Calculation of the Energy Levels of Phosphorus Isotopes (A=31 to 35) by Using OXBASH Code

S. Mohammadi, F. Bakhshabadi

Department of Physics, Payame Noor University, Tehran, Iran

Email address:

Smohammadi1958@yahoo.co.uk (S. Mohammadi)

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Abstract: Phosphorus (P) has 23 isotopes from ^{24}P to ^{46}P, only one of these isotopes, ^{31}Pis stable; such as this element is considered as a monoisotopic element. The longest-lived radioactive isotopes are ^{33}P with a half-life of 25.34 days and the least stable is ^{25}P with a half-life shorter than 30ns. Almost all of them are high energy beta-emitters which have valuable applications in medicine, industry, and tracer studies. Calculations of energy level properties of the Phosphor isotopic chain with A = 31 (N=15) to 35 (N=20) calculated through shell model calculations using the shell model code OXBASH for Windows. A compilation of sd-shell energy levels calculated with the USD Hamiltonian has been published around 1988.A comparison had been made between our results and the available experimental data and USD energies to test theoretical shell model description of nuclear structure in Phosphor nuclei. The calculated energy spectrum is in good agreement with the available experimental data.

Keywords: Phosphorus Isotopes, OXBASH Code, Shell Model Structure, USD Interaction

1. Introduction

Analysis of neutron-rich sd nuclei has been of intense curiosity in recent years as they present new aspects of nuclear structure [11].Traditional shell-model studies have recently received a renewed interest through large scale shell-model computing in no-core calculations for light nuclei, the 1s0d shell, the 1p0f shell and the 3s2d1g$_{7/2}$ shell with the inclusion of the 0h$_{11/2}$ intruder state as well. It is now therefore fully possible to work to large-scale shell-model examinations and study the excitation levels for large systems. In these systems, inter core is assumed and space is determined by considering shell gaps.

The crucial starting point in all such shell-model calculations is the derivation of an effective interaction, based on a microscopic theory starting from the free nucleon-nucleon (NN) interaction. Although the NN interaction is too short but finite range, with typical interparticle distances of the order of 1–2 fm, there are indications from both studies of few-body systems and infinite nuclear matter, both real and effective ones, may be of importance. Thus, with many valence nucleons present, such large-scale shell-model calculations may tell us how well an effective interaction which only includes two-body terms reproduces properties such as excitation spectra and binding energies. The problems of deriving such effective operators and interactions are solved in a limited space, the so-called model space, which is a subspace of the full Hilbert space. Several formulations for such expansions of effective operators and interactions exist. For example, for nuclei with *4 < A < 16* p-shell is used of Cohen-Kurath interaction and USD interaction is suitable for *16 < A < 40*sd-shell. [1, 2]

In order to calculate the nuclear structure properties of both ground and excited states based on the nuclear shell model one needs to have wave functions of those states. These wave functions are obtained by using the shell-model code OXBASH[3].The code OXBASH for Windows has been used to calculate the nuclear structure for Phosphor nucleus, by employing the SD (independent charges) and SDPN (depending charges) model space with three effective interactions[3]. The first interaction for the lower part of the sd-shell is Chung-Wildenthal particle interaction (CW), secondly, the Universal sd-shell Hamiltonian (USD interaction). In the third interaction the New Universal sd-shell Hamiltonian (USDAPN) is used. [3]

Richter *et a1*[4] used this shell model successfully in the p-shell, and fp-shell [5], [6] and Wildenthal [7] and Brown *et*

al[8] in the sd-shell to describe the systematic observed in the spectra and transition strengths.

In the present work, we focus our attention on the description of nuclear structure features, in particular the energy levels of sd shell and nucleuses ^{31}P, ^{32}P, ^{33}P, ^{34}P and ^{35}P[9,10]is studied in the framework shell model nuclear of configuration $0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$.

2. Theoretical Background

One of the approaches to study the structure of a nucleus and NN interactions, named Shell model structure that we deal with all degrees of freedom in this space and consider such all many-body configurations. In this model protons and neutrons move all active single particle orbits with three restrictions, Isospin, Angular momentum and Parity conservation [1, 2]. A *J* orbit has *(2J+1)* degeneracy for J_z, if we put N_π protons and N_v neutrons on such orbits, then the numbers of possible configurations are $_{2J+1}C_{N_\pi} \times _{2J+1}C_{N_v}$. Of course numbers of basis increases in a combinatorial way and the irrelevant numbers must are taken into account.

As is well known, the interaction between two protons, two neutrons or a proton and a neutron is approximately the same, $v_{\pi\pi} = v_{vv} = v_{\pi v}$, so isospin (T) was introduced as a new quantum number.

