accurate.

The requirements of the opacity project go way beyond the available data. As for the other ions, the calculations are *ab initio* and comprehensive. It is typical of iron ions with open $n = 3$ shells that the numerous excited core states overlap with each other and with valence electron states $4l$. For this reason the ci expansions have to be large. Another problem is to find a suitable cutoff of the close coupling expansion. Generally, the target states lie close together and electron correlation effects are very strong. Therefore, even with modern computer power it is only just possible to include the most important configurations and target terms to describe an iron ion. The calculated term energies match the (few!) experimental target term energies only poorly. We cannot expect the calculations for iron to yield the accuracy achieved for the lighter ions. On the other hand, they point to important processes that could not be described by other methods and give a comprehensive range of data that include the most important electron correlation and collisional coupling effects explicitly.

5.1 - Fe VIII

The target ion, with ground configuration $1s^2 \dots 3p^6$ appears to have an argon like core. However, the overlap between the 3p and 3d orbitals makes it necessary to include all terms of the core-excited configurations $3p^5 3d$ and $3s3p^6 3d$ and configuration $3p^4 3d^2$ for correlation. With this target, Storey and Taylor (unpublished, to be referred to as ST) have obtained all bound states with configurations $3p^6 nl$, $3p^5 3dn'l$, $3s3p^6 3dn'l$ and $3p^4 3d^3$ for energies such that n or $n' \leq 10$, and for $l \leq 4$, oscillator strengths for transitions between these bound states, and all the photoionisation cross sections. Oscillator strengths

for transitions between terms of configurations $3p^6 3d$ and $3p^5 3d^2$, $3p^5 3d 4s$ were previously obtained in a ci calculation by Tiwary /18,19/ and recently by Fawcett /17/. These oscillator strengths are very sensitive to electron correlation effects and the different calculations give widely differing results for individual transitions, but show fair agreement for the sums of line strengths between close-lying terms of the same symmetry, see table

Table 1

Linestrengths for transitions $3p^6 3d^2 D - 3p^5 3d^2 {}^2 L^\circ$ and $3p^6 4l {}^2 L^\circ$ in Fe VIII

SS=SUPERSTRUCTURE calculation by Storey (unpublished)

upper term\author	ST	SS	Tiwary	Fawcett
$3p^5 3d^2 ({}^1 D) {}^2 P^\circ$	0.04	0.04	0.02	0.03
..... $({}^1 S) {}^2 P^\circ$	0.29	0.02	0.04	0.14
$3p^6 4p {}^2 P^\circ$	0.47	0.83	—	0.76
$3p^5 3d^2 ({}^3 P) {}^2 P^\circ$	3.30	3.27	3.11	4.15
$3p^5 3d^2 ({}^1 D) {}^2 D^\circ$	0.02	0.01	0.02	0.02
..... $({}^3 P) {}^2 D^\circ$	0.00	0.00	0.00	—
..... $({}^3 F) {}^2 D^\circ$	6.72	6.47	7.38	9.19
$3p^5 3d^2 ({}^1 G) {}^2 F^\circ$	0.06	0.05	0.06	0.02
..... $({}^1 D) {}^2 F^\circ$	0.17	0.16	0.27	0.20
..... $({}^3 F) {}^2 F^\circ$	4.23	4.45	4.58	6.17
$3p^6 4f {}^2 F^\circ$	2.52	2.71	—	2.96

Table 2

Weighted oscillator strengths for transitions $3p^6 3d^2 D - 3p^5 3d ({}^3, {}^1 L) 4s {}^2 L^\circ$ in Fe VIII

upper term\author	ST	Tiwary	Fawcett
$({}^3 P^\circ) {}^2 P^\circ$	0.43	0.43	0.62
$({}^1 P^\circ) {}^2 P^\circ$	0.10	0.20	0.12
$({}^3 D^\circ) {}^2 D^\circ$	0.94	0.92	0.94
$({}^1 D^\circ) {}^2 D^\circ$	0.01	0.09	0.24
$({}^3 F^\circ) {}^2 F^\circ$	1.18	1.19	1.37
$({}^1 F^\circ) {}^2 F^\circ$	0.58	0.48	0.64

