Shell-model studies of the *rp* reaction ^{35}Ar(p,γ)^{36}K

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We present results for levels in ^{36}K (the mirror of nucleus ^{36}Ar) that are used in *rp* reaction rate calculations. The levels are also determined from the isobaric mass multiplet equation and the binding energies of the $T = 1$ analog states as a check on the assignment of spins and parity. Where the analog states are not known, the levels are calculated with two-body interactions that use the *sd*-shell interactions USDA and USDB as the charge-independent parts, with a Coulomb, charge-dependent, and charge-asymmetric Hamiltonian added. The γ-decay lifetimes and ^{35}Al to ^{36}K spectroscopic factors are calculated with the same interactions, and together with experimental information on the levels of excited states, are used to determine the ^{35}Ar(p, γ)^{36}K reaction rates.

I. INTRODUCTION

It has been known that explosive hydrogen burning is not restricted to proton-induced reactions on light target nuclei with masses $A < 20$. If stellar temperatures are sufficiently high or a substantial number of heavier seed nuclei with masses A $\geqslant$ 20 exist before the explosion, proton capture reactions on a variety of heavier target nuclei are bound to occur. In the case of the reaction of interest ^{35}Ar(p, γ)^{36}K, the Q value (1.658 MeV) is relatively low, and the density of states corresponding to (p, γ) resonances is too low to employ statistical methods in estimating the total reaction rates. Thus the contribution of individual levels has to be considered, and detailed information about the level structure is required.

II. PROCEDURE FOR DETERMINING ^{36}K ENERGY LEVELS

There are three different sources for the energies of ^{36}K that are input into the reaction rate calculations: (1) well-established experimental energies, (2) predicted levels based on the isobaric mass multiplet equation (IMME) to calculate the expected energy of levels in ^{36}K by using the measured binding energies of the $T = 1$ partners and a theoretical value of the c coefficient of the IMME [1] (3) level energies calculated with the *sd*-shell interactions USDA and USDB.

The method used for source (2) is explained in Ref. [2]. According to the IMME,

$$B = a + bT_z + cT_z^2, \qquad (1)$$

where B is the binding energy of a state. For the three $T = 1$ isobaric states in $A = 36$ one can then, with $T_z = (N - Z)/2$, substitute $T_z = 1, 0, -1$ alternately, and by rearranging obtain

$$B_p = 2B_o - B_n + 2c \qquad (2)$$

for the proton-rich member (^{36}K), where c can be expressed as

$$c = (B_n + B_p - 2B_o)/2. \qquad (3)$$

For the calculation of the b and c coefficients of the IMME, we use the USDA and USDB Hamiltonians [3] for the charge-independent parts and add the Coulomb, charge-dependent, and charge-asymmetric nuclear Hamiltonian obtained by Ormand and Brown for the *sd* shell [1]. These composite interactions are called usda-cdpn and usdb-cdpn in the NUSHELLX code [4]. The cd refers to "charge-dependent," and pn is used because the calculations are done in the pn formalism. For the nuclei considered in Ref. [1], $A = 18$–22 and $A = 34$–39, the 42 b coefficients were reproduced with an rms deviation of 27 keV and the 26 c coefficients were reproduced with an rms deviation of 9 keV. There is considerable state dependence in the c coefficients (ranging in values from 130 to 350 keV), which is nicely reproduced by the calculations (see Fig. 9 in Ref. [1]).

In Fig. 1, values of c from experiment and theory are compared for states in ^{36}K ordered according to increasing experimental energy. The experimental values are obtained for states where all three members of the multiplet are known. In general a good correspondence can be seen, the largest deviations being less than 30 keV. There is considerable state dependence with c values from experiment ranging from 127 to 235 keV. This IMME method was used in Ref. [5] for the $T = 1$ states of the odd-odd nuclei with masses 28, 32, and 36 and in Ref. [2] for ^{26}Si.