Single-particle wave functions of a neutron and a proton can be expressed with the t = 1/2 spinors .The nuclear states of a nucleus with *N* neutrons and *Z* protons *(A=N+Z)* can be characterized by definite values of T and M_T quantum numbers [1, 2, 11]

$$M_T = 1/2(N-Z), \quad 1/2(N-Z) \le T \le A/2$$

The configuration for a given nucleus partitioned into core part *(N_c, Z_c)* and an active valance part*(N-N_c, Z-Z_c)*. For practical reasons the number of valance nucleons must be small, as the numerical computations increase dramatically in magnitude with this number. Valance nucleons move in a finite number of j-orbits and their Hamiltonian of the valance nucleons is given by [2]

$$H = E_0 + \sum_i \varepsilon_i a_i^+ a_j + 1/2 \sum_{ijkl} \langle ij|V|kl\rangle a_i^+ a_j^+ a_l a_k$$

Where E_0 is the energy of the inert core, $\varepsilon_i's$ are the single particle energies of the valance orbits and $\langle ij|V|kl\rangle$ are the two-body matrix elements (TBME) of residual interaction amongst the valance particles. $\varepsilon_i's$ effectively take account of interaction between a valance particle and those in the inert core and V is taken from theoretical calculations or phenomenological models. The eigenvectors obtained from H-matrix in turn are used to obtain matrix elements of other physically interesting operators such as electric and magnetic moments, *EM* transition probabilities, β-decay matrix elements, one- and two-nucleon transfer probabilities, etc.

Finely, the shell-model calculations are confronted with all the available data. A commonly used procedure is to parameterized the effective interactions and even single particle energies of valance orbits and other such operators

(M1, GT, E2 etc.) and then obtain the values of these parameters which give the best numerical fit to the observed set of data points. Computer programs to construct and diagnolize Hamiltonian matrices have been existence for almost 40 years now. An improved modern version ones is OXBASH [3, 12] that uses the angular momentum coupled (J) scheme. As the interaction between two valence neutrons, we have to know the set of two-body matrix elements (TBME's) $\langle ab; JT|V|cd; JT\rangle$ with $(JT) = (01)$

OXBASH code only works for $J_z=J$. By applying J^+ operator, it predicts a set of m-scheme vectors that if used for projection will produce a good *J*-basis. The treatment that follows cannot be generalized for both spin and isospin to predict exactly a number of m-scheme vectors equal to the good *JT*-basis dimension. One disadvantage of an m-scheme basis is that it is much larger than the corresponding basis consisting of wave functions coupled to J and T. The n/p formalism enters naturally in the m-scheme formalism, since it only needs to skip those unwanted t_z values in each J-orbit in the corresponding SPS_le (Single Particle State _le)

In the second line of approach the two body matrix elements are treated as parameters, and their values are obtained from best fit to experimental data [13].

Brown and coworkers [18] have carried extensive studies of energy level and spectroscopic properties of sd-shell nuclei in terms of a unified Hamiltonian applied in full sd-shell model space. The universal Hamiltonian was obtained from a least square fit of 380 energy data with experimental errors of 0.2MeV or less from 66 nuclei. The USD Hamiltonian is defined by 63 sd-shell two body matrix element and their single particle energies. In more recent work Brown and co-workers have modified USD type Hamiltonian to USDA and USDB based on updated set of binding energy and energy levels of O, F, Ne, Na, Mg and P isotopes.

2.1. OXBASH Code

The calculations have been carried out using the code OXBASH for Windows [3, 12]. The code uses an m-scheme Slater determinant basis and works in the occupation number representation, where the occupancy (vacancy) of a bit in any given position of the computer word symbolizes the presence (absence) of a particle in a specific single particle state (i.e. in a given $|n, l, j, m_j, t_z >$ state). Using a projection technique, wave functions with good angular momentum J and isospin T are constructed. The SDPN and SD model spaces consist of *($0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$)* above the *Z = 8* and *N=8* closed shells for protons and neutrons. CW is an effective interaction that has been used with the SD model space, where the single-particle energies are 0.877, -4.15 and -3.28 MeV for subshells $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively. Also the USD effective interaction has been used with the SD model space, where the single-particle energies are 1.647, -3.948 and -3.164 MeV for subshells $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively. Meanwhile USDAPN is the effective interaction that has been used, where the single-particle energies for protons and neutrons are 1.980, -3.061 and -3.944 for $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively [14].

