Spectral Structure of Electron Antineutrinos from Nuclear Reactors

D. A. Dwyer*
Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

T. J. Langford†
Yale University, New Haven, Connecticut 06520, USA
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Recent measurements of the positron energy spectrum obtained from inverse beta decay interactions of reactor electron antineutrinos show an excess in the 4 to 6 MeV region relative to current predictions. First-principles calculations of fission and beta decay processes within a typical pressurized water reactor core identify prominent fission daughter isotopes as a possible origin for this excess. These calculations also predict percent-level substructures in the antineutrino spectrum due to Coulomb effects in beta decay. Precise measurement of these substructures can elucidate the nuclear processes occurring within reactors. These substructures can be a systematic issue for measurements utilizing the detailed spectral shape.

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Determination of the mixing angle θ_{13} required a new generation of reactor antineutrino experiments with unprecedented statistical precision [1–3]. The Daya Bay and RENO experiments have each detected $\sim 10^6$ reactor $\bar{\nu}_e$ interactions [4,5]. Proper characterization of the $\bar{\nu}_e$ energy spectrum emitted by nuclear reactors is important for such measurements of neutrino properties. The standard approach uses measured energy spectra of the β^- from beta decay to estimate the corresponding $\bar{\nu}_e$ emission. Here we refer to this method as "β^- conversion." For a single measured β^- decay spectrum, the corresponding $\bar{\nu}_e$ spectrum can be predicted with high precision. In the 1980s, foils of the fissile isotopes ^{235}U, ^{239}Pu, and ^{241}Pu were exposed to thermal neutrons from the ILL reactor, and the cumulative β^- spectra of the fission daughters were measured [6–8]. More recently, a similar measurement was made for ^{238}U [9]. The fission of these four main parent isotopes represent $>99\%$ of reactor $\bar{\nu}_e$ emission. Given that each measured β^- spectrum is composed of thousands of unique beta decays, the conversion must be done *en masse*. This introduces uncertainties of a few percent in the corresponding prediction of the cumulative $\bar{\nu}_e$ spectra. Detailed descriptions of such calculations can be found in Refs. [10–12]. A recent study suggested that the uncertainties in converting the β^- spectrum to the $\bar{\nu}_e$ spectrum may have been underestimated due to shape corrections for forbidden beta decays [13].

In this Letter, we discuss an alternative calculation of the $\bar{\nu}_e$ spectrum based on nuclear databases. This *ab initio* approach relies on direct estimation of the $\bar{\nu}_e$ spectrum from the existing surveys of nuclear data. This method suffers from rather large uncertainties in our knowledge of the fission and decay of the >1000 isotopes predicted to be present in a nuclear reactor core. Despite these uncertainties, we find that an *ab initio* calculation involving no fine-tuning predicts an excess of $\bar{\nu}_e$'s with $E_{\bar{\nu}} = 5$–7 MeV relative to the β^- *conversion* method. Recent measurements of the positron energy spectra from $\bar{\nu}_e$ inverse beta decay ($\bar{\nu}_e + p \to e^+ + n$) show a similar $\sim 10\%$ excess from 4 to 6 MeV, consistent with the kinematic relationship $E_{\bar{\nu}} \simeq E_{e^+} + 0.8$ MeV. We also observe substructures at the level of a few percent in the calculated energy spectra, which are difficult to demonstrate from the β^- conversion method. These substructures are due to discontinuities introduced by the Coulomb phase space correction in the $\bar{\nu}_e$ spectrum of each unique decay branch. Precise measurement of these substructures could provide a unique handle on the nuclear processes occurring within a reactor. If not properly accounted for in the model, these substructures can present a systematic problem for measurements relying on the high-resolution features of the reactor $\bar{\nu}_e$ energy spectrum, for example [14,15].

Calculation of the $\bar{\nu}_e$ spectrum.—The collective $\bar{\nu}_e$ emission from a reactor is due to >1000 daughter isotopes with >6000 unique beta decays. The *ab initio* method of calculating the $\bar{\nu}_e$ spectrum follows that presented in Refs. [13,16,17]. The total $\bar{\nu}_e$ spectrum is the combination of many individual beta decay spectra $S_{ij}(E_{\bar{\nu}})$,

$$S(E_{\bar{\nu}}) = \sum_{i=0}^{n} R_i \sum_{j=0}^{m} f_{ij} S_{ij}(E_{\bar{\nu}}). \quad (1)$$

The equilibrium decay rate of isotope i in the reactor core is R_i. The isotope decays to a particular energy level j of the daughter isotope with a branching fraction f_{ij}.

