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HIGH-RESOLUTION MEASUREMENTS OF INTERSYSTEM BANDS OF CARBON MONOXIDE TOWARD X PERSEI[1]

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ABSTRACT

In an echelle spectrum of X Per acquired with the Space Telescope Imaging Spectrograph, we have identified individual rotational lines of 11 triplet-singlet (intersystem) absorption bands of ^{12}CO. Four bands provide first detections for interstellar clouds. From a comparison with the ζ Oph sight line, we find that X Per is obscured by a higher ^{12}CO column density of 1.4×10^{16} cm^{-2}. Together with the high spectral resolution of 1.3 km s^{-1}, this allows (1) an improved measurement of previously published interstellar *f*-values for seven bands and (2) an extraction of the first astrophysical oscillator strengths for *d*–*X* (8–0), (9–0), and (10–0), as well as for *e*–*X* (12–0). The ^{13}CO *d*–*X* (12–0) band, previously suspected to exist toward ζ Oph, is now readily resolved and modeled. Our derived intersystem *f*-values for ^{12}CO include a few mild ($\lesssim$34%) disagreements with recent predictions from a perturbation analysis calculated for the interstellar excitation temperature. Overall, the comparison confirms the superiority of employing multiple singlet levels in the calculations of mixing coefficients over previous single-level predictions.

Subject headings: ISM: abundances — ISM: molecules — molecular data — ultraviolet: ISM

1. INTRODUCTION

Observers of interstellar (IS) sight lines are familiar with the strong $A\,^1\Pi$–$X\,^1\Sigma^+$ permitted absorption bands of CO below 1545 Å. Less familiar to observers are the intersystem bands of CO, which involve the triplet states $a'\,^3\Sigma^+$, $d\,^3\Delta_i$, and $e\,^3\Sigma^-$, whose electric dipole transitions to the ground-state $X\,^1\Sigma^+$ are spin-forbidden. These triplet states have potential energy curves that cross the curve of $A\,^1\Pi$—see Figure 1 of Rostas et al. (2000, hereafter Rostas et al.)—and via mutual perturbations acquire a small percentage of $^1\Pi$ character at the expense of the singlet state. The resulting triplet-singlet *f*-values are relatively small, thus turning the intersystem bands into very useful astrophysical probes along IS sight lines for which the *A*–*X* bands are optically thick (see Morton & Noreau 1994, hereafter MN, and Federman et al. 1994, hereafter F94). To exploit such probes, accurate *f*-values of intersystem transitions are required. Rostas et al. presented predictions from extended calculations of the triplet-singlet mixing coefficients, partly as an attempt to resolve discrepancies between previous theoretical (MN) and astrophysical *f*-values. Rostas et al. also conducted low-resolution laboratory measurements at room temperature to improve upon the experimental results of Eidelsberg et al. (1992). High-resolution laboratory measurements on two intersystem bands were also reported by Stark et al. (2002).

Using the *Hubble Space Telescope* (*HST*), we obtained a high-resolution echelle spectrum of the O9.5 V star X Per (HD 24534) with the Space Telescope Imaging Spectrograph (STIS). Rotationally resolved *A*–*X* bands along this line of sight were first modeled by Kaczmarczyk (2000a), who based his analysis of ^{12}CO on archival *HST* Goddard High Resolution Spectrograph observations. For our STIS observations, the weakest permitted band available for analysis is the *A*–*X* (8–0) band, which still has a large optical depth (τ) in the cores of the strongest lines, $\tau[R(0)] \sim 70$. Therefore, the column density (N) of ^{12}CO toward X Per can be measured more reliably from the observed intersystem bands, which have a much smaller τ. In this Letter, we determine $N(^{12}\mathrm{CO})$ through a comparison with our previous observations of intersystem bands toward ζ Oph (F94). Then we derive IS *f*-values toward X Per for all seven "old" bands and for five intersystem bands seen in IS spectra for the first time. Finally, we compare our *f*-values with the predictions of Rostas et al. Regarding nomenclature, we make use in this Letter of the short notation introduced by Rostas et al., where, e.g., *d*12 stands for *d*–*X* (12–0).