The OXBASH code uses both m-scheme and jj-coupling. It utilizes a basis of the Slater determinants that are antisymmetrized product wave functions. Each of these m-scheme basis states has definite total angular momentum projection quantum number $J_z= M$ and total isospin projection quantum number T_z. An appropriate expression of the shell-model Hamiltonian is given as the sum of one- and two-body operators [8, 15,17]

$$H = \sum_a \varepsilon_a \vec{n}_a + \sum_{a \leq b, c \leq d} \sum_{JT} V_{JT}(ab; cd)\, \hat{T}_{JT}(ab; cd),$$

Where ε_a are the single-particle energies, $\vec{n}_a$ is the number operator for the spherical orbit a with quantum number (n_a, l_a, j_a), $V_{JT}(ab\ cd)$; is a two-body matrix element, and

$$\hat{T}_{JT}(ab; cd) = \sum_{MT_z} A^+_{JMTT_z}\ (ab)\, A_{JMTT_z}(cd),$$

is the scalar two-body transition density for nucleon pairs (a, b) and (c, d), each pair coupled to spin quantum numbers JM.[8, 15, 17]

3. Results

The isotopes of Phosphorus lying between ^{31}P and ^{35}P provide a unique laboratory for examining the foundation of sd shell model calculations. The nucleons of the core (^{16}O) are 8 protons and 8 neutrons which are inert in the $(1s_{1/2}, 0p_{3/2}, 0p_{1/2})J=0, T=0$ configuration and the remaining A-16 nucleons are distributed over all possible combinations of the $0d_{5/2}, 1s_{1/2}$ and $0d_{3/2}$ orbits according to Pauli Exclusion Principle. The package of program called "SHELL" was used to generate the One Body Density Matrix Element (OBDME), and the package of program called "Lpe" is used to calculate the wave functions and energy levels.

We present here some results concerning Ground and excitation energies properties of the P chain for which recent data has been reported in the literature. [18]

3.1. ODD-ODD Nucleus: ^{31}P, ^{33}P, ^{35}P

In Figures 1, 2, 3 it is presented the theoretical, experimental and calculated level schemes for these nucleuses and the result are compared with the experimental data. The calculated spectrum in the Shows the theoretical information is in the exact agreement with the results obtained from OXBASH code and for ^{31}P spectrum obtained with OXBASH is in the best agreement to the experimental data in all the cases. The RMS deviation of ^{31}P and ^{33}P isotopes is 176 and 239 keV, respectively while for ^{35}P the experimental situation is much less documented. According to the tables 1 one can observe that for the ^{31}P isotope which has 8 neutrons ($(0d_{5/2})^6(1s_{1/2})^1$) and 7 protons $(0d_{5/2})^6(1s_{1/2})^2$) of valence, the different between experimental and code data isn't notable where the great value of $|\Delta E|$ is 389keV for the first excited level 11/2. We calculated 27 states of this isotope with T=1/2.

