Determination of Low-Energy Parameters of Neutron–Proton Scattering on the Basis of Modern Experimental Data from Partial-Wave Analyses

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The triplet and singlet low-energy parameters in the effective-range expansion for neutron–proton scattering are determined by using the latest experimental data on respective phase shifts from the SAID nucleon–nucleon database. The results differ markedly from the analogous parameters obtained on the basis of the phase shifts of the Nijmegen group and contradict the parameter values that are presently used as experimental ones. The values found with the aid of the phase shifts from the SAID nucleon–nucleon database for the total cross section for the scattering of zero-energy neutrons by protons, $\sigma_0 = 20.426$ b, and the neutron–proton coherent scattering length, $f = -3.755$ fm, agree perfectly with the experimental cross-section values obtained by Houk, $\sigma_0 = 20.436 \pm 0.023$ b, and experimental scattering-length values obtained by Houk and Wilson, $f = -3.756 \pm 0.009$ fm, but they contradict cross-section values of $\sigma_0 = 20.491 \pm 0.014$ b according to Dilg and coherent-scattering-length values of $f = -3.7409 \pm 0.0011$ fm according to Koester and Nistler.

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1. Along with the deuteron parameters, the low-energy parameters in the effective-range expansion for neutron–proton scattering,

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2} r k^2 + v_2 k^4 + v_3 k^6 + v_4 k^8 + \ldots ,$$

are fundamental quantities that play a key role in studying strong nucleon–nucleon interaction.

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These parameters are of great importance for constructing various realistic nuclear-force models, which, in turn, form a basis for studying the structure of nuclei and various nuclear processes. For this reason, it is highly desirable to determine reliably and accurately the parameters in the effective-range expansion, including the scattering length $a$, the effective range $r$, the shape parameter $v_2$, and higher order parameters $v_n$.

Although low-energy parameters for neutron–proton scattering have been determined and studied since the early 1950s, even the experimental values of such parameters as the scattering length $a$ and the effective range $r$ are ambiguous to date. As for the shape parameter $v_2$, even its sign is unknown at the present time. The theoretical value of this parameter depends greatly on the nuclear-force model used: as we go over from one model to another, the parameter $v_2$ in the triplet state changes within a broad interval, from $-0.95 \, [1, 2]$ to $1.371 \, \text{fm}^3 \, [3]$, whence it follows that the shape parameter is a very subtle and sensitive feature of nucleon–nucleon interaction.

We would like to note that not only does the shape parameter $v_2$ depend on the form of interaction, but it is also strongly dependent on the scattering length $a$ and the effective range $r$. In particular, a change of only a few tenths of a percent in the scattering length $a$ may lead to a severalfold change in the shape parameter $v_2 \, [4]$. The shape parameters $v_n$ of order higher than that of $v_2$ have been still more poorly determined and are more sensitive to details of nucleon–nucleon interaction. The aforesaid highlights once again the importance of reliably determining the scattering length $a$ and the effective range $r$, the more so as these are quantities that are most frequently used as inputs in constructing various models of nucleon–nucleon interaction.

2. It is well known [5] that the neutron–proton system may occur either in the triplet (the total spin is $S = 1$) or the singlet (the total spin is $S = 0$) spin state. In determining the scattering lengths $a$ and the effective ranges $r$ in the triplet ($t$) and singlet ($s$) spin states, one employs the experimental dependence of the total (spin-averaged) cross section for the scattering of slow neutrons by free protons and data characterizing the scattering of zero-energy neutrons by para-hydrogen. In order to determine the triplet and singlet scattering lengths ($a_t$ and $a_s$, respectively), use is usually made of equations that relate these quantities
to the total cross section for the scattering of zero-energy neutrons by protons,

$$\sigma_0 = \pi \left( 3a_t^2 + a_s^2 \right),$$

(2)

and to the coherent scattering length,

$$f = \frac{1}{2} \left( 3a_t + a_s \right).$$

(3)

In this case, the cross section $\sigma_0$ is determined from the results of experiments that study slow-neutron scattering on protons bound in various molecules ($\text{H}_2$, $\text{H}_2\text{O}$, $\text{C}_6\text{H}_6$, $\text{CH}_3\text{OH}$), corrections associated with neutron capture by a proton and with effects of proton binding in molecules being subsequently eliminated. The elimination of binding-effect corrections is a nontrivial many-body problem, since, in addition to proton and neutron motion, it is necessary to take into account the motion of the molecular residue. A number of significant simplifications and approximations are made in solving this problem [6]. A compendium of experimental results from [7–13] on the total cross section for the scattering of zero-energy neutrons by free protons, $\sigma_0$, is given in Table 1.