1. Fawcett's results are 20% higher on average than other calculations. He states in his discussion that he had to omit certain excited core configurations and that he expected these to reduce the oscillator strengths by 10%. ST include the important core-excited configurations but, unlike Fawcett, do not adjust any parameters in order to fit the observed wavelengths. Therefore, Storey and Taylor's results should be more accurate for the sumtotal of linestrengths pertaining to close-lying terms, whereas Fawcett's calculations, reduced perhaps by 20%, should be preferred when oscillator strengths for individual lines

are required, especially so as he also includes spin-orbit interactions. For the more excited states ST's calculations should be reliable even for individual transitions, as term-mixing effects depend strongly on the energy differences and on the overlap of the electron orbitals involved. This is illustrated by the results quoted in table 2, where the agreement between different calculations is seen to be fairly good, with the exception of the gf -value for the transitions between terms $3p^6 3d$ and $3p^5 3d 4s^2 D^\circ$. The energies of the two terms $^2D^\circ$ are much closer in Fawcett's calculation than in the present work. Therefore, the weaker transition obtains a bigger share of the sum of the line strengths in Fawcett's calculation. Fawcett's results - reduced by 20% for *both* transitions - should be the more reliable because of the close agreement with observed wavelengths that he achieves.

Tables 1 and 2 list *all* the 21 dipole-allowed transitions for Fe VIII for which comparisons with other 'accurate' calculations could be made. Taylor and Storey have calculated some 3500 oscillator strengths.

The new calculations for photoionisation cross sections show the importance of photo-excitation of the core electrons (PEC resonances). Figure 1 shows the photoionisation of the ground state $3p^6 3d$. The cross section is enhanced on average by a factor three by resonances of quasi-bound configurations $3p^5 3dnl$ with $l = 0$ or 2 - there are 24 series of resonances of this type contributing. At energies above 15 Rydberg, resonances converging to the terms of configuration $3s3p^6 3d$ stand out clearly. These enhance the cross section only

Fig. 1. Fe VIII: Photoionisation cross section from the ground state $3p^6 3d$.

Fig. 2. Fe VIII: Photoionisation cross section from the excited state $3p\ 4d$

slightly, on average. Figure 2 shows the photoionisation from $3p^6 4d$. Here, the resonances of configuration $3p^5 3dn l$ are only small, narrow features as they couple only through configuration mixing. But right at threshold lie states of configuration $3p^5 3d(^1P^o) 4d$. These enhance the cross section by more than a factor ten. The importance of such features in astrophysical applications is obvious. Only calculations that include the contributing configurations explicitly can describe them.

5.2 - Fe VII

The additional electron in the $n = 3$ shell makes this ion a factor three more prolific than Fe VIII. Storey and Saraph (unpublished) have included all terms of configurations $3p^6 3d$, $3p^6 4l$ with $l = 0, 1, 2$, and 3 , $3p^5 3d^2$ and $3s 3p^6 3d^2$ in their close coupling expansion over target states and configuration $3p^4 3d^3$ for correlation. Calculated bound state energies could be compared with the experimental analysis by Ekberg /20/, table 3 shows typical discrepancies. There are 49 terms of configuration $3p^5 3d^3$ of which only 14 have been determined through observations. There are no experimental determinations for the quintets at all. Figure 3 shows the energy bands covered by various configurations. For comparison with experiment, these bands should be shifted by the amounts indicated in table 3. We list in table 4 the first 111 terms of Fe VII. These too may be adjusted in energy using table 3. Hitherto, very few oscillator strengths had been calculated, and those were obtained in a much simpler approximation /21/. No conclusions could be drawn from a comparison. Instead, we give line strengths for transitions between terms of configurations

Table 3

Differences (in Rydberg) between calculated and experimental ionisation energies for Fe VII					
Config.	error range	exceptions	config.	error range	exceptions
3p ⁶ 3d	-.10 to -.11	¹ S: -.05	3p ⁶ 3d4s	.04	-
3p ⁶ 3d4p	.00 to .01	-	3p ⁶ 3d4f	.01 to .03	-
3p ⁶ 3d5f	.00 to .01	³ H ^o : -.01	3p ⁵ 3d ³	.10 to .32	(⁴ F) ³ D ^o : .39 (⁴ P) ³ S ^o : .48
3p ⁵ 3d ² 4s	.23 to .30	-			