Table 2 shows the results of code for isotope ^{33}P $((0d_{5/2})^6(1s_{1/2})^1)_\pi$, $((0d_{5/2})^6(1s_{1/2})^2(0d_{3/2})^2)_\nu$ and the maximum value for $|\Delta E|$ occurs in the third level excited of 3/2 with 331keV. Our records for ^{35}P are in the extremely accurate with the USD energies.
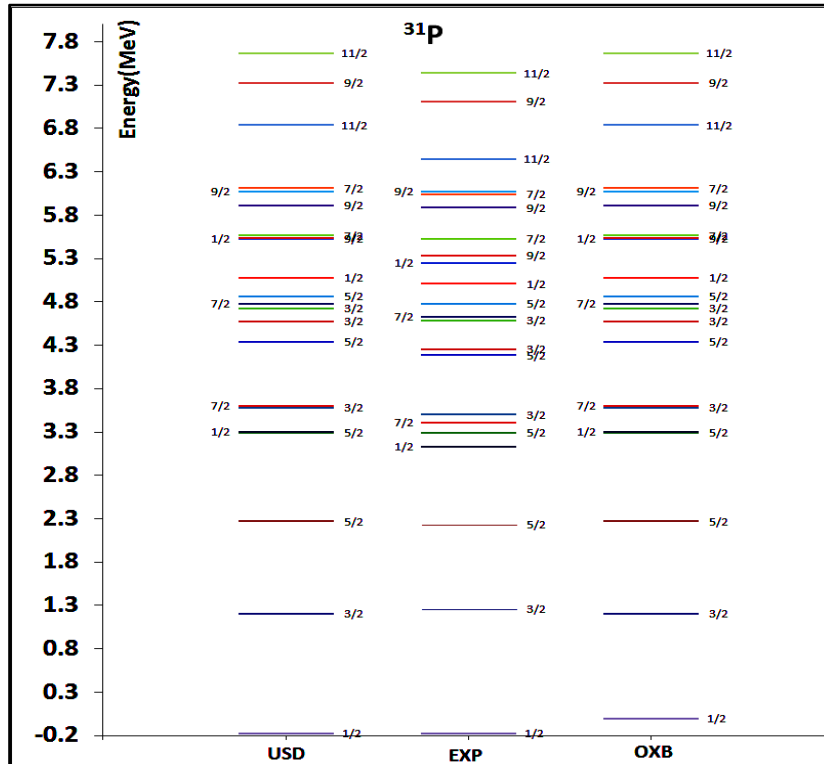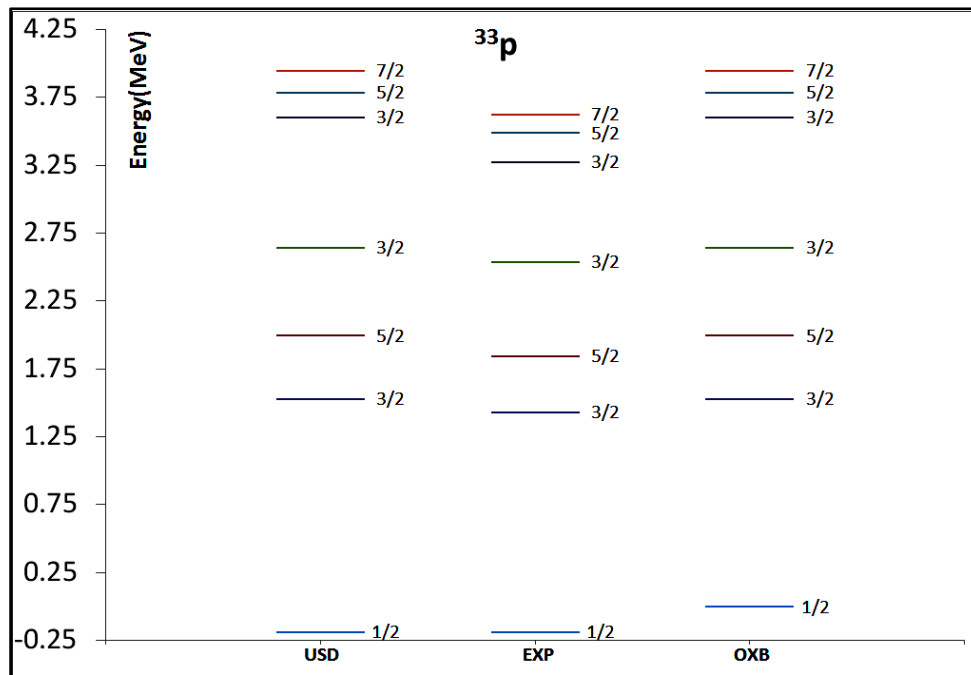

***Figure 1.** Comparison of the experimental and theoretical energy levels with the present calculated work of the bands for ^{31}P nucleus.*

Table 1. Experimental, theoretical and calculated energy levels of $1/2 < J < 17/2$ in ^{31}P spectrum (MeV).

OXB(W)	USD	J	EXP	OXB(W)	USD	J	EXP	OXB(W)	USD	J	EXP
-167.896	-167.895	$(1/2)_1$	-167.753	2.275	2.275	$(5/2)_1$	2.234	5.537	5.537	$(9/2)_1$	5.343
3.31	3.31	$(1/2)_2$	3.134	3.297	3.297	$(5/2)_2$	3.295	5.918	5.918	$(9/2)_2$	5.892
5.084	5.084	$(1/2)_3$	5.015	4.866	4.866	$(5/2)_2$	4.783	6.08	6.08	$(9/2)_2$	6.08
5.536	5.536	$(1/2)_4$	5.256	4.344	4.344	$(5/2)_3$	4.19	7.331	7.331	$(9/2)_4$	7.118
6.531	6.531	$(1/2)_5$	6.337	5.321	5.321	$(5/2)_5$	5.115	6.843	6.843	$(11/2)_1$	6.454
1.21	1.21	$(3/2)_1$	1.266	7.093	7.093	$(5/2)_9$	6.932	7.673	7.673	$(11/2)_2$	7.441
3.587	3.587	$(3/2)_2$	3.506	3.605	3.605	$(7/2)_1$	3.415	9.231 2	9.231	$(13/2)_1$	-
4.581	4.581	$(3/2)_3$	4.261	4.781	4.781	$(7/2)_2$	4.634	10.478	10.478	$(13/2)_2$	-
4.733	4.733	$(3/2)_4$	4.594	6.115	6.115	$(7/2)_2$	6.048	12.063	12.063	$(15/2)_1$	-
5.763	5.763	$(3/2)_5$	5.559	5.571	5.571	$(7/2)_3$	5.529	13.961	13.961	$(17/2)_1$	-

Figure 2. Comparison of the experimental and theoretical energy levels with the present calculated work of the bands for ^{33}P nucleus.