For the fission of a parent nucleus $^{A}_{Z}N_p$, the probability of fragmenting to a particular daughter nucleus $^{A'}_{Z'}N_d$ is given by the instantaneous yield. The majority of these fission daughters are unstable, and will decay until reaching a stable isotopic state. The cumulative yield Y^c_{pi} is the probability that a particular isotope $^{A'}_{Z'}N_i$ is produced via the decay chain of any initial fission daughter. On average, the daughter isotopes of each fission undergo six beta decays until reaching stability. For short-lived isotopes, the decay rate R_i is approximately equal to the fission rate R_p^f of the parent isotope p times the cumulative yield of the isotope i,

$$R_i \simeq \sum_p R_p^f Y_{pi}^c. \quad (2)$$

The Evaluated Nuclear Data File (ENDF) B.VII.1 compiled nuclear data contain tables of the cumulative fission yields of 1325 fission daughter isotopes, including relevant nuclear isomers [18,19]. Evaluated nuclear structure data files (ENSDF) provide tables of known beta decay end-point energies and branching fractions for many isotopes [20]. Over 4000 beta decay branches having end points above the 1.8 MeV inverse beta decay threshold are found. The spectrum of each beta decay $S_{ij}(E_{\bar{\nu}})$ was calculated including Coulomb [21], radiative [22], finite nuclear size, and weak magnetism corrections [13]. In the following calculations, we begin by assuming that all decays have the allowed Gamow-Teller spectral shapes. The impact of forbidden shape corrections will be discussed later in the text.

The upper panel of Fig. 1 shows the β^- spectrum per fission of ^{235}U calculated according to Eq. (1). The β^- spectrum measured in the 1980s using the BILL spectrometer is shown for comparison [6]. Both spectra are absolutely normalized in units of electrons per MeV per fission. The lower panel shows the calculated $\bar{\nu}_e$ spectrum for a nominal nuclear fuel with relative fission rates of 0.584, 0.076, 0.29, 0.05 respectively for the parents ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu. The spectra have been weighted by the cross section of inverse beta decay to more closely correspond to the spectra observed by experiments. Prediction of the $\bar{\nu}_e$ spectrum by β^- conversion of the BILL measurements [11,12] shows a different spectral shape. In particular, there is an excess near 6 MeV in our calculated spectrum not shown by the β^- conversion method. Note that the hybrid approach of Ref. [11] used the *ab initio* calculation to predict most of the β^- and $\bar{\nu}_e$ spectra, but additional fictional β^- branches were added so that the overall electron spectra would match the BILL measurements. The corresponding $\bar{\nu}_e$ spectra for these branches were estimated using the β^- conversion method. Since this method is constrained to match the BILL measurements, it is grouped with the other β^- conversion predictions. An alternate *ab initio* calculation presented in Ref. [17] is consistent with our prediction below 5 MeV, but deviates at 6 MeV.

The significant differences between the calculation and BILL measurements are generally attributed to the systematic uncertainties in the *ab initio* calculation. The 1σ uncertainty bands presented here include only the stated uncertainties in the cumulative yields and branching fractions. Three additional systematic uncertainties are prominent but not included: data missing from nuclear databases, biased branching fractions, and beta decay spectral shape corrections.

