# $^{45}V(p,\gamma)$ thermonuclear reaction rate relevant to $^{44}$ Ti production in core-collapse supernovae: General estimates and shell model analysis

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The lack of knowledge of the  ${}^{45}V(p, \gamma)$  reaction rate has been shown to contribute a large uncertainty to the production of  ${}^{44}$ Ti in core-collapse supernovae. By considering likely contributions from resonances associated with  ${}^{46}$ Cr states that are the isobaric analog of states in  ${}^{46}$ Ti, we have determined that the currently accepted value of the  ${}^{45}V(p, \gamma)$  reaction rate is unlikely to be inaccurate by more than an order of magnitude. These conclusions are confirmed by the shell model calculations with the FPD6 effective interaction.

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# I. INTRODUCTION

The isotope <sup>44</sup>Ti is of interest in astrophysics because of the evidence for its production in supernovae. Recent studies [1,2] estimate the mass of <sup>44</sup>Ti that can be produced in corecollapse supernovae could approach  $10^{-4}$  solar masses. The very high abundance of <sup>44</sup>Ca in the present solar system can be attributed almost entirely to the synthesis of <sup>44</sup>Ti progenitor nuclei [3]. In addition, silicon carbide meteoritic samples have been shown to have large excesses of <sup>44</sup>Ca [4,5]. These are thought to be condensates of presolar supernovae ejecta, forming within a few years after the supernovae and hence reflecting the initial <sup>44</sup>Ti abundance [6]. Recently, gammaray astronomy using several satellite based observatories, most significantly CGRO surveys with COMPTEL [7–9], have directly observed the 1.157 MeV gamma ray that signifies the decay of <sup>44</sup>Ti.

These observations, coupled with the successful efforts to determine the half-life of <sup>44</sup>Ti [10–14], provide a most stringent test of supernova models. Of course there exist many significant uncertainties in the theoretical models used, including the electron fraction [15] and the possibility that nearly fully ionized <sup>44</sup>Ti might be expelled from the core of the star, thus extending its mean half-life [16]. Uncertainties in the hydrodynamics, equation of state, and effects of magnetic fields could also play a role in the <sup>44</sup>Ti production.

However, there are also possible uncertainties in the nuclear reaction rates that could affect the amount of <sup>44</sup>Ti produced. The *et al.* [17] recently performed a systematic variation of the reaction rates used in one such network calculation. They found that the uncertainty in the amount of <sup>44</sup>Ti produced in the alpha-rich freeze-out phase of a corecollapse supernova showed appreciable sensitivity to four reaction rates. Of these, the dominant one was <sup>45</sup>V( $p, \gamma$ ). Although that reaction occurs somewhat to the proton-rich side of the centroid of the alpha-rich freeze-out path, the high temperature environment of alpha-rich freeze-out provides all the constituents necessary to make the  ${}^{45}V(p,\gamma){}^{46}Cr$  reaction important in determining the ultimate  ${}^{44}Ti$  abundance.

The reaction rates would normally be determined in these scenarios through a statistical model approach. However, although the level density in this mass region near the Gamow window would be expected to be sufficiently high to make averaging over resonances a good approximation, strong isolated resonances can nevertheless enhance the cross section within a narrow range of energies. Therefore, it is interesting to identify possible states that could produce strong resonances, based on spectroscopic data, and then to examine their effect on the reaction rates. The present study utilized information about the known states in <sup>46</sup>Ti to predict the location, spin-parity quantum numbers, and spectroscopic factors of excited states in <sup>46</sup>Cr that are likely to be populated via the  ${}^{45}V(p,\gamma)$  reaction, and from this to calculate the reaction rates. Unfortunately, despite there being many relevant experimental studies, the spectroscopic information is far from complete in the region of excitation that is of interest here.

However, an extensive examination of the literature made it clear that there was sufficient information available to at least make a judgment of whether the analogs of states in <sup>46</sup>Ti are likely to contribute strongly enough in <sup>46</sup>Cr to alter significantly the current estimate of the astrophysically important  $(p, \gamma)$  reaction rates. We supplement the estimates based on available information by a direct shell model calculation of low-lying levels of positive parity in a nuclear system with A = 46 using the effective isospin-invariant FPD6 interaction successfully tested earlier for this region of the nuclear chart.