Table 2. Experimental, theoretical and calculated energy levels of $1/2 < J < 21/2$ in ^{33}P spectrum (MeV)

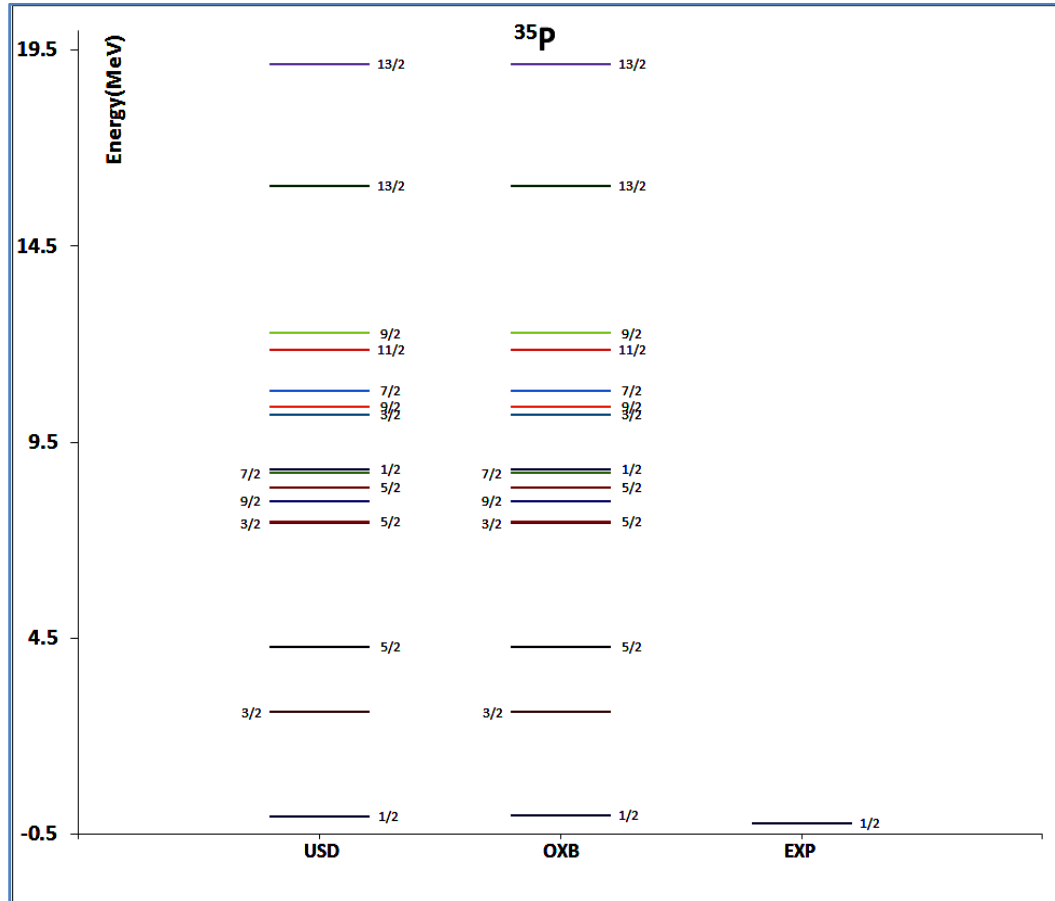| J	USD	EX	OXB(W)	J	USD	EX	OXB(W)
1/2	-0.18598	-0.175645 *	0				
3/2	1.531	1.432	1.531	13/2	9.245	-	9.245
5/2	1.997	1.848	1.997	13/2	10.869	-	10.869
3/2	2.646	2.539	2.646	15/2	13.098	-	13.837
3/2	3.606	3.275	3.606	15/2	13.837	-	14.763
5/2	3.787	3.49	3.787	17/2	15.203	-	15.203
7/2	3.949	3.628	3.949	17/2	16.513	-	16.513
1/2	4.242	-	4.242	19/2	18.936	-	18.936
1/2	5.728	-	5.728	19/2	21.581	-	21.581
7/2	5.905	-	5.905	21/2	22.644	-	22.644
7/2	6.606	-	6.606	21/2	26.16	-	26.16

Figure 3. *Comparison of the experimental and theoretical energy levels [18,9,10] with the present calculate work of the bands for ^{35}P nucleus.*

