Determination of the important ^{30}P(p,γ)^{31}S astrophysical rapid-proton capture reaction rate

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Abstract

The thermonuclear rate of the reaction ^{30}P(p,γ)^{31}S is of major importance for the interpretation of nova nucleosynthesis in the $A \geq 30$ region. Estimates based on shell-model calculations are hampered by the presence of several negative parity states in the resonance region near the proton-emission threshold. We present results of calculations in a full $(0+1)\hbar\omega$ model space which address this problem. Extensive comparisons are also made with recent experimental data for levels of ^{31}S, and it is shown that there are inconsistencies and ambiguities in the data which prevent a one-to-one correspondence with theory. The gamma-decay lifetimes and ^{30}P to ^{31}S spectroscopic factors are calculated for input into the reaction rate equations. Available experimental data is used in conjunction with the calculations to obtain a best estimate for the reaction rate.

1. Introduction

The importance of the ^{30}P(p,γ)^{31}S reaction rate for astrophysics has been extensively discussed [1]. It is, however, not well determined due to uncertainties in the properties of key resonances in the burning region. This lack of knowledge of the thermonuclear reaction rate inhibits the interpretation of observables associated with the underlying astrophysics. The uncertainties in the reaction rate stem from unmeasured quantities, ambiguities in level properties measured in different experiments, and problems with theoretical calculations stemming mainly from the presence of several negative parity states near the threshold energy.

2. Experiments to determine the reaction rate

The halflives for the target (^{30}P) and residual nucleus (^{31}S) are respectively about 2.5 minutes and 2.55 seconds. Thus direct reaction experiments are not currently feasible, so one has to resort to using beta decay, stable targets and nucleon transfer and charge exchange reactions, or alternatively inverse kinematics experiments. A brief summary of reactions used in recent major experiments follow. The dates given with each experiment refer to the date of the first publication or report, and not when the experiment was carried out.

^{32}S(d,t)^{31}S (Irvine et al., 2013) This reaction was used at the Maier-Leibnitz Laboratory (MLL) in Munich to study states in ^{31}S in the energy range 6.3 - 7.1 MeV. [2].

^{32}S(p,d)^{31}S (Ma et al., 2007) In a variation of the above reaction, the (p,d) reaction was utilised at the ORNL-HRIBF to study 26 states in ^{31}S, of which 17 were above the proton-emission threshold [3]. A similar experiment was done at the Yale Wright Nuclear Structure Laboratory (WNSL) by Setoodehnia et al. (2014) [4].

^{31}P(^{3}He,t)^{31}S was employed by Wrede et al. (2007) [5] at the Yale-WNSL and by Parikh et al. [6] at the MLL, Munich (2011) in their studies of ^{31}S states. In a more extensive analysis of the first experiment [7] a total of 17 new levels, and 5 tentative new levels were determined, and 5 tentatively known levels were confirmed. The experimental information was supplemented by data from ^{32}S(d,t)^{31}S measurements. Parikh et al. [6] observed states in the energy region 6.1 - 7.1 MeV.

^{28}Si(α,nγ)^{31}S The fusion-evaporation reaction was employed by Doherty et al. (2014) [8], [8] with the Gammasphere detector array at Argonne National Laboratory using the ATLAS accelerator.

^{12}C(^{20}Ne,nγ)^{31}S (Jenkins et al., 2005 [9],[10]). Excited states in ^{31}S and ^{31}P were populated in the ^{12}C(^{20}Ne,n) and ^{12}C(^{20}Ne,p) reactions, respectively, at a beam energy of 32 MeV, using the ATLAS accelerator at the Argonne National Laboratory. Their resulting γ decay was detected with the Gammasphere array in coincidence with ^{31}S residues at the focal plane of the Fragment Mass Analyzer.