Where data are not available in ^{36}K to determine the c coefficient from experiment, a fairly reliable value can be obtained from a theoretical calculation using Eq. (3). The binding energies for states in ^{36}K can be then be obtained from Eq. (2), with experimental values of binding energy for corresponding states in ^{36}Cl and ^{36}Ar (when they are known in both). Specifically

$$B_{th}(^{36}K) = 2B(^{36}Ar) - B(^{36}Cl) + 2c_{th}. \qquad (4)$$

This is a better procedure than assigning states of the final nucleus with uncertainties by basing the assignments on the correspondences with levels in the mirror nucleus. In addition
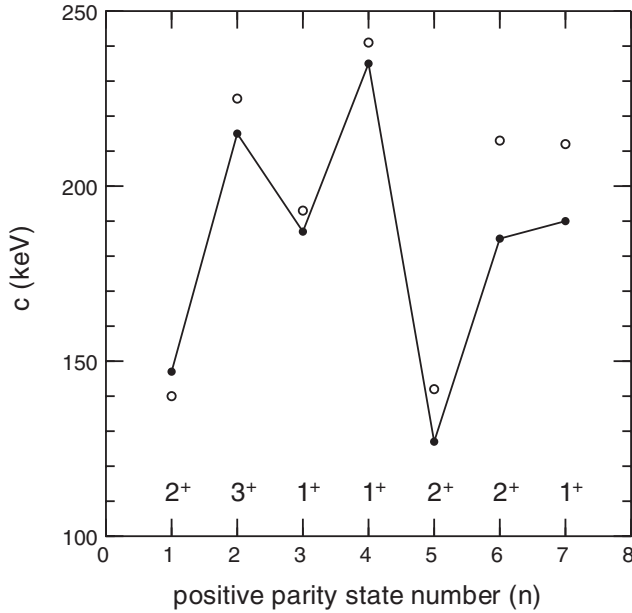
FIG. 1. c coefficients from the IMME ($B = a + bT_z + cT_z^2$) vs state number (in order of increasing energy) in ^{36}K based on experimental energies from Ref. [6] (closed circles) and energies calculated from usdb-cdpn (open circles).

where no levels are known, levels can be predicted provided the analog partners are known.

Figure 2 shows the experimental excitation energies of the $T = 1$ analog states for $A = 36$, where those of ^{36}Ar are relative to the lowest 2^+ $T = 1$ state at 6.611 MeV. A number of levels of ^{36}K recently measured by Wrede *et al.* [7] above the proton separation are included, and all other excitation energies are from Ref. [6]. Three predicted levels with no known experimental counterparts are indicated by crosses.

The third 2^+ state warrants some discussion. In Ref. [7] the assignment of the 2_3^+ state to a level at 2.410 MeV [5] was changed to a level at 2.282 MeV (Table VI in Ref. [7]) that had been observed in their experiment. However, it was assumed that the c coefficients for excited states are the same as those of the lowest $T = 1$ states. Taking into account the variations in the c coefficients seen in Fig. 1, our predicted energy via the IMME method is 2.479 MeV. Equation (4) can be cast in the form of excitation energies relative to the lowest $T = 1$ states:

$$B_p^* = 2B_o^* - B_n^* + 2[c - c(\text{lowest } T = 1)], \qquad (5)$$

From Table VI of Ref. [7] one then obtains a calculated energy of 2.186 MeV for the 3^- state and 2.336 MeV for the 2_3^+ state of ^{36}K if one sets $c - c(\text{lowest } T = 1) = 0$. These values are close to the measured values of the last two states in Table VI (2.197 and 2.282 MeV, respectively). However, if one more correctly calculates the c-coefficient terms in Eq. (4) from Eq. (3) (in this case from usdb-cdpn) for the 2_3^+ state, then $2[c - c(\text{lowest } T = 1)] = 146$ keV, and the predicted energy is 2.482 MeV. This agrees better with the original energy of 2.410 MeV of Ref. [6] and also the measured energy of 2.446 MeV in Table III of Ref. [7], as shown in Fig. 2. Thus we associate the 2_3^+ state with the level observed at 2.446 MeV. The two lower states at 2.197 and 2.282 MeV we assign to the
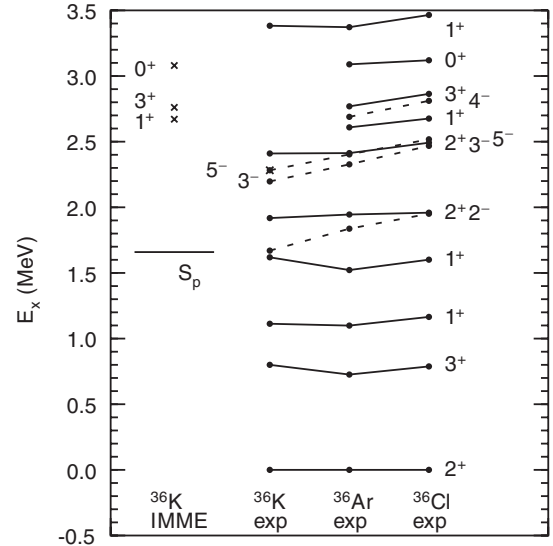

FIG. 2. Experimental energies of the isobaric $T = 1$ triplets for $A = 36$. The energies of ^{36}Ar are relative to the lowest 2^+ $T = 1$ state at 6.611 MeV. Negative parity states are connected by dashed lines. The solid lines connect positive parity states considered to be analogs on the basis of our IMME predictions. The proton separation energy in ^{36}K is shown by the horizontal line on the left-hand side. The data are from Endt [6] except for those above the proton separation energy in ^{36}K for which we use the newer values from Wrede *et al.* [7]. The cross on the 2.282 MeV 5^- state in ^{36}K indicates what this level was associated with the 2_3^+ state by Wrede *et al.* Our reasons for associating the 2_3^+ level with the higher state at the 2.446 MeV state are discussed in the text. The levels labeled ^{36}K IMME are based on Eq. (4) with experimental binding energies of ^{36}Cl and ^{36}Ar and with the theoretical c coefficient [Eq. (3)]. The crosses correspond to predicted energies without experimental counterparts.

negative parity states 3^- and 5^-, respectively. In Ref. [7] a state was also observed at 3.383 MeV, and although it was not assigned a spin-parity, they associated it in Table VI with the 3.360 level of Ref. [6], where it was given a 1^+ assignment. Our IMME method also predicts a level at 3.417 MeV. Thus we associate the observed 3.383 MeV level with the 1_4^+ state.

The important states used in the calculation of the rp reaction rate are given in Table I. When experimental energies are not available, the energies calculated with usdb-cdpn are used in the input.

A. Contribution of negative parity states

When measurements for negative parity states are not available, one could in principle estimate their effect from a theoretical calculation. However, this is often not practical because of the increase in size of the model space required. An alternative would be to use experimental values of the mirror nucleus.

B. Using data from the mirror nucleus

When properties of levels in the final nucleus are uncertain, the crucial parameters of the reaction rate calculations, viz.,

TABLE I. Properties of states in ^{36}K. For negative parity states, experimental values for the mirror nucleus from Ref. [6] are given. Spectroscopic factors are given for $\ell = 0$ and 2 for positive parity states and $\ell = 1$ and 3 are for negative parity states. The spectroscopic factors and decay widths for positive parity states are from usdb-cdpn calculations.