## **II. ESTIMATES OF S FACTORS AND REACTION RATES**

The states of interest will be near an excitation in <sup>46</sup>Cr equal to the proton separation energy (4.890 MeV) plus the energy region of the Gamow window. In the case of the

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<sup>45</sup>V(*p*, *γ*) reaction, for temperatures of about 1 000 000 000 000–2 000 000 000 K ( $T_9$ =1 or 2), which are thought to be the temperatures at which the cooling alpha-rich freeze-out material falls out of nuclear statistical equilibrium, this is a range of excitation energies in <sup>46</sup>Cr of around 5.3–7 MeV.

Since currently no  ${}^{45}V(p, \gamma) {}^{46}Cr$  experimental data exist in this region, we have attempted to determine the likely location and nuclear properties of the relevant <sup>46</sup>Cr states by calculating where the isobaric analog states in the wellknown nucleus <sup>46</sup>Ti would occur in <sup>46</sup>Cr. We also attempted to infer which of the possible analog states might be important to the  ${}^{45}V(p,\gamma) {}^{46}Cr$  reaction. Since likely nuclear configurations in <sup>46</sup>Ti consist of a <sup>44</sup>Ti core with two extra nucleons located in the fp shell, naive shell model arguments suggest that only positive parity states of spin J=1-6 and orbital momentum transfer of  $l_{tr}=1$  or 3 need be considered. In reality, the positive parity level density at excitation energy higher than 3 MeV in <sup>46</sup>Ti is only by a factor of 2 higher than that of negative parity. However, due to a strong suppression of the electric dipole transition in the lower part of the spectrum (see below) the presence of the negative parity levels should not significantly change our estimates. Given the proton energies considered here, p-wave scattering is most likely and this, together with the  $7/2^{-}$  spin of the ground state of <sup>45</sup>V, further limits us to typical spin parities of 2<sup>+</sup>,3<sup>+</sup>,4<sup>+</sup>, and 5<sup>+</sup>. Furthermore, one would expect states of interest to be strongly populated in one- and two-nucleon stripping reactions, such as  ${}^{45}Sc({}^{3}He,d)$ ,  $^{45}$ Sc(<sup>4</sup>He,t), and <sup>44</sup>Ca(<sup>3</sup>He,n), while pickup reactions will populate these states much less strongly.

Since relatively high resolution is needed to provide the required information, probably the best data that exist for our purposes are the  ${}^{45}Sc({}^{3}He,d)$  data of Banu and Gupta [18] and of Bromen and Pullen [19]. From comparison of these data with measurements from other reactions, we have identified eight states that appear to have the right character to be included in this study. The most notable of these other data sets are the  ${}^{44}Ca({}^{3}He,n)$  data of Evers *et al.* [20], the  ${}^{45}Sc({}^{4}He,t)$  data of Priest and Vincent [21], and the  ${}^{48}Ti(p,t)$  data of Kouzes *et al.* [22] and of Rapaport *et al.* [23]. Our criteria for selection included the above arguments, together with a requirement (in the absence of spectroscopic factor information) that the measured cross section for the population of a state was significant.

#### A. Thomas-Ehrman shift calculations

The excitation energy at which these states will occur in <sup>46</sup>Cr can be calculated from the energies of their analogs in <sup>46</sup>Ti using the formalism of Thomas and Ehrman [24], which takes into account the different spatial distributions of the protons within a nucleus compared to the neutrons in their isobaric analog.

Following this prescription, the level shift of a bound nucleon-nucleus state in <sup>46</sup>Ti,  $\Delta_b$ , from the energy by which it is bound,  $E_b$  (in this case equal to the neutron separation energy minus the excitation of the state in <sup>46</sup>Ti), is given by

TABLE I. Selected positive parity levels in <sup>46</sup>Ti, their possible spins, and the proton partial decay widths of their <sup>46</sup>Cr analogs.