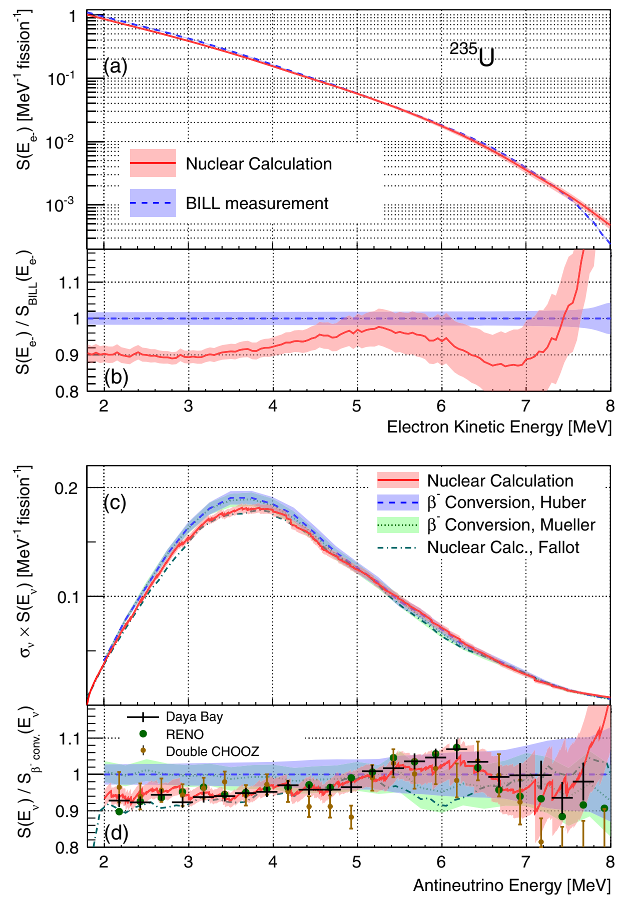

FIG. 1 (color online). (a) *Ab initio* nuclear calculation of the cumulative β^- energy spectrum per fission of ^{235}U exposed to thermal neutrons (solid red), including 1σ uncertainties due to fission yields and branching fractions. The measured β^- spectrum from Ref. [6] is included for reference (dashed blue). (b) Ratios of each spectrum relative to the BILL measurement. (c) The corresponding $\bar{\nu}_e$ spectrum per fission in a nominal reactor weighted by the inverse beta decay cross section (solid red), compared with that obtained by the β^- conversion method (dashed blue [12], dotted green [11]), and an alternate *ab initio* calculation (dash-dotted blue-green [17]). See text for discussion of uncertainties. (d) Ratios of each relative to the Huber calculation. Measurements of the positron spectra (green [23], brown [24], black [25]) are similar to our *ab initio* calculation, assuming the approximate relation $E_{\bar{\nu}} \simeq E_{e^+} + 0.8\,\mathrm{MeV}$. To compare with the calculated spectral shape, measurement normalizations were adjusted approximately −5%.

Missing data.—It is possible that the ENDF/B tabulated fission yields lack data on rare and very short-lived isotopes far from the region of nuclear stability. In Ref. [16], it was argued that this missing data would favor higher-energy decays. For the known fission daughters, ~6% of the yielded isotopes have no measured beta decay information. Both of these effects result in an underprediction of the $\bar{\nu}_e$ spectrum at all energies.

Biased branching fractions.—The branching information of known isotopes may be incomplete or biased. For example the Pandemonium effect can cause a systematic bias, enhancing branching fractions at higher energies

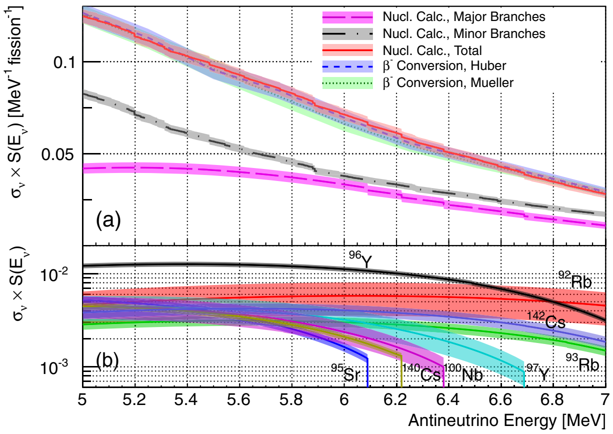

FIG. 2 (color online). (a) Calculated reactor $\bar{\nu}_e$ spectrum per fission in a nominal nuclear power reactor multiplied by the cross section for inverse beta decay (solid red), in the 5–7 MeV region. The eight most prominent decay branches in this region provide 42% of the total counts (long dashed magenta), and combine to produce a local excess relative to the β^- conversion method (dashed blue [12], dotted green [11]). The remaining >1100 decay branches each provide less than 2% of the total rate in this region, and combined provide a smooth shape (dash-dotted black). (b) Individual spectra from the eight most prominent branches. Uncertainties are the same as for Fig 1.

relative to those at lower energies [26]. Such a bias would cause an underprediction of the $\bar{\nu}_e$ spectrum at low energies and an overprediction at high energies, as examined in detail in Ref. [17].