2. OBSERVATIONS AND MODELING

STIS spectra of X Per were acquired in 2001 February and March with grating E140H during 10,728 s over five orbits, yielding the data sets o64812010-030 and o64813010-020. The star was observed through the smallest aperture (0.″1 × 0.″03), which was designed to provide the highest resolving power, $R = 200{,}000$ (Jenkins & Tripp 2001). Elaborate reduction procedures had to be employed in order to correct for odd-even subpixel effects in the unbinned (2048 pixel) exposures. Normal reduction routines were then followed by processing the spectra in the STSDAS environment of IRAF. The five orbital exposures were co-added into a single spectrum of 42 orders between 1316 and 1517 Å, sporting a signal-to-noise ratio of 70, or 100 for features detected and combined from two adjacent overlapping orders. Since the continuum is modulated by shallow photospheric features from X Per, short spectral segments centered on features (bands) of interest were rectified and normalized before being compared to a fitted synthetic model of the pertinent feature. Flux and wavelength calibrations were performed by the Space Telescope Science Institute pipeline and supplied with the binned, 1024 pixel exposures.

A previous analysis of ^{12}CO by Kaczmarczyk (2000b) implied that this line of sight involves two unresolved velocity components. However, the significantly higher resolution of our spectrum shows profile asymmetries due to underlying structure, which required four components for a good fit. This is the same number of components found in preliminary fits of high-resolution K I spectra of X Per (D. E. Welty 2000, private communication), although we derived a different set of relative velocities, fractions, and component widths. Some 87% of the total $N(^{12}\mathrm{CO})$ resides in a main component with a Doppler

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TABLE 1
INTERSYSTEM BANDS OF CO TOWARD X PER

Isotopomer (1)	Band (2)	λ (Å) (3)	W_λ (mÅ) (4)	$W_\lambda^{XP}/W_\lambda^{\zeta\ Oph}$ (5)	$f_{XP} \times 10^5$ (6)	f_{XP}/f_{MN} (7)	f_{F94}/f_{MN} (8)	f_{R00}/f_{MN} (9)	f_{XP}/f_{R00} (10)
^{12}CO	$a'11$ [$A2$]	1480.8	6.52 ± 0.39	4.6 ± 0.8	3.04 ± 0.51	1.06 ± 0.18	1.06 ± 0.18	1.14	0.93 ± 0.16
	$a'14$ [$A4$]	1419.5	44.67 ± 0.40	2.6 ± 0.1	83.1 ± 13.0	0.94 ± 0.15	0.76 ± 0.04	0.94	1.00 ± 0.16
	$a'17$ [$A6$]	1366.2	6.38 ± 0.29	6.0 ± 1.2	3.03 ± 0.49	1.19 ± 0.19	1.01 ± 0.20	1.00	1.20 ± 0.20
	$d7$ [$A2$]	1464.1	4.73 ± 0.21	5.0 ± 0.7	1.92 ± 0.31	4.78 ± 0.77	5.00 ± 0.75	5.07	0.94 ± 0.15
	$d12$ [$A6$]	1366.4	9.62 ± 0.23	5.3 ± 0.7	5.26 ± 0.83	0.67 ± 0.11	0.58 ± 0.07	0.69	0.97 ± 0.15
	$e4$ [$A2$]	1471.2	4.33 ± 0.33	7.2 ± 1.6	1.74 ± 0.30	0.72 ± 0.13	0.51 ± 0.10	0.81	0.89 ± 0.15
	$e5$ [$A3$]	1449.5	15.99 ± 0.23	6.8 ± 0.5	7.70 ± 1.21	0.78 ± 0.12	0.53 ± 0.04	0.69	1.13 ± 0.18
	$d8$ [$A3$]	1442.7	2.09 ± 0.27	…	0.86 ± 0.18	0.39 ± 0.08	…	0.52	0.76 ± 0.15
	$d9$ [$A4$]	1422.3	6.89 ± 0.26	…	3.42 ± 0.55	…	…	…	(0.88 ± 0.14)
	$d10$ [$A5$]	1402.8	1.30 ± 0.22	…	0.57 ± 0.13	…	…	…	(0.66 ± 0.15)
	$e12$ [$A8$]	1323.1	3.09 ± 0.24	…	1.52 ± 0.26	1.07 ± 0.19	…	(0.96)	(1.12 ± 0.19)
^{13}CO	$d12$ [$A6$]	1370.9	4.59 ± 0.19	…	173 ± 11	1.13 ± 0.07	…	…	…