Table 3. *Experimental, theoretical and calculated energy levels of $1/2 < J < 13/2$ in ^{35}P spectrum (MeV)*

J	USD	EXP	OXB(W)	J	USD	EXP	OXB(W)
$(1/2)_1$	8.83	-	8.83	$(7/2)_1$	7.452	-	7.452
$(1/2)_2$	11.751	-	11.751	$(7/2)_2$	8.727	-	8.727
$(1/2)_3$	12.127	-	12.127	$(7/2)_3$	10.828	-	10.828
$(3/2)_1$	7.448	-	7.448	$(7/2)_4$	11.658	-	11.658
$(3/2)_2$	10.219	-	10.219	$(9/2)_1$	8.015	-	8.015
$(3/2)_3$	10.595	-	10.595	$(9/2)_2$	10.428	-	10.427
$(3/2)_4$	10.595	-	10.595	$(9/2)_3$	12.299	-	12.299
$(5/2)_1$	4.298	-	4.298	$(9/2)_4$	15.219	-	15.219
$(5/2)_2$	7.494	-	7.494	$(11/2)_1$	11.869	-	11.869
$(5/2)_3$	8.369	-	8.369	$(13/2)_1$	16.053	-	16.053
$(5/2)_4$	10.178	-	10.178	$(13/2)_2$	19.156	-	19.156

3.2. ODD-EVEN Nucleus: ^{32}P, ^{34}P

In Figures 4 and 5, the theoretical, experimental and calculated level schemes for two isotopes are presented, and the results are compared with the experimental data. In cases of ^{32}P and ^{34}P, ordering of levels is correctly reproduced by W and USD interactions. The root mean square (RMS) deviation is 257 and 234 keV for ^{32}P and ^{34}P, respectively. The calculated levels spectra up to the state J=12 for ^{32}P,

$((0d_{5/2})^6(1s_{1/2})^1)_\pi$, $((0d_{5/2})^6(1s_{1/2})^2(0d_{3/2})^1)_\nu$ in Figure 4, are compared with the available experimental information. The maximum value for $|\Delta E|$ occurs in the fourth level excited of 1 with $487keV$. We calculated 22 states of this isotope with T=1. The calculated energies for isotope ^{34}P $((0d_{5/2})^6(1s_{1/2})^1)_\pi$, $((0d_{5/2})^6(1s_{1/2})^2(0d_{3/2})^3)_\nu$ up to the state J=9 is shown in Figure5 with their values tabulated in Table 5.
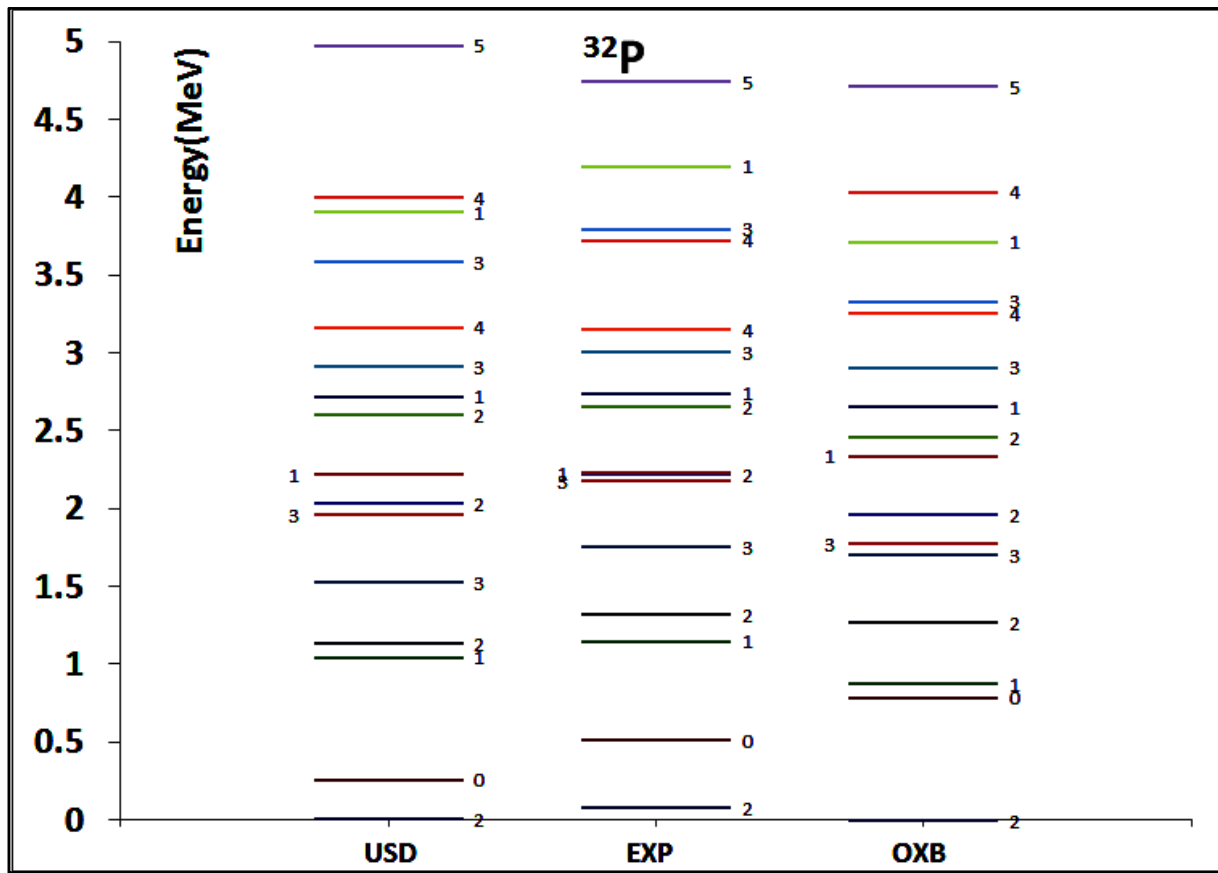
Figure 4. *Comparison of the experimental and theoretical energy levels [18,9,10]with the present calculate work of the bands for* ^{32}P *nucleus.*