Shape corrections.—The beta decay spectra of each branch may vary from the allowed shape, depending on the nuclear matrix elements connecting initial and final states. In general, these corrections are small for allowed or slightly forbidden decays, but can be more significant for those decays involving a large ΔJ or cancellations between matrix elements. In Ref. [13] it was shown that ∼25% of known reactor β^- decay branches are forbidden, and that shape corrections could in principle impact the β^- conversion method.

These systematic uncertainties are difficult to quantify and do hinder prediction of the absolute $\bar{\nu}_e$ rate and spectrum from a reactor. To correctly model and incorporate all of these uncertainties requires an extensive study not considered for this manuscript. Instead we focus here on two characteristics of the calculation which appear robust to these uncertainties. First, the combined distribution of the beta decay branches predicts an excess from 5 to 7 MeV in the antineutrino spectrum. Second, the Coulomb corrections introduce fine structures to the $\bar{\nu}_e$ spectrum that are not reflected in the corresponding β^- conversion.

Spectral shape in the 5–7 MeV region.—Recent measurements show a ∼10% excess of events from 4 to 6 MeV in the positron spectrum [23–25], similar to the *ab initio* calculation. In this region, the spectral shape is dominated by eight prominent decay branches which contribute 42% of the calculated rate. All eight branches are transitions between the ground states of the initial and final isotopes, and all are first forbidden nonunique decays. While the remaining 58% is composed of ∼1100 decay branches, none individually contribute more than 2%. Therefore each of these minor branches has little influence on the shape of the 5–7 MeV excess. Figure 2 shows the *ab initio* prediction broken into the eight major branches and the remaining minor branches. Table I summarizes these prominent decay branches. While the spectra calculated for each fissile parent isotope show slightly different excesses in this region, these variations are small when compared with the differences in spectral slopes.

The impact of each unquantified systematic uncertainty on this spectral feature can be examined. Contributions from missing nuclear data could add additional decay branches in this region, increasing the overall normalization and difference from the β^- conversion model. To remove this local excess, it would require that the additional branches have a particular distribution of end points just below and just above the excess. While possible, this seems contrived. For the eight prominent branches, six are 0^- decays. These decays are not expected to have any significant deviation from allowed shapes [27]. The ft

TABLE I. Most prominent beta decay branches with $E_{\bar{\nu}} = 5$–7 MeV. The table presents the decay parent, end-point energy, half-life, and decay ft value. The decay type describes the parent and daughter states. The moderate ft values and lack of significant change of J^π suggest that all but possibly ^{140}Cs decay with allowed spectral shapes. The rate each branch contributes to the total between 5–7 MeV is N, accounting for the inverse beta decay cross section. The 1σ uncertainty due to the fission yield and branching fraction is σ_N.

Isotope	Q(MeV)	$t(s)$	Log(ft)	Decay type	N (%)	σ_N (%)
^{96}Y	7.103	5.34	5.59	$0^- \to 0^+$	13.6	0.8
^{92}Rb	8.095	4.48	5.75	$0^- \to 0^+$	7.4	2.9
^{142}Cs	7.308	1.68	5.59	$0^- \to 0^+$	5.0	0.7
^{97}Y	6.689	3.75	5.70	$1/2^- \to 1/2^+$	3.8	1.1
^{93}Rb	7.466	5.84	6.14	$5/2^- \to 5/2^+$	3.7	0.5
^{100}Nb	6.381	1.5	5.1	$1^+ \to 0^-$	3.0	0.8
^{140}Cs	6.220	63.7	7.05	$1^- \to 0^+$	2.7	0.2
^{95}Sr	6.090	23.9	6.16	$1/2^+ \to 1/2^-$	2.6	0.3