Table 4

The 111 lowest bound states of Fe VII

No	configuration	term	E(Ryd)	No	configuration	term	E(Ryd)
* 1	3s ² 3p ⁶ 3d ²	³ F	0.0000	*57	3s ² 3p ⁵ 3d ³ (² D _a)	³ D ^o	5.2845
* 2		¹ D	0.1618	58	3p ⁶ 2d4d	¹ D	5.3157
* 3		³ P	0.1839	59		³ P	5.3250
* 4		¹ G	0.2597	*60	3p ⁵ 3d ³ (² G)	¹ F ^o	5.3252
* 5		¹ S	0.6601	61	3p ⁶ 3d4d	¹ G	5.3474
* 6	3d4s	³ D	3.2889	62	3p ⁵ 3d ³ (² D _b)	³ D ^o	5.4040
* 7		¹ D	3.3327	63	3p ⁶ 3d4d	¹ S	5.4713
8	3p ⁵ 3d ³ (⁴ P)	⁵ S ^o	3.6816	*64	3p ⁵ 3d ³ (² D _g)	³ P ^o	5.5272
9		⁴ F	³ D ^o 3.7514	*65		⁴ F	³ F ^o 5.5857
10		⁴ F	³ F ^o 3.8213	*66		² P	¹ P ^o 5.7245
11		⁴ F	⁵ G ^o 3.9135	*67		² H	¹ G ^o 5.7460
*12	3p ⁶ 3d4p	¹ D ^o	3.9855	*68		² D _b	¹ P ^o 5.9840
*13		³ D ^o	4.0098	69		² F	¹ F ^o 5.9847
*14		³ F ^o	4.0366	*70		⁴ F	³ D ^o 5.9910
*15		³ P ^o	4.0834	71	3p ⁶ 3d5s	³ D	6.0556
16	3p ⁵ 3d ³ (² G)	¹ F ^o	4.1222	72		¹ D	6.0701
17		² G	³ F ^o 4.1483	73	3d4f	³ H ^o	6.0909
*18	3p ⁶ 3d4p	¹ P ^o	4.1574	*74		¹ G ^o	6.1416
19	3p ⁵ 3d ³ (² G)	³ G ^o	4.1866	*75		³ F ^o	6.1436
20		² F	³ D ^o 4.1878	*76		³ G ^o	6.1618
21		² P	³ P ^o 4.1938	*77		¹ D ^o	6.1651
22		² G	¹ G ^o 4.2651	*78		¹ F ^o	6.1775
23		² G	³ H ^o 4.3036	*79		³ D ^o	6.1972
24		² P	¹ S ^o 4.3087	*80		³ P ^o	6.2105
25		² H	³ I ^o 4.3243	*81		¹ H ^o	6.2165
26		⁴ P	⁵ D ^o 4.3274	*82		¹ P ^o	6.2616
27		⁴ P	⁵ P ^o 4.3410	*83	3p ⁵ 3d ³ (⁴ P)	³ S ^o	6.2646
28		² F	³ F ^o 4.3886	84	3p ⁶ 3d5p	¹ D ^o	6.3535
29		² P	³ D ^o 4.3938	85		³ D ^o	6.3645
30		² D _b	¹ F ^o 4.4082	86		³ F ^o	6.3740
31		² F	¹ D ^o 4.4626	87		³ P ^o	6.3918
32		² H	¹ I ^o 4.4643	88		¹ F ^o	6.4086
33		⁴ F	³ G ^o 4.4944	89		¹ P ^o	6.4172
*34		² G	¹ H ^o 4.4947	90	3s3p ⁶ 3d ³	⁵ F	6.6962
35		⁴ P	³ P ^o 4.5119	91	3s ² 3p ⁶ 3d5d	¹ F	6.8346
36		² P	³ S ^o 4.5420	92		³ D	6.8433
37		² H	³ H ^o 4.5541	93		¹ P	6.8485
38		² D _a	¹ P ^o 4.5744	94		³ G	6.8507
39		⁴ P	³ D ^o 4.5803	95		³ S	6.8688
40		² P	¹ D ^o 4.6056	96		³ F	6.8693
41		² D _b	³ F ^o 4.6363	97		³ P	6.8963
*42		² F	³ G ^o 4.6512	98		¹ D	6.8967
*43		² F	¹ G ^o 4.7465	99		¹ G	6.9114
44		² D _b	³ P ^o 4.7861	100	3s3p ⁶ 3d ³	⁵ P	6.9203
45		² D _a	³ F ^o 5.0139	101	3s ² 3p ⁶ 3d5d	¹ S	6.9666
46		² H	³ G ^o 5.0282	102	3p ⁵ 3d ² (⁴ D ^o)4s ⁵ D ^o		7.0228
47	3p ⁶ 3d4d	¹ F	5.1381	103	3s3p ⁶ 3d ³	³ G	7.0246
48	3p ⁵ 3d ³ (² D _a)	¹ F ^o	5.1473	104		³ H	7.0815
49	3p ⁶ 3d4d	³ D	5.1609	105		³ P	7.0876
50		¹ P	5.1737	106		³ F	7.0953
51	3p ⁵ 3d ³ (² H)	¹ H ^o	5.1737	107		³ D	7.1159
52	3p ⁶ 3d4d	³ G	5.1791	*108	3s ² 3p ⁵ 3d ² (⁴ D ^o)4s ⁵ D ^o	³ D ^o	7.1412
*53	3p ⁵ 3d ³ (² D _a)	¹ D ^o	5.1814	109	3s3p ⁶ 3d ³	¹ G	7.2086
54	3p ⁶ 3d4d	³ S	5.2214	*110	3s ² 3p ⁶ 3d5f	³ H ^o	7.2443
*55	3p ⁵ 3d ³ (² D _b)	¹ D ^o	5.2412	*111		¹ G ^o	7.2477
56	3p ⁶ 3d4d	³ F	5.2658	* for exp. E see Ekberg, 1981.