Two values of the total cross section $\sigma_0$ are recommended at the present time. These are the value obtained by Houk (1971) [12],

$$\sigma_0 = 20.436(23) \text{ b},$$

(4)

and the value obtained by Dilg (1975) [13],

$$\sigma_0 = 20.491(14) \text{ b}.$$  

(5)

Since these two values of $\sigma_0$ are inconsistent, their weighted-mean value

$$\sigma_0 = 20.476(12) \text{ b}$$

(6)

can also be used in determining the scattering lengths.

It should be noted that the total cross section $\sigma_0$ has not been measured since 1975.

The coherent scattering length $f$, which is determined by relation (3), is found either from experiments where slow neutrons are scattered by pure para-hydrogen [8, 14, 15] or by crystals
or — and this is a more precise method — from experiments where neutrons are reflected by a liquid mirror and where use is made of a number of pure hydrocarbons [9, 10, 17–22]. Also, a method for determining the coherent scattering length by means of neutron interferometry from experiments to study neutron scattering on molecular hydrogen was proposed in [23]. The values found by various authors for the neutron–proton coherent scattering length $f$ are quoted in Table 2, whence it can be seen that the value of this quantity is even more ambiguous than the value of $\sigma_0$.

In determining the scattering lengths in the triplet and the singlet state ($a_t$ and $a_s$, respectively), one employs most frequently, at the present time, the coherent-length value obtained by Koester and Nistler [22],

$$f = -3.7409(11) \text{ fm},$$  \hfill (7)

and the coherent-length value presented in the compilation of Dumbrajs et al. [24],

$$f = -3.738(1) \text{ fm}.$$  \hfill (8)

Recent experiments aimed at determining the neutron–proton coherent scattering length by means of neutron interferometry [23], which were mentioned above, yielded the value

$$f = -3.7384(20) \text{ fm}.$$  \hfill (9)

Within the experimental errors, the value in (9) agrees with the result of Koester and Nistler in (7) and with the value in (8), which was used by Dumbrajs et al. [24].

Table 3 presents values obtained in a number of previous studies [9, 10, 13, 18, 21, 22, 24–28] for the scattering lengths and effective ranges in the triplet and singlet spin states. All of them have been used as experimental values. The values of the triplet ($a_t$) and singlet ($a_s$) scattering lengths from Table 3 were obtained on the basis of formulas (2) and (3) by using various values for the total cross section $\sigma_0$ and the neutron–proton coherent scattering length $f$.

The values of the triplet effective range $r_t$ in Table 3 were determined primarily in an approximation that does not depend on the form of interaction; that is,

$$r_t \equiv \rho(-\varepsilon_d, 0) = 2R \left(1 - \frac{R}{a_t}\right),$$  \hfill (10)
where \( \rho(-\varepsilon_d, 0) \) is the mixed effective radius of the deuteron;

\[
R = \frac{1}{\alpha}
\]

is a parameter that characterizes the spatial dimensions of the deuteron; and \( \alpha \) is the deuteron wave number, which is related to the deuteron binding energy \( \varepsilon_d \) by the equation

\[
\varepsilon_d = \frac{\hbar^2 \alpha^2}{m_N}.
\]

In a number of studies \[24, 26\], the triplet effective range was determined in accordance with the formula

\[
r_t = \rho(-\varepsilon_d, 0) + \delta r_t,
\]

where the correction \( \delta r_t \) is a model-dependent quantity. According to the estimates obtained by Noyes on the basis of the dispersion relations \[26\], the correction \( \delta r_t \) arising owing to one-pion exchange is

\[
\delta r_t = -0.013 \text{ fm}.
\]

According to other estimates \[24\], this correction is

\[
\delta r_t \simeq -0.001 \text{ fm},
\]

which is an order of magnitude smaller in absolute value than the estimate in (14). In the latter case, the effective range \( r_t \) is therefore nearly coincident with the mixed effective radius \( \rho(-\varepsilon_d, 0) \).