^{30}P(d,nγ)^{31}S (Kankainen, 2013 [11]) This transfer reaction was studied in inverse kinematics at the NSCL, East Lansing to study key astrophysical resonances in ^{31}S. The ^{31}S ions were analyzed by the S800 spectrometer and identified by energy loss and time-of-flight measurements. γ rays from the decays of excited states in ^{31}S were detected in coincidence with the recoiling ^{31}S ions using GRETINA.

^{31}Cl(β,γ) An alternative approach is to populate $l = 0$ resonances with ^{31}Cl decay. This was done in an experiment in February and March, 2014 at the NSCL, East Lansing (Bennett et al.) [12]. Fast beams of ^{31}Cl were produced using projectile fragmentation of a ^{36}Ar beam on ^{9}Be. Gammas were detected with the Yale Clovershare array of HPGe detectors.

^{31}Cl(β,p) and ^{31}Cl(β,γ) (Saastamoinen, PhD Thesis, 2011, Dept. of Physics, University of Jyväskylä,). The experiments detecting both protons and gammas from excited states in ^{31}S were carried out at Texas A&M University. In an earlier similar experiment at IGISOL (Kankainen et al., 2006 [13]) ^{31}Cl nuclei were produced via ^{32}S(p,2n) fusion-evaporation reactions induced by a 40 MeV or 45 MeV proton beam on a ZnS target. The beta decay of ^{31}Cl was studied with a silicon detector array and a HPGe detector.

Comparisons of results from these experiments with theory are made in a later section.

3. Theoretical calculation of the reaction rate

The theory for positive parity states is based on the USDB-cdpn Hamiltonian as used in our previous (p,γ) rate calculations for positive parity final states in the *sd*-shell [14], [15], [16]. At the high excitation energies considered here, many negative parity states start to appear. We consider for the first time a microscopic model for these states. The basis consists of a complete $1\hbar\omega$ basis made from all possible excitations of one nucleon from $0p$ to $1s-0d$ or the excitation of one nucleon from $1s-0d$ to $0p-1f$. The M-scheme dimension in this basis is on the order of two million and they are calculated with NuShellX in a proton-neutron basis [17]. We use the WBP Hamiltonian from [18] that was designed to reproduce the energies of $1\hbar\omega$ states for $A = 10-20$. WBP also contains the $sd-pf$ Hamiltonian from [19] that was designed to reproduce energies of $1\hbar\omega$ states in nuclei with $A = 35-43$. WBP has not before been applied to the middle of the sd shell due to the large dimensions involved. The single-particle energies for the $0p$ and $0p-1f$ orbitals were fixed by energies of low-lying negative parity states in $A = 27$ and $A = 29$.

Table 1: Properties of levels in ^{31}S between 5.9 and 7 MeV. See text for details.