values are mostly in the 5 to 6 range, consistent with allowed shapes. Only ^{140}Cs has a large ft value and decay type consistent with a possible forbidden shape correction. Since this isotope contributes only 2.7% of the rate, the resulting correction should be small. Forbidden shape corrections to the numerous minor branches can only negligibly impact the overall structure, although a cumulative effect could slightly impact the normalization and slope. The current uncertainty band includes the stated uncertainties on the branching fractions. Biases such as the Pandemonium effect would need to be significantly larger than these uncertainties on the eight major branches in order to remove the local excess. Pandemonium corrections on the large number of minor branches could slightly reduce the total normalization and change the slope in this region. In particular, ^{92}Rb suffers from significant uncertainty in the branching fraction to the ground state. Our calculation used a branching fraction of $51 \pm 18\%$ from Ref. [28]. In Ref. [29], it was changed to $95 \pm 0.7\%$ to correct for a corresponding overestimation of branching fractions for known excited levels. Recent measurements suggest this may actually be due to unknown excited levels, providing a preliminary result of 74% [30]. Assuming 95% ground-state branching would further increase our predicted rate in the 5–7 MeV region by ∼6%. Awaiting a definitive measurement, we retain the more conservative older value with larger uncertainty. While these uncertainties could reasonably impact the normalization and slope of the spectrum in this region, the prediction of a local excess seems robust provided the tabulated data for these prominent branches is correct.

Figure 1 includes the recently measured deviations in the positron spectrum from reactor $\overline{\nu}_e$ inverse beta decay interactions [23–25]. The relation $E_{\bar{\nu}} \simeq E_{e^+} + 0.8$ MeV was used to compare these deviations with the calculated $\overline{\nu}_e$ spectrum. Normalization was adjusted to provide a comparison of only spectral shape. Each experimental spectrum includes percent-level systematic effects from detector resolution and nonlinearity not present in the calculation, providing only an illustrative comparison. Given these assumptions and the model uncertainties already discussed, the overall agreement between the measurements and *ab initio* calculation is surprising.

Spectral substructures.—The *ab initio* calculated spectrum shows detailed substructures due to the Coulomb corrections in beta decay. The Coulomb correction for a single decay branch produces a sharp discontinuity at the end point of the $\overline{\nu}_e$ spectra. There is no corresponding detailed structure in the β^- spectrum since the Coulomb correction impacts the low-energy end of the spectrum. The substructures are most apparent in the comparison to a smooth analytic approximation of the $\overline{\nu}_e$ spectrum [31],

$$F(E_{\bar{\nu}}) = \exp\left(\sum_i \alpha_i E_{\bar{\nu}}^{i-1}\right). \quad (3)$$

A fit to the calculated $\overline{\nu}_e$ spectrum provides $\alpha = \{0.4739, 0.3877, -0.3619, 0.04972, -0.002991\}$. A significant number of discontinuities are present with amplitudes of a few percent or greater, as shown in Fig. 3.

Systematic uncertainties in the *ab initio* calculation introduce variation in the specific pattern of these substructures. In alternative calculations, random Gaussian fluctuations were applied to the yields and branching fractions according to the tabulated 1σ uncertainties. Parameters were not allowed to fluctuate to negative values, introducing a bias toward enhancing the overall spectrum. For illustration, Fig. 3 shows five spectra from these calculations.

Figure 3 demonstrates the spectral structure after accounting for detector resolution in the measurement of positrons from inverse beta decay. Current reactor $\overline{\nu}_e$ experiments have sufficient resolution (6 to $8\% \times \sqrt{E_{e+}/1\ \mathrm{MeV}}$) to measure the larger scale features. Proposed measurements with 3% resolution (e.g., Refs. [14,15]) may resolve the most prominent decay end points. Measurements reaching percent-level resolution would reveal more details of the nuclear processes occurring within a reactor.