$E_x(^{46}\text{Ti})$ (MeV)	J	$l_{tr}$	$\Gamma_p$ (MeV)
5.080	2 or 4	1	$1.0 \times 10^{-14}$
5.080	2 or 4	3	$9.0 \times 10^{-9}$
5.321	2	1	$2.2 \times 10^{-9}$
5.363	2	1	$8.0 \times 10^{-9}$
5.363	2	3	$4.9 \times 10^{-7}$
5.515	2	1	$2.8 \times 10^{-7}$
5.515	2	3	$2.4 \times 10^{-6}$
6.025	2 or 4	1	$1.9 \times 10^{-4}$
6.118	2	1	$4.1 \times 10^{-4}$
6.118	2	3	$1.5 \times 10^{-4}$
6.424	2 or 4	1	$2.9 \times 10^{-3}$
6.550	2 or 4	1	$5.4 \times 10^{-3}$
6.550	2 or 4	3	$1.1 \times 10^{-3}$

$$\Delta_b = \frac{3\hbar^2 \theta_b^2 k W_l'}{2\,\mu R W_l},\tag{1}$$

where  $\theta_b$  is the reduced width of the state, *k* the wave number, *R* the nuclear radius,  $\mu$  the reduced mass of the system, and  $W_l$  and  $W'_l$  the Whittaker function and its derivative, respectively, as a function of  $E_b$ ,  $l_{tr}$ , *k*, and *R*.

Similarly, the level shift of an unbound state in the analog nucleus, from the energy by which it is unbound,  $E_r$  (in this case equal to the the excitation energy in <sup>46</sup>Cr minus the proton separation energy),  $\Delta_r$ , is given by

$$\Delta_r = -\frac{3\hbar^2 \theta_r^2}{2\mu R^2} P_l(F_l F_l' + G_l G_l'), \qquad (2)$$

where  $\theta_r$  is the reduced width of the unbound state, and  $F_l$ ,  $F'_l$ ,  $G_l$ , and  $G'_l$  the regular and irregular Coulomb wave functions and their derivatives, which are functions of  $E_r$ ,  $l_{tr}$ , k, and R. The Coulomb penetrability factor  $P_l$  is given by

$$P_{l} = \frac{kR}{F_{l}^{2} + G_{l}^{2}}.$$
 (3)

Hence, the method used to determine the excitation of a state in <sup>46</sup>Cr is to pick a state in <sup>46</sup>Ti and guess where its analog will appear. One then calculates  $\Delta_b$  and  $\Delta_r$  and tests the equality

$$E_b - E_r = \Delta_b - \Delta_r, \qquad (4)$$

modifying the excitation in <sup>46</sup>Cr until agreement is found.

Table I lists the deduced properties of the eight states we have determined as being of possible interest, subdivided into the spin and transferred angular momentum combinations allowed for these states by the experimental data. Included are the predicted proton partial decay widths, calculated using the relation of Blatt and Weisskopf [25],

$$\Gamma_p = \frac{2\hbar P_l \theta_p^2}{R} \left(\frac{2E}{\mu}\right)^{1/2}.$$
(5)

In the calculations we take  $\theta_b \approx \theta_r = \theta_p$ ; we slightly modify  $\theta_b$  in order to get the resonance energies corresponding to the same state in <sup>46</sup>Ti equal for both l=1 and l=3. This adjustment will affect mostly l=3 shifts by no more than few hundred keV. This will have a negligible effect on the  $(p, \gamma)$  cross sections, as the l=3 proton captures are greatly hindered compared with l=1 captures. Assuming  $\theta_p^2 = 0.1$  in all cases one gets the proton widths listed in Table I. Although this is a somewhat arbitrary choice, it was deemed to be reasonable in view of the number of states (~10) over which the strength appears to be shared.

### **B.** Direct capture

In the regime of well separated narrow resonances, direct capture will contribute significantly to the cross section between the resonance energies. Since we do not assume narrowly spaced resonances *a priori*, we have to consistently include the direct capture contribution. Due to the lack of information on bound states in <sup>46</sup> Cr, as well as on spectroscopic factors, we limit ourselves to an attempt to estimate an upper limit of the direct capture contribution.

Assuming the first two excited states in <sup>46</sup>Cr to be the analogs of the corresponding states in <sup>46</sup>Ti and setting the  $(p, \gamma)$  spectroscopic factors to 1.0, we calculated direct E1, E2, and M1 capture to the ground state and the first two excited states. The calculation was similar to that of Rauscher *et al.* [26], which utilized a folding potential [27] but determined the open parameter  $\lambda$  with the parametrization given in Ref. [28].