n		Experiment						Theory						
	E_{res} (keV)	E_x (keV)	$(2J)\pi$	$(2J)\pi$	$(2J)\pi$	$(2J)\pi$	$(2J)\pi$	$(2J)\pi k$	E_x (keV)	$(2J)\pi k$	E_x (keV)	ℓ	C^{2}S	
		NDS 2013 [20]	NDS 2013 [20]	Wrede 2014 [1]	Doherty et al. 2012 [8]	Parikh et al. 2011 [6]	Jenkins et al. 2006 [9]	USDB-cdpn		$1\hbar\omega$				
1		5896	3+,5+					3+6(t)	5965			0	0.018	
2		5959	3+,5+	*				5+7(t)	6044			2	0.042	
3		5978	(9+)					9+3(g)	5829			2	0.023	
4	8	6139	(7+)	b	(3,7)+	9		3+7(t)	6141			0	0.013	
5	29	6160	(5−,7+)	b	7[+]	5	[5−]			5−2(t)	5825			
6	124	6255	1+	1+	[1+]	1+	[1+]	1+5(g)	6259			0	0.0017	*p*1
7	149	6280	3+	3+	[3+]	3+	[3+]	3+8(g)	6280			0	0.00024	*p*2
8	196	6327	(3)	b	3[−]	1+				3−2	6327	1	0.29	
9	226	6357	(5−)	b	5[−]	3+	[(5+)]							
10	246	6377	(9−)	(9)	(5,9) [9−]	[9−]	[9−]			9−1(g)	6313	3	0.39	
11	261	6392	(5+)	a,(5+)	5+			5+8	6402			2	0.061	*p*3
12	263	6394	(11+)	a,(11)	11[+]	[11+]	[11+]	11+1(g)	6364					
13	270	6401		a,c	[7(−)]			7+6(t)	6298			2	0.053	
14	289	6421	(1+,3+,5+)	*										
15	411	6542	(3−)	b	3[−]	(7,9)	[(3,5)−]			3−3	6757	1	0.037	
16	451	6583	(7)	(7)	(3,5,7)[−]	7	[7]			5−3	6792	1	0.0043	
17	505	6636	(9−)	(9)	(5,9)[9−]	9[−]	[9−]			9−2(g)	6682	3	0.11	
18	589	6720	(5)			5	[(3,7)]	5+9(t)	6862			2	0.081	*p*4
19	618	6749	3+			3+	[(3,7)]	3+9	6965			0	0.0045	*p*5
20	665	6796		*			[(3,7)]							
21	702	6833	(11−)			11[−]				11−1(g)	6833			
22	705	6836		*										
23	717	6848		*										
24	741	6872	(11)			11	[(3,5)]							
25	806	6937	(1+,3+,5+)			(1-5)+								
26	830	6961				1+		1+6	6995			0	0.0026	
27	844	6975	1+					1+7	7028			0	0.000015	
28										5−2	5825	1	0.067	
29	116									1−2	6247	1	0.23	
30	471									1−3	6602	1	0.068	
31	252									7−3	6838	3	0.0058	
32	712									9−3	6843	3	0.10	
33	760									7−4	6891	3	0.18	
34	765									3−4	6896	1	0.19	
35	790									5−4	6921	1	0.48	
36	767							9+4	6898					
37	848							7+7	6979			2	0.00092	

4. Comparison between experiment and theory

Selected experimental and the theoretical results are shown in Table I and Fig. 1. The first columns 2-8 give the experimental data. Columns 3-4 are the values given in the recent Nuclear Data Sheets (NDS) compilation [20], and the 2nd column is the resonance energy based on the NDS energy. The 5th column gives the spin-parity assignments from the recent review by Wrede [1] that are based purely on the data for ^{31}S and excludes spin-parity assignments based upon assumed correspondence with mirror levels in ^{31}P, that are indicated by the spin-parity inside the square brackets in columns 6-8. The letters (a,b,c) in column 5 correspond to the footnotes given by Wrede. For (a) there is some question of whether there are two or three levels between E_x = 6390 keV and 6405 keV. If one assumes that the two levels seen in Ref [8] are at their reported energies, then one of the two levels reported in Refs. [5], [6] and [2] is different and there would be three levels all together. For (b) there are conflicting spin-parity assignments between Parikh et al. [6] and Doherty et al. [8]. The spin-parity of the 6139 keV state assigned by Doherty et al. [8] is based only on a possible match to a level in ^{31}P and it was changed by Irvine et al. [2]. For (c) the spin-parity is unconstrained. The * indicate levels of questionable existence. The levels at 5959 and 6848 keV that are only seen in a low resolution (p,d) experiment [3] are probably amalgams of neighboring levels. The level at 6421 keV has only been seen a ^{31}Cl beta-decay experiment [13] and not confirmed in a reaction experiment. The level at 6796 keV has only been seen in a low resolution (^{3}He,n) experiment and has not been confirmed. The placement of two nearby levels at 6833 and 6836 keV was inferred from the fact that a significant proton emission was observed at this energy that may not be expected for a level with $J = 11/2$ that would decay by ℓ=5 [1]. Wrede has suggested that increased communication between the relevant experiment groups would facilitate some resolution of the conflicting spin-parity assignment [1], and a workshop was held to this end in 2014; the results will be published in an upcoming Focus Issue of Eur. Phys. J. Plus.