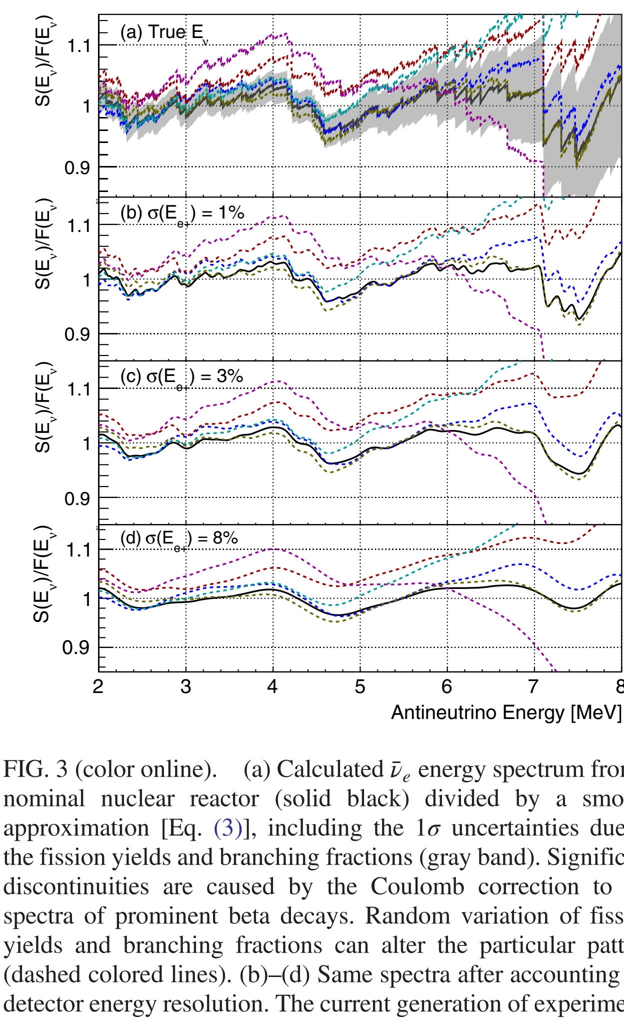

FIG. 3 (color online). (a) Calculated $\bar{\nu}_e$ energy spectrum from a nominal nuclear reactor (solid black) divided by a smooth approximation [Eq. (3)], including the 1σ uncertainties due to the fission yields and branching fractions (gray band). Significant discontinuities are caused by the Coulomb correction to the spectra of prominent beta decays. Random variation of fission yields and branching fractions can alter the particular pattern (dashed colored lines). (b)–(d) Same spectra after accounting for detector energy resolution. The current generation of experiments with ∼8% energy resolution is sensitive to the larger variations. Future high-resolution experiments would detect some of the substructures.

The unquantified systematic uncertainties can also modify the predicted substructures. Missing nuclear data would introduce additional isotopes and decay branches, thereby increasing the number of discontinuities. The Pandemonium effect would slightly reduce the amplitude of discontinuities at high energies, and enhance those at low energies. Shape corrections can increase or decrease the amplitude of a particular discontinuity. While these uncertainties can make the exact pattern of substructures difficult to predict, it is clear that substructures of the scale shown will be present.

Discussion.—While the *ab initio* calculation of the reactor $\overline{\nu}_e$ energy spectrum has significant uncertainties, two specific characteristics are predicted. A local spectral excess due to prominent beta decay branches in the 5–7 MeV region is similar to that seen in recent measurements. Dedicated studies of the fission yields and branching fractions of these prominent decays would help confirm the spectral shape in this region. It is unclear why the predictions based on β^- conversion, which are expected to be more accurate, are inconsistent with the observed $\overline{\nu}_e$ spectra. Given the large normalization uncertainties in the *ab initio* prediction, it is difficult to address the overall flux deficit discussed in Ref. [32].

Calculation predicts percent-level substructures in the $\overline{\nu}_e$ energy spectrum, although the exact pattern is uncertain. A high-resolution measurement of the reactor antineutrino spectrum could provide a unique diagnostic of the nuclear processes within a reactor. The structure may pose a systematic issue for measurements probing high-resolution features in the spectrum. For example, the neutrino mass hierarchy presents itself as percent-level differences in the high-frequency oscillatory pattern in the spectrum as shown in Fig. 2 of Ref. [33].

These conclusions demonstrate the value of precise measurement of the $\overline{\nu}_e$ energy spectra from nuclear reactors, reinforcing the conclusion of Ref. [13]. Research reactors could provide a model system (primarily ^{235}U) for comparison of measurement and calculation.

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[*]dadwyer@lbl.gov
[†]thomas.langford@yale.edu

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