An additional effect was taken into account which can prove important in stellar plasmas. As the target nucleus is in thermal equilibrium with its environment, not only the ground state but also low-lying excited states can be populated. This effect is usually included in the calculated stellar rates whereas laboratory measurements can only measure the rate with the target being in the ground state. In the case of <sup>45</sup>V, the first excited state will still be populated half as strongly as the ground state at a temperature of  $T_9=1.5$ . Therefore, we also included capture on the first excited state of the target, assuming equal potentials and spectroscopic factors as for the target being in the ground state but weighting the cross section contribution by the thermal population.

The resulting direct capture reaction rate is shown in the next section. Since there are no experimental data on bound states, scattering lengths, and spectroscopic factors, the resulting *S* factors and rates are only approximate. However, as will be seen, the contribution is several orders of magnitude smaller than the resonance part of the cross section, a conclusion that is not likely to be altered by more accurate or sophisticated calculations.

## C. Astrophysical S factors

The astrophysical *S* factors for each of these states can be determined using the Breit-Wigner single-level resonance formula [29],

$$S(E) = \pi \frac{(2J+1)}{(2j_t+1)(2j_p+1)} \times \frac{\Gamma_{\gamma}\Gamma_p}{(E-E_r)^2 + \Gamma^2/4} \exp(2\pi\eta),$$
(6)

where *J* is the spin of the state in the compound nucleus,  $j_t$  is the spin of the target nucleus,  $j_p$  is the spin of the projectile proton, and  $\eta$  is the Sommerfeld parameter. The total width,  $\Gamma$ , is assumed to be the sum of the proton and gamma partial decay widths. Following the method of Rolfs and Rodney [30], the value calculated by this equation at the resonance energy,  $S(E_r)$ , can then be used in conjunction with energy dependent gamma and proton partial decay widths to determine an energy dependent *S* factor,

$$S(E) = S(E_r) \frac{\exp[2\pi\eta(E)]}{\exp[2\pi\eta(E_r)]} \frac{\Gamma_p(E)}{\Gamma_p(E_r)} \frac{\Gamma_{\gamma}(E)}{\Gamma_{\gamma}(E_r)}$$
$$\times \frac{[\Gamma(E_r)]^2/2}{(E - E_r)^2 + [\Gamma(E)]^2/4}.$$
(7)

A rough estimate of the  $\gamma$  widths may be inferred from the results of several <sup>45</sup>Sc( $p, \gamma$ ) works. In particular, Rahman *et al.* [31] and Molla *et al.* [32] have looked at gamma decays in <sup>46</sup>Ti up to around 6 MeV excitation. Typically they find *E*1 or *E*2 transitions of 2–3 MeV, which for the *E*1 transitions would be consistent with decays to the two known negative parity states that occur at just above 3 MeV excitation energy in <sup>46</sup>Ti.

For comparison to our results, we use the statistical model calculations performed with the NON-SMOKER code [33,34], which is an improvement of the well-known SMOKER code [35,36]. Among other changes, NON-SMOKER features improved optical potentials and level densities [37]. The statistical model [38] assumes a number of overlapping resonances, which allows the use of average resonance properties. Although this requirement is usually satisfied for nuclei in this mass region, strong and widely spaced analog resonances could contribute significantly.

Figure 1 shows, as an example, the calculated *S* factors for the analog to the 5.515 MeV state in <sup>46</sup>Ti, assuming  $l_{tr}$ = 1 or 3, and for 3.0 MeV *E*1 or *E*2 gamma decay transition probabilities; for comparison, the prediction of NON-SMOKER is also shown. The solid curve shows the predicted astrophysical *S* factor assuming the *E*1 transition proceeds with a strength of 10<sup>-3</sup> W.u. which is typical for this scenario.