Columns 11-12 give the results obtained with the $1\hbar\omega$ Hamiltonian. The format in the 11th column is $(2J) - k$, where $-$ indicates negative parity and k is the number of the state for a given J. Columns 13-14 give the calculated spectroscopic factors. The labels in the last column indicate the largest contributions for positive parity p. For negative parity see the comments in section 5.

Columns 9-10 give the results obtained with the USDB-cdpn Hamiltonian. The format in the 9th column is $(2J) + k$ where $+$ indicates positive parity and k is the number of the state for a given J. All of the USD-cdpn energies given have been shifted down by 240 keV in order to align theory and experiment for the well established $3/2^+$ T=3/2 level at 6280 keV. This gives energies for other positive parity states in the region of interest within 100 keV of possible associations with experiment as shown in Table I. A similar energy shift is also found for the comparison of theory and experimental levels in ^{31}P, and is about the same with the USDA Hamiltonian. This shift indicates a possible systematic failure of the USD Hamiltonians at high energy. For future work it may be interesting to include some these levels in the determination of the empirical two-body matrix elements [21]. Since the reaction rate is exponentially sensitive to the resonance energy, the association with experimental energies levels is important. Some of the associations in Table I are rather certain (good, g) but others are very tentative (t). All unmarked and t matches need to be confirmed. Unmatched theoretical levels are given at the bottom.

The energies for the $1\hbar\omega$ states in Table I are shifted down by 354 keV in order to align theory and experiment for the well established $11/2^-$ level at 6824 keV. The theoretical levels have been associated with known experimental levels in the Table with the labels good (g) and tentative (t). This association is crucial for a precise calculations of the rates. Thus, the rates we obtain will depend upon a confirmation of the experimental and theoretical associations. The $1\hbar\omega$ states that cannot be matched with experiment are given in the bottom of the Table I. All levels up to 6.8 MeV can be tentatively matched with theory except for the experimental levels at 6160, 6420 and 6796 keV; but the latter two of these are of questionable experimental existence. There are two $1/2^-$ negative-parity states predicted at 6247 and 6602 that cannot be matched to know experimental levels. Above 6.8 MeV the two $1/2^+$ levels at 6961 and 6975 MeV have a good association with theory with the upper of these in theory being the $1/2^+$ T=3/2 level. In addition, between 6.8 and 7.0 MeV there are four unmatched experiment levels and seven theoretical levels, indicating that there are several levels in this region that have not yet been observed.

The experimental information on the states in the mirror nucleus ^{31}P in the 6-8 MeV energy range is not complete enough to help resolve the spin-parity ambiguities in the ^{31}S or to help with the associations between experiment and theory we have made in Table I.

5. Calculation of the reaction rate

Our calculated rates are shown in Fig. 1 based on the resonance energies and spectroscopic factors given in Table I. They are based on the Eqs. used in [16] with the information in Table I together with gamma-decay lifetimes for positive-parity states obtained with the USDB-cdpn Hamiltonian and the effective gamma-decay operator for M1 and E2 from [22]. (Fig. 1 and Table II of Ref. [23] did not include the contribution from the theoretical $3/2^-_2$ state that was associated with the experimental state at 6327 keV in Table I. The corrected versions are given here.) The most important negative parity states are labeled in panel (c). The spectroscopic properties of the $3/2^-_3$ and $1/2^-_2$ states are given in Table III of Ref. [23]. The spectroscopic properties of the $3/2^-_2$ state shown in panel (c) are: Γ_γ = (0.009) eV, $\Gamma_p = 6.7 \times 10^{-6}$