The singlet effective range \( r_s \) is usually determined on the basis of an analysis of the total cross section for neutron–proton scattering, \( \sigma(E) \), in the low-energy region at fixed values of the parameters \( a_t, a_s, \) and \( r_t \). The values found in this way for the singlet effective range \( r_s \) appear to be even more ambiguous than the values of the triplet effective range. As can be seen from Table 3, the scattering-length and effective-range values used as experimental ones change within rather broad ranges. The scatter of these values is due first of all to the fact that different experimental values of the cross section for the scattering of zero-energy neutrons by free protons, \( \sigma_0 \), and of the neutron–proton coherent scattering length \( f \) are used
to determine these quantities. The ambiguity in determining the singlet effective range $r_s$ is also associated with an insufficient accuracy of the experimental total cross sections for neutron–proton scattering at energies below 5 MeV. The values found by different authors for the singlet effective range $r_s$ change within a broad range, from 2.42 [9] to 2.81 fm [13].

Thus, the accuracy of the experiments performed in the 1950s–1970s is insufficient for unambiguously determining the low-energy parameters of neutron–proton scattering. At the same time, these parameters play an important role in the theory of few-nucleon systems, which is based on nucleon–nucleon interaction. As was shown in [29, 30], the binding energies of the $^3$H and $^4$He nuclei depend greatly on the singlet effective range $r_s$, increasing as $r_s$ becomes smaller. By way of example, we indicate that, as $r_s$ decreases by 0.1 fm, the binding energies of the $^3$H and $^4$He nuclei increase by 0.3 and 1.5 MeV, respectively. We note that the decrease of 0.01 fm in the triplet scattering length $a_t$ also leads to the increase of 0.025 MeV in the triton binding energy [31, 32]. At the same time, it is well known that, in calculations with realistic nucleon–nucleon potentials, the binding energies of few-nucleon systems prove to be underestimated. In such calculations, the $^3$H binding energy is as a rule underestimated by 1 MeV. A reliable and precise determination of the low-energy parameters of neutron–proton scattering and their use in calculating the binding energies of systems that contain three or more nucleons may contribute to solving the problem of underestimating the binding energies of few-nucleon systems without introducing three-particle forces, quark degrees of freedom, and other concepts that would require revising basic points in the traditional theory of nuclear forces, which relies on pair nucleon–nucleon interaction.

To conclude this section, we present, for low-energy parameters, values that are currently used as experimental ones. Most frequently, the present-day literature quotes two sets of low-energy parameters. These are the set from [24],

\[
\begin{align*}
    a_t &= 5.424(4) \text{ fm}, \quad r_t = 1.759(5) \text{ fm}; \\
    a_s &= -23.748(10) \text{ fm}, \quad r_s = 2.75(5) \text{ fm},
\end{align*}
\]

which is matched with the experimental value (5) of the total cross section at zero energy due to Dilg [13] and with the value in (8) for the neutron–proton coherent scattering length from
\[ a_t = 5.419(7) \text{ fm}, \quad r_t = 1.753(8) \text{ fm}; \]
\[ a_s = -23.740(20) \text{ fm}, \quad r_s = 2.77(5) \text{ fm}, \]

which corresponds to the weighted-mean value (6) of the cross sections presented by Houk [12] and Dilg [13] and to the value in (7) for the coherent length due to Koester and Nistler [22].

It should be noted that the experiments performed in the 1950–1970s were the main source of information used to deduce the values in (16) and (17) for the low-energy parameters of neutron–proton scattering.

3. In recent years, the accuracy of experimental data on nucleon–nucleon scattering has been improved considerably; moreover, methods of their partial-wave analysis, which make it possible to describe the results of scattering experiments in terms of phase shifts, have also been refined [33, 34]. Owing to this, the triplet and singlet low-energy parameters of neutron–proton scattering can be determined independently of one another by using the $^3S_1$- and $^1S_0$-state phase shifts [4, 35]. The results of the partial-wave analysis performed by the GWU group [33] (data from the well-known SAID nucleon–nucleon database) and by the Nijmegen group [34] are presently the most precise and most widely used data on the phase shifts for nucleon–nucleon scattering. The most popular modern realistic nucleon–nucleon potentials constructed within the last decade, which include the Nijm-I, Nijm-II, Reid93 [36], Argonne V18 [37], CD-Bonn [28, 38], and Moscow [39] potentials, are based on fits to data of the Nijmegen group [34]. However, it should be noted that the partial-wave analysis of the Nijmegen group is a result of processing and averaging experimental data on nucleon–nucleon scattering over a period from 1955 to 1992, but this analysis provides an insufficiently accurate description of modern experimental data on nucleon–nucleon scattering. Despite the proximity of the phase shifts for neutron–proton scattering that were obtained by the GWU and Nijmegen groups, the corresponding values of the low-energy parameters in the effective-range expansion are markedly different [4], this difference being not only quantitative but also qualitative.