#### **D.** Thermonuclear reaction rates

The reaction rate is obtained by numerically integrating the *S*-factor information with the thermal energy distribution. The contribution from a single narrow resonance may be obtained using the equation [39]

$$N_A\langle\sigma v\rangle = \left(\frac{8}{\pi\mu}\right)^{1/2} \frac{N_A}{(kT)^{3/2}} \int_0^\infty S(E) \exp\left[-\frac{E}{kT} - \frac{b}{E^{1/2}}\right] dE$$
(8)



FIG. 1. Astrophysical *S* factor calculated using the single resonance formula as a function of proton center-of-mass energy for the resonance in  ${}^{46}$ Cr corresponding to the first  ${}^{46}$ Ti level in Table II. The results of the statistical code NON-SMOKER are included for comparison.

in  $\text{cm}^3 \text{s}^{-1} \text{ mole}^{-1}$ , where *T* is temperature in Kelvin, *E* is in MeV, and the parameter *b* is given by

$$b = (2\mu)^{1/2} \pi e^2 Z_1 Z_2 / \hbar, \qquad (9)$$

where  $Z_1$  and  $Z_2$  are the atomic numbers of the projectile and target nuclei.

In summing the contributions from several states in this way it is necessary to consider whether interference from many states of the same spin and similar proton decay width might significantly affect our findings. To judge this to first order, we have considered pairwise interference between neighboring states using the simple approximation that the total *S* factor for the pair is then given by [40]

$$S(_{tot}) = S_{r1}(E) + S_{r2}(E) + 2[S_{r1}(E)S_{r2}(E)]^{1/2} \cos(\delta_{r1} - \delta_{r2}), \quad (10)$$

where  $S_{r1}(E)$  and  $S_{r2}(E)$  are energy dependent *S* factors of the two neighboring states, and the phase shifts,  $\delta$ , are given by

$$\delta_r = \tan^{-1} \frac{2(E - E_r)}{\Gamma(E)} - \frac{\pi}{2},\tag{11}$$

where  $E_r$  is the resonance energy of each of the two states.

In the vicinity of the peaks, which is the only region which makes a significant contribution to the reaction rate, the interference term makes little difference. Hence we believe it is justified, within the context of the current work, to continue by just taking the sum of all the possible contributing states, so as to form an approximate estimate of the maximum total reaction rate.

# **III. SHELL MODEL CALCULATIONS**

A quantitative analysis based on the levels included in Table I is likely to be inaccurate due to missing information about the spectroscopic factors, spin, and parities of the selected levels. Examination of the known <sup>46</sup>Ti level structure suggests that individual analogs of the states that appear in <sup>46</sup>Cr might be able to alter significantly the <sup>45</sup>V( $p, \gamma$ )<sup>46</sup>Cr reaction rate. To complement and refine this information, in particular, to minimize the possibility of important missing states, we have performed a shell model calculation. Such analyses have proven very effective in predicting the properties of relatively low-lying nuclear states and transition probabilities. The region of nuclei between Ca and Ni is currently under extensive study both experimentally and by shell model practitioners [41,42].

The model which can be treated with sufficient precision covers the fp major shell consisting of (in increasing energy)  $f_{7/2}$ ,  $p_{3/2}$ ,  $p_{1/2}$ , and  $f_{5/2}$  subshells. The many-body dimensions of the relevant Hamiltonian matrices are still tractable, exactly or with the help of the exponential extrapolation

TABLE II. Shell model <sup>46</sup>Ti levels corresponding to resonances in the Gamow window in <sup>46</sup>Cr, selected according to the magnitude of the spectroscopic factors for relative l=1 and l=2 proton waves (last two columns). The width  $\Gamma_W$  corresponds to an *E*1 transition to a negative parity level (3<sup>-</sup> or 4<sup>-</sup>) assuming a Weisskopf unit for the *B*(*E*1) reduced transition probability.  $\Gamma_{+\rightarrow+}$  are the shell model results for the transition widths from the selected states to all other positive parity states lower than 5 MeV.