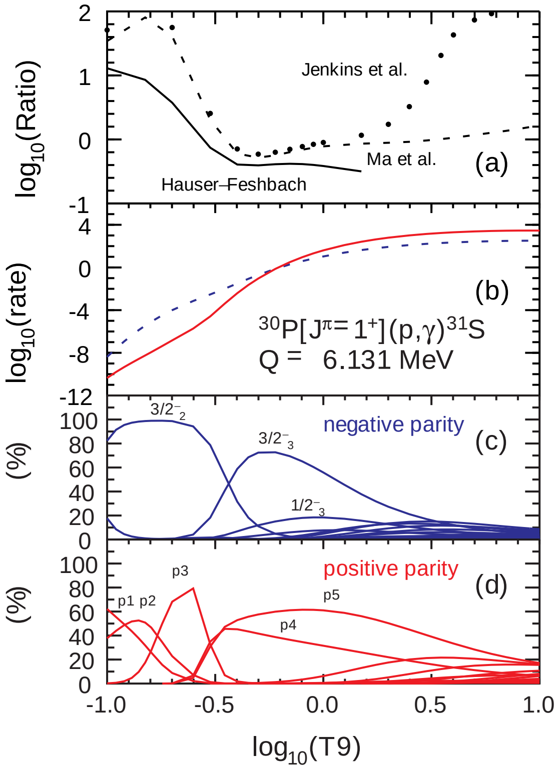

Fig. 1: The total *rp* reaction rate versus temperature T9 (GigaK) (top panel) and the contribution of each of the final states (lower panels) obtained with the data from Table I. The results are separated into the contributions from positive and negative parity states. The total rate is shown separately for the positive parity (red line) and negative parity (blue dashed line) final states. The top panel shows the present rate divided those form other models as discussed in the text.

eV, $\omega\gamma = 4.5 \times 10^{-6}$ eV and $C^2S(\ell{=}1){=}0.29$. The rate in the region near $\log_{10}(T9) = -0.8$ is one to two orders or magnitude larger than those from previous works. This large increase demonstrates the importance of confirming the spin-parity assignments of levels in the excitation energy range of 6.1 to 6.7 MeV in ^{31}S.

The bottom parts of the figure show the contributions from individual final states. The labels for the most important positive-parity contributions in Fig. 1 are given on the right-hand side of Table I. For the hottest ONe novae on white dwarfs close to the Chandrasekhar limit the rate up to T9 = 0.5 [$\log_{10}(T9){=}-0.3$] is important [24]. For most of these $\Gamma_\gamma >> \Gamma_p$ and the gamma lifetime is thus not important. The experimental associations of the $3/2^-_2$, $3/2^-_3$ and $5/2^+_8$ ($p3$) states need to be verified, and the gamma widths of the $3/2^-_2$ and $3/2^-_3$ states need to be measured. The $1/2^-_3$ state has not yet been associated with experiment. The experimental association of the $3/2^+_8$ ($p2$) state enters only because of its calculated small isospin-forbidden proton decay spectroscopic factor - this needs to be verified. Overall, the rate we obtain is still uncertain. But our results provide the essential ingredients that will need to be combined with experiment when the spin-parity and decay properties of these states in ^{31}S are verified.

The top panel of Fig. 1 shows the present rate divided by those give by the Hauser-Feshbach (HF) model [25], and the resonance state results based on the assumptions made by Jenkins et al. [9] and Ma et al. [3]. The rates for these are given in the Reaclib data base [26]. These previous rates are based on assumptions that are much less microscopic than the present.

6. Conclusions

In summary, in view of the importance of the ^{30}P(p,γ)^{31}S reaction, we considered the major aspects leading to uncertainties in calculating the reaction rate. Because of the high excitation energies involved in the resonance region, several negative parity states appear. Calculations were done for the first time in this mass region in a full (0+1) $\hbar\omega$ model space to take their contributions into account. It turns out that that the negative parity states make contributions to the reaction rate comparable to the positive parity states. The theoretical energies were correlated with available experimental energies, which required a review of ambiguities and uncertainties in the experimental data. A number of cases are suggested where improved data are required. It is evident that there are several experimental inconsistencies and ambiguities which would require further investigation to resolve.

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