NOTE.—The nearest "parent" A–X permitted band is given in square brackets. References to XP are this Letter, and references to R00 are Rostas et al. The f-values are computed for $N(^{12}CO) = 1.41 \times 10^{16}$ cm^{-2}, and for $N(^{13}CO) = 1.94 \times 10^{14}$ cm^{-2}. Since R00 did not have f-values for $d9$, $d10$, and $e12$, the comparison is with unpublished results from M. Eidelsberg.

parameter (b-value) of 0.39 km s^{-1}. The other three components have between 2% and 9% shares of N, with b-values between 0.17 and 2.09 km s^{-1}, as will be fully described in a future paper. The highly saturated A–X bands could be fitted only once the total N was established via the intersystem bands. Our method of analysis employed a multiparametric spectrum synthesis code based on Voigt profile line transfer equations given in Black & van Dishoeck (1988). The computed absorption spectrum was convolved with a Gaussian instrumental profile (Jenkins & Tripp 2001) and then matched with the data via rms minimization down to relative parameter steps of 10^{-4} or less.

3. THE COLUMN DENSITY OF ^{12}CO

In order to determine f-values for intersystem bands, $N(^{12}CO)$ toward X Per must be known. For optically thin features, the equivalent width (W_λ) is proportional to τ, i.e., $W_\lambda \propto fN$. We can, therefore, utilize the published value of N toward ζ Oph and the ratio of W_λ's for optically thin bands toward the two stars in the determination of N toward X Per. The result should be independent of the intersystem f-values and of the modeled cloud structure, provided we exclude the W_λ ratio for the optically thick $a'14$. Column (5) of Table 1 lists the ratios of band W_λ toward X Per over band W_λ toward ζ Oph. Among the optically thin bands, the highest W_λ ratio belongs to $e4$, which was the faintest intersystem band analyzed by F94. In addition, $e4$ also sports the largest deviation of derived f-value in the low-τ sample of F94. It is clear that F94 underestimated the low-resolution W_λ for $e4$ as a result of placing the continuum too low (see their Fig. 1). Dropping the $e4$ band, and thus avoiding a 5% increase in the average, we obtain W_λ(X Per)/$W_\lambda(\zeta\ \mathrm{Oph}) = 5.54 \pm 0.87$. Under the necessary and fulfilled condition of optical thinness, this is also the ratio of N(X Per) over $N(\zeta$ Oph). Here we shall adopt the Lambert et al. (1994) column density toward ζ Oph, $N(^{12}CO) = (2.54 \pm 0.16) \times 10^{15}$ cm^{-2}, which was also employed by F94. Based on the measured N ratio, we infer that $N(^{12}CO)$ toward X Per is $(1.41 \pm 0.22) \times 10^{16}$ cm^{-2}. Kaczmarczyk (2000b) found $(1.0 \pm 0.2) \times 10^{16}$ cm^{-2} from an analysis of permitted A–X bands; the agreement between the two determinations is at the 2σ level. Recall, however, that Kaczmarczyk's model has fewer cloud components and larger b-values, readily accounting for its reduced column density.

4. BAND OSCILLATOR STRENGTHS

The crossings of vibrational levels in a triplet state and vibrational levels in the $A\ ^1\Pi$ state occur near certain rotational J' levels. Therefore, mixing coefficients depend on J', and thus intersystem f_{band}-values generated by interaction with $A\ ^1\Pi$ have a dependence on T_{ex}. Whereas all previous calculations of mixing coefficients focused on the vibrational level of the A state (v_A) closest to the perturbing triplet level, i.e., a single-v_A treatment, Rostas et al. were the first to use multi-v_A computations that included all A levels with $v' = 0$–12. They derived f_{band}-values that for some intersystem bands were in better agreement with their own experimental results ($T_{ex} = 300$ K) and/or with the IS results of F94 ($T_{ex} = 4.2$ K). Still, the calculated f-values of Rostas et al. are "a few percent" off, because the changes in $f_{v'v''}$ of the "parent" A–X bands induced by mixing with other triplet levels were ignored. In addition, differences of a few percent are expected owing to the adopted sources for A–X f-values: MN and we used values from Chan, Cooper, & Brion (1993), while Rostas et al.'s preference lies with values published by Eidelsberg et al. (1999).