Using the approximation of the effective-range function $k \cot \delta$ at low energies by polynomials and Padé approximants within the least squares method, we calculated the triplet and singlet low-energy parameters of neutron–proton scattering for the experimental data on the
GWU [33] and Nijmegen [34] phase shifts. The results obtained for the low-energy parameters in the present study by employing the data from the partial-wave analysis of the GWU group,

\[
\begin{align*}
a_t &= 5.4030 \text{ fm}, \quad r_t = 1.7494 \text{ fm}, \quad v_{2t} = 0.163 \text{ fm}^3; \\
a_s &= -23.719 \text{ fm}, \quad r_s = 2.626 \text{ fm}, \quad v_{2s} = -0.005 \text{ fm}^3;
\end{align*}
\]

(18)

differ significantly from the parameter values

\[
\begin{align*}
a_t &= 5.420 \text{ fm}, \quad r_t = 1.753 \text{ fm}, \quad v_{2t} = 0.040 \text{ fm}^3; \\
a_s &= -23.739 \text{ fm}, \quad r_s = 2.678 \text{ fm}, \quad v_{2s} = -0.48 \text{ fm}^3,
\end{align*}
\]

(19)

which were obtained on the basis of the data from the partial-wave analysis of the Nijmegen group. The triplet low-energy parameters calculated here for the phase shifts of the Nijmegen group are virtually coincident with the analogous parameters obtained previously in [35]. Unfortunately, the data presented by the Nijmegen group do not contain the singlet low-energy parameters of neutron–proton scattering. The value of the singlet shape parameter \(v_{2s}\) for the Nijmegen phase shifts was calculated in [1], and it is in agreement with our value.

Using expressions (18) and (19) for the scattering lengths and relying on formulas (2) and (3), we find for the cross section \(\sigma_0\) and for the coherent scattering length \(f\) that

\[
\sigma_0 = 20.426 \text{ b}, \quad f = -3.755 \text{ fm}
\]

(20)

in the case of the GWU phase shifts and that

\[
\sigma_0 = 20.473 \text{ b}, \quad f = -3.7395 \text{ fm}
\]

(21)

in the case of the Nijmegen phase shifts.

The values in (21) are in good agreement with the weighted mean of the cross sections obtained by Houk and Dilg, \(\sigma_0 = 20.476(12) \text{ b}\), and with the coherent-scattering-length value of \(f = -3.7409(11) \text{ fm}\) according to Koester and Nistler [22]. It should be emphasized, however, that this agreement is not accidental; it is directly related to the fact that, in the partial-wave analysis of the Nijmegen group, the cross-section values obtained by Houk [12] and Dilg [13] and the coherent-scattering-length value obtained by Koester and Nistler [22] were used as
input experimental parameters. It is precisely the reason why all of the experimental low-energy parameters in (17), with the exception of the singlet effective range, agree within the experimental error with the corresponding parameters in (19), which were calculated on the basis of the Nijmegen phase shifts.

The singlet-effective-range value of $r_s = 2.678$ fm, which was calculated for the phase shifts obtained by the Nijmegen group, is much smaller than the experimental value of $r_s = 2.77(5)$ fm, which was quoted by Dilg in [13]. In this connection, it should be noted that, in [13], the singlet effective range $r_s$ was determined from experimental data on the total cross section for neutron–proton scattering at energies below 5 MeV at the scattering-length values fixed at $a_t = 5.423(4)$ fm and $a_s = -23.749$ fm and the triplet-effective-range value fixed at $r_t = 1.760(5)$ fm, but, as was indicated above, this method for determining the effective range is highly unreliable (see Table 3). A determination of the singlet effective range $r_s$ directly from the singlet phase shift irrespective of the triplet parameters is more correct and consistent, which reduces substantially the uncertainty in this quantity.