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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$E_x$ (MeV)	$J^{\pi}$	$\Gamma_W$ (MeV)	$\Gamma_{+ \to +}$ (MeV)	$\overline{\theta}_p^2(1)$	$\overline{\theta}_p^2(3)$
$5.410$ $3^+$ $3.21 \times 10^{-5}$ $9.99 \times 10^{-8}$ $0.17326$ $0.024384$ $5.528$ $2^+$ $4.23 \times 10^{-5}$ $7.74 \times 10^{-8}$ $0.14431$ $0.12649$ $5.683$ $4^+$ $4.72 \times 10^{-5}$ $5.62 \times 10^{-8}$ $0.19603$ $0.012333$ $5.820$ $4^+$ $5.74 \times 10^{-5}$ $2.87 \times 10^{-8}$ $0.29935$ $0.027444$ $5.917$ $2^+$ $7.25 \times 10^{-5}$ $2.96 \times 10^{-8}$ $0.10968$ $0.025836$ $5.917$ $5^+$ $2.07 \times 10^{-5}$ $16.44 \times 10^{-8}$ $0.16332$ $0.077744$ $6.180$ $5^+$ $2.87 \times 10^{-5}$ $13.94 \times 10^{-8}$ $0.23898$ $0.013617$ $6.232$ $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.002699$ $6.373$ $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.033714$	5.191	4+	$2.11 \times 10^{-5}$	$1.41 \times 10^{-8}$	0.10969	0.024388
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.410	3+	$3.21 \times 10^{-5}$	$9.99 \times 10^{-8}$	0.17326	0.024388
5.683 $4^+$ $4.72 \times 10^{-5}$ $5.62 \times 10^{-8}$ $0.19603$ $0.012333$ 5.820 $4^+$ $5.74 \times 10^{-5}$ $2.87 \times 10^{-8}$ $0.29935$ $0.027440$ 5.917 $2^+$ $7.25 \times 10^{-5}$ $2.96 \times 10^{-8}$ $0.10968$ $0.025830$ 5.917 $5^+$ $2.07 \times 10^{-5}$ $16.44 \times 10^{-8}$ $0.16332$ $0.077743$ 6.180 $5^+$ $2.87 \times 10^{-5}$ $13.94 \times 10^{-8}$ $0.23898$ $0.013617$ 6.232 $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.002699$ 6.373 $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.033718$	5.528	$2^{+}$	$4.23 \times 10^{-5}$	$7.74 \times 10^{-8}$	0.14431	0.126491
5.820 $4^+$ $5.74 \times 10^{-5}$ $2.87 \times 10^{-8}$ $0.29935$ $0.027444$ 5.917 $2^+$ $7.25 \times 10^{-5}$ $2.96 \times 10^{-8}$ $0.10968$ $0.025836$ 5.917 $5^+$ $2.07 \times 10^{-5}$ $16.44 \times 10^{-8}$ $0.16332$ $0.0777436$ 6.180 $5^+$ $2.87 \times 10^{-5}$ $13.94 \times 10^{-8}$ $0.23898$ $0.0136176$ 6.232 $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.0026996$ 6.373 $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.0337166$	5.683	$4^{+}$	$4.72 \times 10^{-5}$	$5.62 \times 10^{-8}$	0.19603	0.012338
$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.820	$4^{+}$	$5.74 \times 10^{-5}$	$2.87 \times 10^{-8}$	0.29935	0.027440
5.917 $5^+$ $2.07 \times 10^{-5}$ $16.44 \times 10^{-8}$ $0.16332$ $0.077744$ 6.180 $5^+$ $2.87 \times 10^{-5}$ $13.94 \times 10^{-8}$ $0.23898$ $0.013617$ 6.232 $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.002694$ 6.373 $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.033714$	5.917	$2^{+}$	$7.25 \times 10^{-5}$	$2.96 \times 10^{-8}$	0.10968	0.025836
6.180 $5^+$ $2.87 \times 10^{-5}$ $13.94 \times 10^{-8}$ $0.23898$ $0.013617$ 6.232 $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.002699$ 6.373 $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.033718$	5.917	5+	$2.07 \times 10^{-5}$	$16.44 \times 10^{-8}$	0.16332	0.077748
$6.232$ $3^+$ $10.02 \times 10^{-5}$ $48.33 \times 10^{-8}$ $0.26471$ $0.002699$ $6.373$ $4^+$ $11.47 \times 10^{-5}$ $14.30 \times 10^{-8}$ $0.10239$ $0.033718$	6.180	5+	$2.87 \times 10^{-5}$	$13.94 \times 10^{-8}$	0.23898	0.013617
$6.373 \qquad 4^{+}  11.47 \times 10^{-5}  14.30 \times 10^{-8}  0.10239  0.033713$	6.232	3+	$10.02 \times 10^{-5}$	$48.33 \times 10^{-8}$	0.26471	0.002699
	6.373	4+	$11.47 \times 10^{-5}$	$14.30 \times 10^{-8}$	0.10239	0.033718



FIG. 2. Astrophysical *S* factor calculated using the single resonance formula as a function of proton's center-of-mass energy for the resonances in  $^{46}$ Cr corresponding to all ten  $^{46}$ Ti levels in Table II.

method [41,43]. The necessary effective interactions suggested for this region have been shown to work well. Thus, the FPD6 effective interaction [44] should give a very good description of nuclear structure in our region of interest around A = 46.