n	J^π	k	E_x(usdb-cdpn) (MeV)	E_x(expt) (MeV)	E_{res} (MeV)	C^2S $\ell = 0$	C^2S $\ell = 2$	Γ_γ (eV)	Γ_p (eV)	$\omega\gamma$ (eV)
1	2^+	1	0.000	0.000		1.1×10^{-2}	7.9×10^{-1}	0	0	0
2	3^+	1	0.854	0.800		0	2.0×10^{-1}	9.3×10^{-5}	0	0
3	1^+	1	1.080	1.113		8.3×10^{-2}	2.1×10^{-1}	9.8×10^{-5}	0	0
4	1^+	2	1.749	1.619		1.6×10^{-2}	2.8×10^{-2}	1.4×10^{-3}	0	0
5	2^+	2	2.013	1.890	0.232	5.2×10^{-2}	1.3×10^{-2}	9.5×10^{-3}	6.9×10^{-7}	4.3×10^{-7}
6	3^-	1		2.197	0.539	1.3×10^{-1}	6.5×10^{-1}	4.7×10^{-4}	1.2×10^{-1}	4.1×10^{-4}
7	5^-	1		2.282	0.624	0	9.3×10^{-1}	7.5×10^{-7}	1.7×10^{-2}	1.0×10^{-6}
8	2^+	3	2.474	2.446	0.788	3.5×10^{-2}	1.6×10^{-2}	2.5×10^{-2}	6.2	1.5×10^{-2}
9	1^+	3	2.571	2.671	1.013	9.6×10^{-3}	1.2×10^{-2}	8.1×10^{-3}	1.5×10^{1}	3.0×10^{-3}
10	3^+	2	3.055	2.761	1.103	0	5.0×10^{-2}	1.1×10^{-1}	3.3	9.1×10^{-2}
11	0^+	1	3.183	3.080	1.422	0	3.9×10^{-3}	2.8×10^{-2}	2.0	3.5×10^{-3}
12	1^+	4	3.397	3.360	1.702	5.3×10^{-3}	1.9×10^{-4}	1.4×10^{-2}	2.8×10^{2}	5.2×10^{-3}
13	4^+	1	3.683		2.025	0	6.5×10^{-4}	9.0×10^{-3}	3.8	1.0×10^{-2}
14	0^+	2	4.435		2.777	0	1.6×10^{-4}	6.7×10^{-2}	5.9	8.3×10^{-3}
15	3^+	3	4.570		2.912	0	8.8×10^{-3}	1.7×10^{-1}	4.1×10^{2}	1.5×10^{-1}
16	2^+	4	4.593		2.935	5.3×10^{-3}	4.8×10^{-3}	3.0×10^{-1}	3.6×10^{3}	1.8×10^{-1}

single-nucleon spectroscopic factors connecting the target and final states, and the lifetimes of the states in the final nucleus are frequently used and can be justified on the basis of isospin symmetry. The calculated and experimental (d, p) spectroscopic factors for the reaction ^{35}Cl$(d, p)^{36}$Cl to the lower levels of ^{36}Cl to states in ^{36}Cl are given in Table II, and the theoretical and experimental lifetimes of states in ^{36}Cl are given in Table III. The theoretical values are based on usda-cdpn and usdb-cdpn. Optimal g factors and effective charges for the γ-decay calculations are used that were determined from least-squares fits to 48 magnetic moments, 26 quadrupole moments, 111 $M1$ transitions and 144 $E2$ transitions [9] for USDA and USDB separately.

The general agreement between theory and experiment in Table II is quite reasonable, particularly for the stronger

transitions. For the lifetimes in Table III the agreement is also fairly good on the whole. The fact that the interactions usda-cdpn and usdb-cdpn generally give a good reproduction for the mirror nucleus of the crucial parameters in a rate calculation, namely, energy levels, single-nucleon spectroscopic factors, and lifetimes, suggests that the results for ^{36}K should be of similar quality. This lends credibility to using calculated values for these parameters in ^{36}K when the experimental values are not available.

In view of the correspondence between mirror states for $A = 36$ it would be reasonable to substitute an experimental value from the mirror nucleus in a case where a calculation is not feasible, as for the 3^- state at 2.468 MeV. In this way the contribution from this level, which lies close to some of the most important resonances, can be taken into account approximately.