For the sake of comparison, the low-energy parameters for neutron–proton scattering that correspond to the GWU (GWU PWA) and Nijmegen (Nijm PWA) phase shifts are given in Table 4, along with the values of these parameters for a number of the realistic potentials (Argonne V18 [37], CD-Bonn [28, 38], and Moscow [39] potentials) whose parameters were matched with the Nijmegen nucleon–nucleon database. Also quoted there are the experimental values of the low-energy parameters. Table 4 shows that the values of the low-energy parameters obtained for the Nijmegen phase shifts are in perfect agreement with the corresponding parameters for the potentials fitted to the Nijmegen nucleon–nucleon database.

A significant distinction between the values of the triplet low-energy parameters for the GWU and Nijmegen data was discussed in detail in our previous article [4]. Here, we only indicate that the difference of the triplet scattering lengths by 0.3% is in fact a more important circumstance than the fourfold distinction between the values of the triplet shape parameters. This is because many important features of the neutron–proton system — such as the asymptotic deuteron normalization factor $A_S$ and the root-mean-square radius $r_d$ of the deuteron — are highly sensitive to variations in the triplet scattering length [40]. We also note that,
Although the triplet effective ranges obtained from experimental data of the two main groups are close to each other, the values of the difference $\delta r_t$ of the effective range $r_t$ and the mixed effective radius $\rho(-\epsilon_d, 0)$ for the GWU [33] and Nijmegen [34] phase shifts differ significantly. For example, the correction $\delta r_t$ for the phase shifts of the GWU group is positive, taking the value

$$\delta r_t = 0.0163 \text{ fm}. \quad (22)$$

For the phase shifts of the Nijmegen group, this correction is negative and, in absolute value, is an order of magnitude smaller than the correction in (22): $\delta r_t = -0.001 \text{ fm}$. The value of the singlet effective range for the phase shifts of the GWU group also differs from its counterpart for the Nijmegen phase shifts (by about 2%), and the corresponding difference of the singlet shape parameters is formidable, reaching two orders of magnitude.

In contrast to the partial-wave analysis of the Nijmegen group, the partial-wave analysis of the GWU group does not employ the values of the cross section $\sigma_0$ and the coherent scattering length $f$ as input parameters. The theoretical values of $\sigma_0 = 20.426 \text{ b}$ and $f = -3.755 \text{ fm}$, which we obtained here for the cross section in question and for the neutron–proton coherent scattering length from data of the partial-wave analysis performed by the GWU group, are in perfect agreement with the experimental cross-section value of $\sigma_0 = 20.436(23) \text{ b}$ according to Houk [12], and the experimental coherent-scattering-length value obtained by Houk and Wilson [9, 10],

$$f = -3.756(9) \text{ fm}, \quad (23)$$

but they contradict the cross-section value of $\sigma_0 = 20.491(14) \text{ b}$ according to Dilg [13] and the coherent-scattering-length value of $f = -3.7384(20) \text{ fm}$, which was obtained recently by the neutron-interferometry method in [23]. Thus, we see that a reliable experimental determination of the total cross section for neutron–proton scattering at zero energy, $\sigma_0$, and of the coherent scattering length, $f$, is now quite a pressing problem. Precise values of these quantities would make it possible to determine unambiguously the triplet and singlet scattering lengths and to solve the problem of choosing a correct set of the low-energy parameters and phase shifts among currently recommended experimental values.
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Table 1. Total cross section for neutron scattering on a proton at zero energy

| No. | References                  | $\sigma_0$, b  |
|-----|-----------------------------|----------------|
| 1   | Melkonian [7] (1949)        | 20.36(10)      |
| 2   | Stewart and Squires [8] (1953) | 20.41(14)  |
| 3   | Houk and Wilson [9] (1967) | 20.37(2)       |
| 4   | Houk and Wilson [10] (1968) | 20.442(23)    |
| 5   | Neill et al. [11] (1968)   | 20.366(76)     |
| 6   | Houk [12] (1971)           | 20.436(23)     |
| 7   | Dilg [13] (1975)           | 20.491(14)     |
Table 2. Amplitude for coherent neutron–proton scattering