The MN line oscillator strength, $f_{J'J''}$, which we use as input for the fits, includes $f_{v'v''}$ for the permitted A–X band and the usual Hönl-London rotational factor, as well as the single-v_A strength of the perturbation. According to Rostas et al., for triplet levels that cross the A levels at low values of J', single-v_A and multi-v_A calculations should not differ by a large factor since the interaction with the nearest "parent" v_A level is predominant. Therefore, using $f_{J'J''}$-values from MN is a valid approach while searching for relatively small corrections due to multi-v_A interactions. This condition is appropriate for all bands studied here, except for $d7$, $d10$, and to a lesser extent, $e4$. On the other hand, intersystem bands that are farther from their nearest parents have "J-independent" f_{band}-values owing to their high-J' crossing, especially under IS conditions. Again, using $f_{J'J''}$-values from MN poses no difficulties for scaling the integrated band f-values thanks to negligible high-J'' level populations. Indeed, we made no attempt to fit rotational lines independently of each other; our syntheses did not indicate a need to adjust individual $f_{J'J''}$-values. Rather than varying the f-values, our variable parameters were $N(^{12}CO)$, which scales the entire band, and T_{ex}, which determines its shape. Eleven ^{12}CO bands exhibit similar excitation temperatures with averages of $T_{1,0} = 6.1 \pm 1.0$ K and $T_{2,0} = 5.9 \pm 0.4$ K. Lower

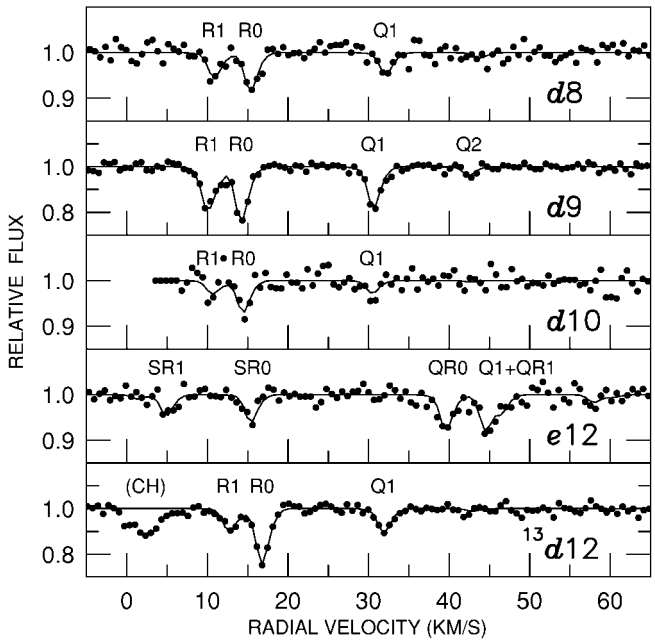

FIG. 1.—Montage of five newly detected intersystem CO bands toward X Per. STIS data are shown as filled circles, while a solid line depicts individual fits for the four-cloud model of ^{12}CO. Heliocentric radial velocity is shown for the $R(0)$ line of all bands.

T_{ex} were suggested by the fit to $a'14$, presumably owing to effects of higher τ. Although f_{band} depends on T_{ex}, the difference in f-values between $T_{ex} = 4.2$ K and $T_{ex} = 6.0$ K is $\lesssim$1%, which we ignore here. One additional variable fitting parameter was the heliocentric radial velocity. For the main component, the average value from nine ^{12}CO intersystem bands is 14.7 ± 1.0 km s^{-1}, where the 1 σ error is dominated by STIS wavelength calibration uncertainties. This radial velocity is in very good agreement with the K I fits mentioned in § 2.