TABLE II. Spectroscopic factors for ^{35}Cl$(d, p)^{36}$Cl from Ref. [10]. * refers to negative parity. The convention for the state number n follows that for ^{36}K given in Table I.

n	J^π	k	E_x uscb-cdpn (MeV)	E_x expt (MeV)	C^2S usda-cdpn $\ell = 0(1^*)$	C^2S usdb-cdpn $\ell = 0(1^*)$	C^2S expt $\ell = 0(1^*)$	C^2S usda-cdpn $\ell = 2(3^*)$	C^2S usdb-cdpn $\ell = 2(3^*)$	C^2S expt $\ell = 2(3^*)$
1	2^+	1	0.000	0.000	0.010	0.011	0.038	0.73	0.78	1.18
2	3^+	1	0.850	0.788				0.18	0.19	0.32
3	1^+	1	1.105	1.165	0.096	0.085	0.11	0.21	0.21	0.31
4	1^+	2	1.808	1.601	0.017	0.014	0.073	0.024	0.021	
5	2^+	2	2.061	1.959	0.072	0.061	0.028	0.078	0.015	
6	3^-	1		2.468			0.129			0.654
8	2^+	3	2.513	2.492	0.026	0.028	0.024	0.013	0.013	0.060
7	5^-	1		2.518						0.925
9	1^+	3	2.583	2.676	0.0011	0.0010	0.012	0.010	0.013	
10	3^+	2	3.062	2.864				0.064	0.050	0.136

TABLE III. Lifetimes for ^{36}Cl levels from Ref. [6] compared to the theoretical results. The convention for the state number n follows that for ^{36}K given in Table I.

n	J^π	k	E_x(usdb-cdpn) (MeV)	E_x(expt) (MeV)	$T_{1/2}$(usda-cdpn) (ps)	$T_{1/2}$(usdb-cdpn) (ps)	$T_{1/2}$(expt) (ps)
2	3^+	1	0.850	0.788	12.5	6.6	13.8(12)
3	1^+	1	1.105	1.165	11.8	6.5	6.4(4)
4	1^+	2	1.808	1.601	0.089	0.33	0.65(4)
5	2^+	2	2.061	1.959	0.031	0.037	0.044(2)
6	3^-	1		2.468			0.97(10)
7	2^+	3	2.513	2.492	0.020	0.025	0.042(10)
8	5^-	1		2.51			1610(80)
9	1^+	3	2.583	2.676	0.036	0.036	0.021(4)
10	3^+	2	3.062	2.864	0.0061	0.0064	0.015(1)

III. RESULTS FOR THE REACTION RATE

The resonant reaction rate for capture on a nucleus in an initial state i, $N_A\langle\sigma v\rangle_{\mathrm{res}\,i}$, for isolated narrow resonances is calculated as a sum over all relevant compound nucleus states f above the proton threshold [11], i.e.,

$$N_A\langle\sigma v\rangle_{\mathrm{res}\,i} = 1.540 \times 10^{11}(\mu T_9)^{-3/2}$$
$$\times \sum_f \omega\gamma_{if}\, e^{-E_{\mathrm{res}}/(kT)} \quad \mathrm{cm}^3\,\mathrm{s}^{-1}\,\mathrm{mole}^{-1}. \quad (6)$$

Here T_9 is the temperature in gigaK, $E_{\mathrm{res}} = E_f - E_i$ is the resonance energy in the center-of-mass system, the resonance strengths in MeV for proton capture are

$$\omega\gamma_{if} = \frac{(2J_f + 1)}{(2J_p + 1)(2J_i + 1)} \frac{\Gamma_{p\,if}\Gamma_{\gamma f}}{\Gamma_{\mathrm{total}\,f}}. \quad (7)$$

The $\Gamma_{\mathrm{total}\,f} = \Gamma_{p\,if} + \Gamma_{\gamma f}$ is a total width of the resonance level, and J_i, J_p, and J_f are target (^{35}Ar), the proton projectile ($J_p = 1/2$), and states in the final nucleus (^{36}K),

respectively. The proton decay width depends exponentially on the resonance energy via the single-particle proton width and can be calculated from the proton spectroscopic factor $C^2 S_{if}$ and the single-particle proton width $\Gamma_{sp\,if}$ as $\Gamma_{p\,if} = C^2 S_{if}\Gamma_{sp\,if}$. The single-particle proton widths were calculated from [12]

$$\Gamma_{sp} = 2\gamma^2 P(\ell, R_c), \quad (8)$$

with $\gamma^2 = \frac{\hbar^2 c^2}{2\mu R_c^2}$ and where the ℓ-dependent channel radius R_c was chosen to match the widths obtained from an exact evaluation of the proton scattering cross section from a Woods-Saxon potential well for ^{25}Al for $Q = 0.1$–0.4 MeV. The simpler model of Eq. (8) matches the results obtained from the scattering cross sections as well as those used in Ref. [13] to within about 10%. We use a Coulomb penetration code from Barker [14].