| No. | References                        | $f$, fm    |
|-----|-----------------------------------|------------|
| 1   | Shull et al. [16] (1948)          | $-3.900(100)$ |
| 2   | Hughes et al. [17] (1950)         | $-3.75(3)$  |
| 3   | Burgy et al. [18] (1951)          | $-3.78(2)$  |
| 4   | Stewart and Squires [8] (1955)    | $-3.80(5)$  |
| 5   | Dickinson et al. [19] (1962)      | $-3.740(20)$ |
| 6   | Koester [20] (1967)               | $-3.719(2)$ |
| 7   | Houk and Wilson [9, 10] (1967, 1968) | $-3.756(9)$ |
| 8   | Koester and Nistler [21] (1971)   | $-3.740(3)$ |
| 9   | Koester and Nistler [22] (1975)   | $-3.7409(11)$ |
| 10  | Callerame et al. [15] (1975)      | $-3.733(4)$ |
| 11  | Schoen et al. [23] (2003)         | $-3.7384(20)$ |
Table 3. Low-energy parameters of neutron–proton scattering from various studies

| No. | References                   | $a_t$, fm | $a_s$, fm | $r_t$, fm | $r_s$, fm |
|-----|------------------------------|-----------|-----------|-----------|-----------|
| 1   | Burgy et al. [18] (1951)     | 5.377(21) | −23.690(55) | 1.704(28) | −         |
| 2   | Noyes [25] (1963)            | 5.396(11) | −23.678(28) | 1.727(14) | 2.51(11)  |
| 3   | Houk and Wilson [9] (1967)   | 5.392(6)  | −23.689(13) | 1.724(7)  | 2.42(9)   |
|     |                              | 5.399(11) | −23.680(28) | 1.732(12) | 2.48(11)  |
|     |                              | 5.411(4)  | −23.671(12) | 1.747(4)  | 2.59(8)   |
| 4   | Houk and Wilson [10] (1968)  | 5.405(6)  | −23.728(13) | 1.738(7)  | 2.56(10)  |
| 5   | Koester and Nistler [21] (1971) | 5.414(5) | −23.719(13) | −         | −         |
| 6   | Noyes [26] (1972)            | 5.413(5)  | −23.719(13) | 1.735     | 2.66      |
|     |                              | 5.423(5)  | −23.712(13) | 1.748(6)  | 2.75(10)  |
| 7   | Lomon and Wilson [27] (1974) | 5.414(5)  | −23.719(13) | 1.750(5)  | 2.76(5)   |
| 8   | Dilg [13] (1975)             | 5.423(4)  | −23.749(9)  | 1.760(5)  | 2.77(5)   |
|     |                              |           |            |           | 2.81(5)   |
|     |                              |           |            |           | 2.78(5)   |
| 9   | Koester and Nistler [22] (1975) | 5.424(3) | −23.749(8)  | 1.760(5)  | 2.81(5)   |
| 10  | Dumbrajs et al. [24] (1983)  | 5.424(4)  | −23.748(10) | 1.759(5)  | 2.75(5)   |
| 11  | Machleidt [28] (2001)        | 5.419(7)  | −23.740(20) | 1.753(8)  | 2.77(5)   |
Table 4. Low-energy parameters of neutron–proton scattering that were obtained on the basis of the present-day data of the partial-wave analysis and modern realistic models of nucleon–nucleon interaction

| No. | Model       | $a_t$, fm | $a_s$, fm | $r_t$, fm | $r_s$, fm | $\sigma_0$, b | $f$, fm  |
|-----|-------------|-----------|-----------|-----------|-----------|---------------|----------|
| 1   | GWU PWA     | 5.4030    | −23.719   | 1.7494    | 2.626     | 20.426        | −3.755   |
| 2   | Nijm PWA    | 5.420     | −23.739   | 1.753     | 2.678     | 20.473        | −3.7395  |
| 3   | Argonne V18 | 5.419     | −23.732   | 1.753     | 2.697     | 20.461        | −3.7375  |
| 4   | CD Bonn     | 5.4199    | −23.738   | 1.751     | 2.671     | 20.471        | −3.7392  |
| 5   | Moscow      | 5.422     | −23.740   | 1.754     | 2.66      | 20.476        | −3.7370  |
| 6   | Expt. [10, 12] | 5.405(6) | −23.728(13)| 1.738(7) | 2.56(10) | 20.436(23) | −3.756(9) |
| 7   | Expt. [24]  | 5.424(4)  | −23.748(10)| 1.759(5) | 2.75(5)  | 20.491(14) | −3.738(1) |
| 8   | Expt. [28]  | 5.419(7)  | −23.740(20)| 1.753(8) | 2.77(5)  | 20.476(12) | −3.7409(11)|