Fig. 3. Energy bands below the ionisation threshold covered by low configurations of Fe^{6+} .

$3p^6 3d^2$ and $3p^5 3d^3$ and the embedded configurations $3p^6 4p$ and $-4f$, see table 5. However, the same criticisms will apply to these data as have been found to apply to the data for

Table

Oscillator strengths that are larger than 0.25 for transitions between the first 111 terms of Fe VII. Calculated wavelengths are given.

$\lambda(\text{\AA})$	config. ₁	term ₁	config. ₂	term ₂	f
147.9	3p ⁶ 3d ²	³ F	3p ⁶ 3d4f	³ G ^o	0.673
148.3		³ F		³ F ^o	0.472
149.9		³ P		³ S ^o	0.556
151.2		³ P		³ P ^o	0.456
151.5		¹ D		¹ F ^o	0.677
151.5		³ P		³ D ^o	0.962
151.8		¹ D		¹ D ^o	0.414
152.1		³ F		³ D ^o	0.888
153.0		¹ G		¹ H ^o	0.635
154.9		¹ G		¹ G ^o	0.564
156.5		¹ D	3p ⁵ 3d ³ (² D _b)	¹ P ^o	0.730
159.2		¹ G		² F ¹ F ^o	1.011
162.7		¹ S		¹ P ^o	1.768
163.1		³ F		³ F ^o	0.715
166.1		¹ G		² H ¹ G ^o	0.795
170.5		³ P		² D _a ³ P ^o	0.455
171.2		¹ S		² D _b ¹ P ^o	0.615
174.6		³ P		² D _b ³ D ^o	0.405
176.5		¹ D		² G ¹ F ^o	0.550
179.9		¹ S		² P ¹ P ^o	0.520
181.2		³ F	3p ⁶ 3d4d	² H ³ G ^o	0.293
181.5		¹ D		² D _a ¹ D ^o	0.321
685.0	3p ⁶ 3d4p	¹ D ^o		¹ D	0.298
731.3		³ D ^o		³ F	0.515
733.9		³ P ^o		³ P	0.393
743.8		¹ F ^o		¹ G	0.747
786.7		¹ P ^o		¹ D	0.372
790.6		¹ D ^o		¹ F	0.479
791.6		³ D ^o		³ D	0.288
797.7		³ F ^o		³ G	0.641
845.7		³ P ^o		³ D	0.286
896.6		¹ P ^o		¹ P	0.364
908.1	3d4d	¹ F	3d4f	¹ G ^o	0.567
919.2		¹ P		¹ D ^o	0.586
921.3		³ S		³ P ^o	0.932
927.3		³ D		³ F ^o	0.566
999.4		³ G		³ H ^o	0.702
1006.		³ F		³ G ^o	0.622
1045.		³ P		³ D ^o	0.510
1049.		¹ G		¹ H ^o	0.727
1057.		¹ D		¹ F ^o	0.552
1153.		¹ S		¹ P ^o	0.781
1154.	3d4s	¹ D	3d4p	¹ F ^o	0.353
1218.		³ D		³ F ^o	0.316
3216.	3d5s	¹ D	3d5p	¹ D ^o	0.374

Fe VIII. Figure 4 shows sample photoionisation cross sections. As in the case of Fe VIII, core-excitation processes dominate the cross sections.

Fig. 4. Fe VII: Photoionisation cross sections for terms of P symmetry.

6 - CONCLUSIONS

The programme of atomic data calculations that was initiated by the Opacity Project has produced comprehensive sets of radiative data for ions of stellar abundance. The amount of data produced exceeds by one or more orders of magnitude what was previously available in the literature. Yet a standard of accuracy is maintained that satisfies present requirements

of the astronomers for the lighter ions. For the iron ions discussed here, the quality of the data is limited by the computer power. In all cases, the calculations have pointed to the importance of electron correlation and core excitation effects.

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