The total rp reaction rates have been calculated for each of the interactions usd-cdpn, usda-cdpn, and usdb-cdpn. The
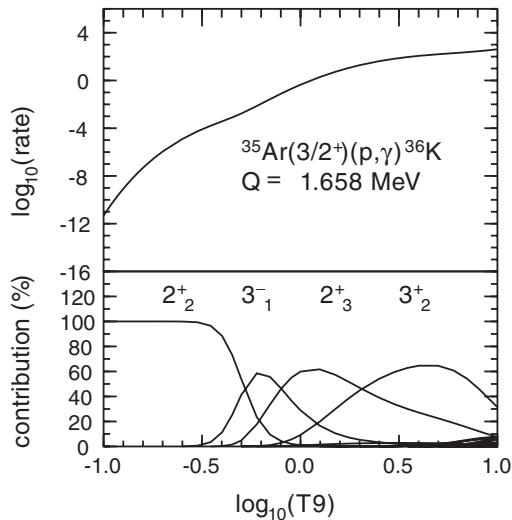

FIG. 3. Total rp reaction rate vs temperature $T9$ (gigaK) (top panel) and the contribution of each of the final states (lower panel) with usdb-cdpn. Γ_γ was calculated for ^{36}K levels.
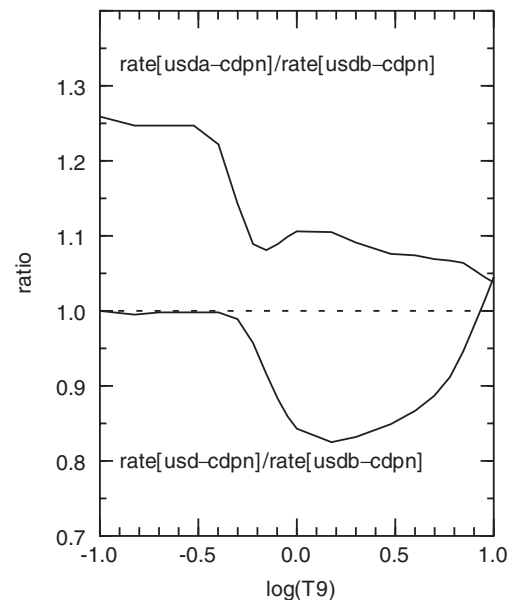

FIG. 4. Total rp reaction rates of usda-cdpn and usd-cdpn vs usdb-cdpn compared.
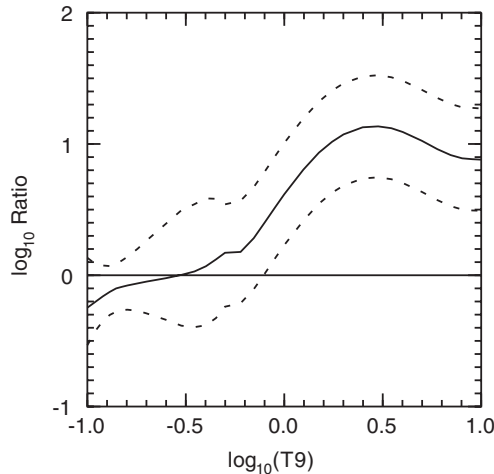
FIG. 5. The usdb-cdpn present rate divided by the rate given in the 2010 evaluation (Table B.58 of Ref. [8]); solid line for the median rate and the dashed lines for the low and high rates.

Q values required were based on measured energies in ^{36}K; and where they were not known, values calculated from Eq. (4) were used. Figure 3 shows the results for the resonance-capture rate obtained using the properties of ^{36}K given in Table I. The Γ_p and Γ_γ in this case are all based on the usdb-cdpn Hamiltonian.