In this model we describe only positive parity states in nuclei <sup>46</sup>Ti or <sup>46</sup>Cr. An excitation of negative parity requires the creation of a hole in the sd shell. Unfortunately the full sdfp space leads to matrix dimensions that are too large for direct diagonalization. For applying approximate approaches one needs to carefully eliminate the spurious excitations associated with center-of-mass motion. One can calculate a few low-lying states including only  $1\hbar\omega$  excitations. However, the negative parity states corresponding to the Gamow window in the  ${}^{45}V(p,\gamma)$  reaction are intractable due to the very high density of negative parity states at that excitation energy in the analog nucleus <sup>46</sup>Ti. We can study the potential implication of the negative parity states by calculating the occupation probabilities of the  $2s_{1/2}$  and  $1d_{3/2}$  proton single particle levels in the ground state of <sup>45</sup>V. In the calculation we truncated the  $0+2\hbar\omega sdpf$  shell model space up to 10 000 000 m-scheme states, following an ordering procedure described in Refs. [41,43]. As an effective interaction we used a combination of FPD6 for the fp shell, USD [45] for the sd shell, and a modified form of the Millener-Kurath interaction [46] for the cross-shell part. The resulting occupation probability is 1.96 (very close to the maximum value of 2), and that for  $d_{3/2}$  is 3.9 (close to the maximum value of 4). When this strength is spread over many states, it suggests that the s- and d-wave spectroscopic factors of typical negative parity states in the Gamow window are smaller than, or of the order of,  $10^{-3}$ . This number supports our approach of keeping only the positive parity states in the analysis of the  $^{45}$ V $(p, \gamma)$ <sup>46</sup>Cr reaction rate.

Experimentally, 57 levels are known for <sup>46</sup>Ti in the excitation energy range below 5 MeV and 59 levels between 5 and 7 MeV. Many levels do not have certain assignments of spin, although, for the majority, the parity is known. We performed the shell model diagonalization with the isospininvariant FPD6 effective interaction calculating with the core of  $^{40}$ Ca the positive parity levels up to 7 MeV excitation energy. The shell model reproduces the collective yrast band in agreement with data [47] (mean square deviation less than 300 keV), and the overall level density is also reasonable (18 out of the total of 23 positive parity, fully identified states, with excitation energy lower than 5 MeV, are obtained). Therefore we expect that the average properties of the relevant states within the Gamow window, such as typical single-particle occupation numbers and spectroscopic factors, can be used as representative quantities for reliable estimates of the reaction rates.

With the shell model wave functions we find the spectroscopic factors  $S_p(jl)$  for the proton capture from the continuum state (jl) by the ground state  $J^{\pi} = 7/2^{-}, T = T_3 = 1/2$ of <sup>45</sup>V with the excitation of the state  $|JT\rangle$  in <sup>46</sup>Cr as the triple-barred reduced matrix element

$$S_p(jl) = \frac{1}{\sqrt{(2J+1)(2T+1)}} \langle JT || |a_{jl}^{\dagger} || |^{45} \mathbf{V}_{g.s.} \rangle.$$
(12)

The reduced widths for given final states can be written, after averaging over the proton spin, as

$$\theta_p^2(l) = \frac{1}{3} \sum_j \left[ S_p(jl) \right]^2 \equiv \frac{1}{3} \ \overline{\theta}_p^2(l).$$
(13)

We need the spectroscopic factors and the reduced widths of the individual states for the proton orbital momenta l=1and l=3. The resulting states of positive parity give rise to dipole radiation to final states of negative parity or to *E*2 and *M*1 gamma transitions to the lower-lying positive parity states. In Table II we show the calculated reduced widths for the shell model states at energies close to those selected for Table I. The reduced widths for l=3 are smaller than for l= 1; the difference can reach two orders of magnitude. The column  $\Gamma_W$  shows the radiation widths for those states in the Gamow window that can decay by a dipole radiative transition to the analog of the lowest negative parity



FIG. 3. Reaction rate as a function of temperature; the solid curve, denoted as  $\Gamma_{\gamma}$ , corresponds to the width of *E*1 transitions under assumption of  $10^{-3}$  W.u. for the *B*(*E*1) reduced transition probability, and the dashed curve shows the results of the NON-SMOKER statistical calculation.