Table 4. *Experimental, theoretical and calculated energy levels of* $0 < J < 12$ *in* ^{32}P *spectrum (MeV)*

| OXB(W)	USD	J	EXP	OXB(W)	USD	J	EXP
0.788	0.26	$(0)_1$	0.513	3.258	3.168	$(4)_1$	3.149
-0.255	0.005	$(1)_1$	-0.175	3.649	3.727	$(4)_2$	4.035
2.342	2.224	$(1)_2$	2.23	4.717	4.977	$(5)_1$	4.743
2.656	2.722	$(1)_3$	2.745	5.354	5.614	$(5)_2$	-
3.716	3.909	$(1)_4$	4.203	5.746	6.006	$(5)_3$	-
-0.266	-0.175	$(2)_1$	0.078	6.093	6.353	$(5)_4$	-
1.268	1.135	$(2)_2$	1.323	7.133	7.393	$(6)_1$	-
1.964	2.036	$(2)_3$	2.219	7.401	7.661	$(6)_2$	-
2.462	2.602	$(2)_4$	2.658	8.563	8.823	$(7)_1$	-
3.327	3.518	$(2)_5$	3.445	12.498	12.757	$(8)_1$	-
3.467	3.592	$(2)_6$	3.88	12.26	12.52	$(8)_2$	-
1.705	1.528	$(3)_1$	1.754	13.918	14.178	$(9)_1$	-
1.776	1.965	$(3)_2$	2.178	17.199	17.459	$(10)_1$	-
2.908	2.916	$(3)_3$	3.005	21.063	21.322	$(11)_1$	-
3.332	3.587	$(3)_4$	3.797	22.818	23.078	$(11)_2$	-
4.373	3.976	$(3)_5$	4.312	27.057	27.316	$(12)_1$	-
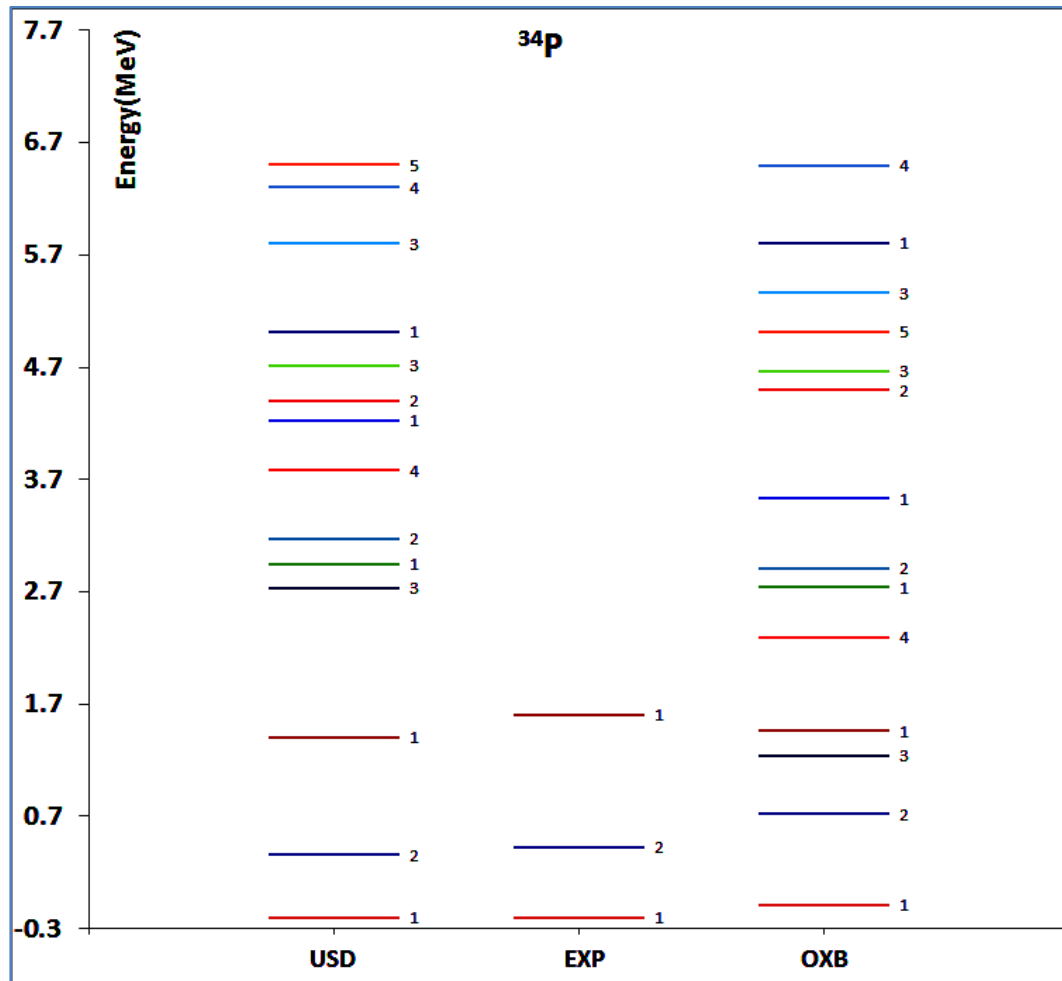
Figure 5. *Comparison of the experimental and theoretical energy levels with the present calculate work of the bands for ^{34}P nucleus.*