4.1. *Bands Previously Seen toward ζ Oph*

Table 1 lists results of synthetic fits for 12 intersystem bands detected in our spectrum of X Per. For the reference f-values, we used the MN $f_{J'J''}$-values of the $R(0)$ lines, which agree to $\pm$1% of f_{band}-values calculated for $T_{ex} = 4.2$ K, except for $a'14$ and $a'17$, which have low-J' crossings and for which the $R(0)$ f-values are off by $\lesssim$2%. Each ratio of a fitted f_{band}-value over the reference MN value was computed from the ratio of each band's fitted $N(^{12}\mathrm{CO})$ over the actual N determined in § 3. Column (6) lists the resulting band f-values toward X Per. For comparison, in columns (7) through (9) we list ratios of f_{band} from this Letter, from F94, and from theoretical predictions in Rostas et al. over the values from MN. The Rostas et al. values are based on multi-v_A calculations, while the MN values refer to single-v_A results. The theoretical ratios in column (9) lack formal error bars, although deviations due to the presence of other triplet levels and to absolute scales should amount to a few percent. Column (10) directly compares f-values from X Per to those from Rostas et al.

The first seven bands listed in Table 1 were previously detected toward ζ Oph by F94. As discovered by F94, the measured f-value of $d7$ toward X Per is 5 times greater than the value listed by MN in their Tables 5 and 14. However, MN list another f-value for $d7$ in their Table 7, based on measurements by Eidelsberg et al. (1992); the latter result is more in line with both IS f-values and was confirmed in room temperature experiments by Rostas et al. The more rigorous multi-v_A calculation reproduces the astronomical f-values much better than a single-v_A prediction because $d7$ is relatively far from its nearest parent, $A2$. Our new f-value is 6% (0.4 σ) lower than the prediction by Rostas et al., while the F94 result differs by 1% only. Consequently, we do not confirm the recent laboratory result by Stark et al. (2002) that $f_{band}(d7)$ should be reduced by 29% $\pm$ 15% relative to Rostas et al.

Our synthesis of the optically thick $a'14$ toward X Per returns an f-value 6% smaller than that listed by MN, versus the F94 result of -24%. The agreement with the newer predictions is better: the F94 f-value is lower by 19%, whereas the X Per result is identical to that of Rostas et al. According to them, single-v_A and multi-v_A f-values are also identical: 8.3×10^{-4}. Thus, ironically, the strong $a'14$ cannot help to distinguish between the two methods because its (single) interaction with $A4$ is extremely predominant. All other five bands, $a'11$, $a'17$, $d12$, $e4$, and $e5$, are also found to be in very good agreement with the multi-v_A predictions of Rostas et al., i.e., to within 20%. Of these, the F94 a' bands already showed an excellent agreement with MN ($\lesssim$6%) and are within 7% of Rostas et al. The last three F94 bands showed large differences (down to -49%) from MN predictions. All three show better agreement with Rostas et al.: $d12$ now differs by -16%, $e5$ differs by -23%, while $e4$ is off by -37% (3.1 σ). The F94 f-value for $e4$ remains their most discrepant result (after $d7$). This weakest band of F94 was affected by an improper continuum placement, forcing its exclusion from our derivation of $N(^{12}\mathrm{CO})$ in § 3. The result of Stark et al. (2002) for $e4$, that its f-value is marginally too small by 17% $\pm$ 15% relative to Rostas et al., is very similar to the X Per measurement: $-11\% \pm 15\%$. Out of the seven bands under discussion, the largest X Per difference relative to Rostas et al.'s predictions belongs to $a'17$ ($+20\% = +1.0$ σ), a band for which a few weaker $J'' = 2$, 3 lines are blended with another intersystem band, $d12$.

4.2. *Bands Newly Detected toward X Per*

In our spectrum, there are first IS detections of four ^{12}CO intersystem bands: $d8$, $d9$, $d10$, and $e12$. Of these, f_{band} was predicted by Rostas et al. for $d8$, while single-v_A f-values were listed by MN for $d8$ and $e12$. We identified $d9$ and $d10$ as intersystem CO features thanks to their characteristic shapes. Final confirmation was provided by a comparison with laboratory band head wavelengths in Table 27 of Tilford & Simmons (1972) or through the use of molecular state constants from Tilford & Simmons to compute reasonably accurate line positions. The newly detected bands are shown in Figure 1. Our wavelength calculations with the constants for the $d\,^3\Delta_1$ state identify the new d–X bands as the F_3 ($\Omega = 1$) branch of the $d\,^3\Delta_i$ state. According to the lists of MN, F_2 ($\Omega = 2$) components are at least 10 times weaker.