IV. UNCERTAINTIES IN THE RESONANT-CAPTURE REACTION RATES

A detailed analysis of error sources in the rate calculations has been given in Ref. [2]. A general indication of the variation caused by the use of different interactions can be obtained by comparing the corresponding reaction rates. As an example this is shown in Fig. 4 for the reaction ^{35}Ar$(p, \gamma)^{36}$K.

The usdb-cdpn present rate divided by the rate given in the 2010 evaluation (Table B.58 of Ref. [8]) is shown in Fig. 5. The data used for Γ_γ and Γ_p in the 2010 evaluation are the same as those in Ref. [5]. Below about $\log_{10}(T9) = -0.2$, the two rates are in agreement. But near $\log_{10}(T9) = 0.5$, the present rate is a factor of 10 larger than the 2010 evaluation. This increase comes from the 2_3^+ and 3_2^+ states (see the bottom panel in Fig. 3). For these two states, $\Gamma_\gamma \ll \Gamma_p$ and their contribution to the rate is proportional to Γ_γ. For 2_3^+ the 2010 evaluation uses the experimental value in ^{36}Cl whereas we use the theoretical value of $T_{1/2} = 0.019$ ps for ^{36}K. From the $T_{1/2}$ values given in Table III we find $[\Gamma_\gamma(\text{usdb-cdpn})/\Gamma_\gamma(\text{expt})](2_3^+) = 2.3(5)$, which gives an increase in our rate compared to the 2010 evaluation.

The 2010 evaluation does not include the 3_2^+, but as we see from the bottom of Fig. 3, this state dominates the

rate near $\log_{10}(T9) = 0.7$. From Tables I and III we find $[\Gamma_\gamma(\text{usdb-cdpn})/\Gamma_\gamma(\text{expt})](3_2^+) = 3.5(2)$, so if we were to use the experimental value from ^{36}Cl the rate near $\log_{10}(T9) = 0.7$ would be decreased by a factor of 3.5. We note in Table 36e of the Endt compilation [6], that there is an inconsistency between measurements for the 2.864 MeV 3_2^+ level, with one experiment giving $T_{1/2} < 0.010$ ps and another experiment giving $T_{1/2} = 0.015(1)$ ps. If the ^{35}Ar$(p, \gamma)^{36}$K rate in the region of $\log_{10}(T9) = 0.5$ turns out to be important for an astrophysical process, the γ decay rates for the 2.492 MeV 2_3^+ and 2.864 MeV 2_3^+ states in ^{36}Cl should be experimentally confirmed.

V. CONCLUSIONS

Because the calculation of the *rp* reaction rate for the ^{35}Ar$(p, \gamma)^{36}$K requires a knowledge of the energy levels in ^{36}K, and some levels are uncertain, we have adopted the method of Ref. [5] for determining levels, which is partly based on experiment and partly on theory. For the experimental part we used well-known binding energies of the $T = 1$ analog states of ^{36}K. For the theoretical part we used calculated c coefficients of the isobaric mass multiplet equation. We have demonstrated that a good correspondence between theoretical and experimental values of the c coefficient for sd-shell nuclei exists. The method leads to a reliable prediction of energy levels in ^{36}K. Where experimental energies were not available, we used energy values in ^{36}K constrained by our method for the Q values of the proton capture process on ^{35}Ar. The required spectroscopic factors and γ-decay lifetimes for rate calculations were obtained from shell-model calculations using the new sd-shell interactions USDA and USDB for the charge-independent parts of the interactions.

Because some negative parity states occur in the region close to the threshold energy, their contributions to the reaction rate were estimated by using spectroscopic factors and lifetimes of their mirror counterparts in ^{36}Cl. It was found that the 3^- state at 2.197 MeV (our assigned energy) contributed significantly to the *rp* reaction rate. We also furthered arguments for changing the assignment made in Ref. [7] for the 2_3^+ state to an energy of 2.446 MeV, measured in Ref. [7], and in consequence thereof, made assignments of the 3^- and 5^- states just above the threshold to 2.197 and 2.282 MeV, respectively.

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