Table 5. *Experimental, theoretical and calculated energy levels of $0 < J < 9$ in ^{34}P spectrum (MeV)*

J	USD	EXP.	OXB.(W)	J	USD	EXP.	OXB.(W)
$(1)_1$	1.408	1.609	1.467	$(4)_1$	3.788	-	2.301
$(1)_2$	2.954	-	2.745	$(4)_2$	6.308	-	6.503
$(1)_3$	4.232	-	3.537	$(5)_1$	6.509	-	5.022
$(1)_4$	5.025	-	5.816	$(6)_1$	7.671	-	9.88
$(2)_1$	0.363	0.429	0.729	6	9.455	-	12.352
$(2)_2$	3.176	-	2.919	7	11.367	-	11.488
$(2)_3$	4.406	-	4.503	7	13.839	-	13.508
$(3)_1$	2.737	-	1.25	8	15.46	-	13.973
$(3)_2$	4.719	-	4.669	8	17.722	-	16.235
$(3)_3$	5.806	-	5.368	9	21.809	-	20.322

4. Conclusions

As can be seen from ^{31}P diagram, very good agreement is obtained for most of energy levels and the ordering of levels is correctly reproduced. For isotope ^{32}P one can see differences between experimental and calculated values in which for the first levels, discrepancies are approximately large. For example in the first excited level of $(0)_1$, relative error is about 50% since the experimental and calculated values are 0.513 and 0.788, respectively, even though in the higher levels discrepancies are getting smaller. In the case of isotope ^{33}P, as seen from the Figure 2 very good agreements is obtained for most of energy levels, but for higher J values like $(7/2)_1$, there is a discrepancy of about (8 % keV). For isotopes ^{34}P and ^{35}P the same comparison were made in Figures 5 and 3, respectively. Unfortunately, although enough experimental data are not available, but regarding the USD data we can judge that almost all calculations have meet the reasonable success in reproducing the observed level structure.

In general the best and most complete results are found with the largest model space while calculations in an infinite space are not possible and the computation time increases exponentially with model space size so some truncation is required. Also an interaction used must be appropriate for the

model space. The empirical interactions are (usually) better determined for smaller model spaces. The model space in OXBASH is defined by the active valance nucleon orbits and our calculated results are reasonably consistent with experimental data, although the structure of odd-even nuclei is much more complicated than their odd-odd neighbours. Especially, in the energies more than 3.5 MeV, the states in ^{32}P are more sporadic than ^{31}P.

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