Whereas $d8$ was already mentioned by MN, who adopted the room temperature f-value of Eidelsberg et al. (1992), the newer experiments of Rostas et al. led to a refined value. Our determination clearly favors the new value of Rostas et al. calculated for an IS temperature, since the X Per f-value is -24% (-1.7 σ) away from their value but is -61% (-7.6 σ) away from the value listed by MN. The strongest of the new bands, $d9$, has a W_λ between those of $d7$ and $d12$. Its strong detection contradicts its noninclusion in the tables of MN, who imposed a limiting f-value smaller than inferred here. The third

d–X band, $d10$, has the smallest secure f-value found in this study, $\sim 6 \times 10^{-6}$. The $d10$ band also lacks a previously published f-value. Toward X Per, it is blended with the red wing of the much wider Si IV λ1402, which was successfully removed by profile rectification. The new IS detection of $e12$ close to $A8$ confirms to within 7% the f-value given by MN, but it was not included in the study of Rostas et al. However, in column (10) of Table 1 we compare $d9$, $d10$, and $e12$ f-values with unpublished multi-v_A calculations (M. Eidelsberg 2002, private communication). Two bands agree to $\pm 12\%$ with these predictions, while the f-value of our faintest band, $d10$, is -34% ($-2.3\ \sigma$) away from its predicted value.

The high N(CO) toward X Per also provides us with a clean detection of a fully resolved intersystem band from the ^{13}CO isotopomer, namely, $d12$. This band was suggested to exist by MN in the ζ Oph spectrum of $A6$ analyzed by Sheffer et al. (1992). For ^{13}CO, the $d12$ band was predicted to have substantial mixing, borrowing 19% of the $A6$ f-value according to MN versus the mere 1% borrowed by $d12$ from $A6$ in ^{12}CO. Since the $A8$ band of ^{13}CO has $\tau < 1$, we could find $N(^{13}\mathrm{CO})$ toward X Per directly. Using the four-component model from ^{12}CO, we derived $N(^{13}\mathrm{CO}) = (1.94 \pm 0.08) \times 10^{14}$ cm^{-2}, which yields a ^{12}CO/^{13}CO ratio of 73 ± 12 toward X Per. As can be seen in Table 1, the measured f-value of ^{13}CO $d12$ is 13% ($2\ \sigma$) larger than the single-v_A prediction in MN. Unfortunately, multi-v_A calculations for ^{13}CO have yet to be performed.

5. CONCLUDING REMARKS

The agreement between the band f-values determined from our measurements of absorption along the IS line of sight to X Per and the calculations of Rostas et al. is very good. Rostas et al. suggested that multi-v_A computations are superior for intersystem f-values whenever the spin-forbidden band is not fully overlapped by the permitted band. We concur, because the 11-band average of column (10) in Table 1 is 0.95 ± 0.16, i.e., the -5% difference can be accounted for by known T_{ex} approximations and A–X f-value uncertainties, the latter estimated to be $\approx 10\%$ by Rostas et al. As a caveat, had we retained the $e4$ band in the calculation of $N(^{12}\mathrm{CO})$ in § 3, the average would have changed to 0.90 ± 0.15 owing to a systematic adjustment of all f-values by -5%. Individually, nine intersystem bands show very good agreement with their predictions: $a'11$, $a'14$, $d7$, and $d12$ differ by $\leq 0.4\ \sigma$ (7%), while $a'17$, $e4$, $e5$, $d9$, and $e12$ agree to within $1\ \sigma$ (20%). Such small differences between empirical and predicted f-values may be primarily attributed to assigned observational uncertainties ($\leq$17% for the STIS data; 16% for N toward X Per) rather than to the possibility that current quantum mechanical treatments are inadequate. The bands $d9$, $d10$, and $e12$ were not included in Rostas et al., but a comparison with unpublished multi-v_A calculations shows that two f-values agree to within 12%, while $d10$, our weakest and deblended band, is -34% off. The agreement between empirical results and theoretical predictions assures that accurate column densities can be extracted from IS spectra showing very strong absorption in the permitted bands of ^{12}CO. Finally, there is a need for theoretical multi-v_A calculations of triplet-singlet mixing coefficients in ^{13}CO.

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