 $3^{-}(3059)$  keV and  $4^{-}(3441)$  keV states in <sup>46</sup>Ti. The dipole transitions to the 3<sup>-</sup> state are estimated assuming the reduced transition probability equal to a Weisskopf unit,  $B(E1) = 0.064 A^{2/3} e^2 \text{ fm}^2$ . Individual states differ by the gamma-ray energy and we show the radiation width in MeV,  $\Gamma_W(E1) = 6.75 \times 10^{-8} E_{\gamma}^3$  (MeV). The resulting widths range from  $\sim 10^{-4}$  to  $10^{-5}$  MeV. It is well known that the low-lying dipole transitions are considerably overestimated by Weisskopf units. According to the known systematics [48], in the region beyond  $^{40}$ Ca the hindrance factor for the isospin allowed dipole transitions is  $10^{-4} - 10^{-6}$ . (It is interesting to notice that the isospin forbidden dipole transitions in N=Z nuclei as is <sup>44</sup>Ti manifest in average the same hindrance factor.) For the measured gamma transitions from the negative parity levels in <sup>46</sup>Ti, the lifetimes vary from 0.05 ps to 60 ps, which corresponds to the radiation widths from  $10^{-8}$  MeV to  $10^{-11}$  MeV, in agreement with the above systematics. Preliminary shell model results in the sdpf model space are also consistent with this analysis.

The column labeled  $\Gamma_{+\rightarrow+}$  in Table II shows the summed widths of all transitions allowed by angular momentum and parity from a given individual positive parity entrance state to all positive parity states below excitation energy of 5 MeV. These widths were calculated with the full shell model wave functions of initial and final states. The resulting total widths vary from  $10^{-8}$  MeV to  $5 \times 10^{-7}$  MeV. Figure 2 shows the incoherent sum of possible contributions to the astrophysical *S* factor from the ten resonances in <sup>46</sup>Cr corresponding to the states in <sup>46</sup>Ti indicated in Table II. Assuming for the dipole transitions the summed radiation width  $\Gamma_{\gamma} = 10^{-3}\Gamma_{W}$  and using the expressions (6) and (8) for the reaction rate we come to the temperature dependence shown in Fig. 3. The general behavior of the temperature curve is similar to that obtained in a NON-SMOKER statistical calculation. The magnitude of the resulting rate is slightly lower; the difference grows with temperature reaching one order of magnitude at  $T_9=3.5$ . The missing negative parity states, whose density is smaller than that of positive parity states only by a factor of 2, can contribute to an additional increase of the total reaction rate, but not by a factor that is expected to be large. Thus, the first attempt of the shell model analysis confirms the indications of the simpler approach used in the previous parts of this paper.

The shell model results are sensitive to the details of nuclear structure through gamma strengths and proton spectroscopic factors. The inclusion in the analysis of individual negative parity states is an important problem of the nuclear shell model to be considered in the near future.

# **IV. CONCLUSIONS**

The estimates and calculations presented above show that the  ${}^{45}V(p, \gamma)$  reaction rate, the uncertainty of which has recently been recognized by The et al. [17], as being important in the predictions of <sup>44</sup>Ti nucleosynthesis in core-collapse supernovae, is unlikely to be more than an order of magnitude away from the predictions of the statistical model code NON-SMOKER. However, it cannot be excluded that one or more isobaric analogs to states in <sup>46</sup>Ti may contribute significantly to this reaction rate. The first shell model analysis performed here does not show any states that would lead to a striking enhancement of the reaction rate. Of course, additional experiments to identify potential important states in <sup>46</sup>Cr, measure their spins and parities, and determine relevant spectroscopic information would be useful. Such experiments necessitate radioactive beam facilities. However, they will be extremely difficult to perform with the current generation thereof. The next problem from the theoretical side is the extension of calculations in this region of the nuclear chart in order to include the cross-shell excitation and levels of negative parity.

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