Benchmark potential energy curve for collinear H₃

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Abstract
A benchmark-quality potential energy curve is reported for the H₃ system in collinear nuclear configurations. The electronic Schrödinger equation is solved using explicitly correlated Gaussian (ECG) basis functions using an optimized fragment initialization technique that significantly reduces the computational cost. As a result, the computed energies improve upon recent orbital-based and ECG computations. Starting from a well-converged basis set, a potential energy curve with an estimated sub-parts-per-billion precision is generated for a series of nuclear configurations using an efficient ECG rescaling approach.

Keywords: H₃, ECG

1. Introduction
The simplest chemical reaction H₂ + H → H + H₂—and its isotopologues—is possibly one of the most exhaustively studied chemical processes [1]. Furthermore, the H₃ system has qualitatively interesting features: a shallow van-der-Waals minimum for collinear nuclear structures and a conical intersection for equilateral triangular configurations. These features pose challenges when investigating the quantum dynamics of the system and require a high-level description of the electronic structure. The first potential energy surface (PES) for collinear H₃ was obtained by Liu in 1973 [2]. Since then, several full-dimensional surfaces have been published [3, 4, 5, 6, 7, 8, 9] and refined [10, 11, 12, 13, 14, 15, 16] using increasingly accurate quantum chemical methods. More recently, a multireference configuration interaction (MRCI) PES was developed, using a hierarchy of correlation consistent basis sets followed by extrapolation to the complete basis set (CBS) limit [17] with an estimated μE₉ level of precision. This complete configuration interaction (CCI) surface has been the most accurate full-dimensional PES of H₃, and it was used to resolve long-standing discrepancy of experimental and theoretical thermal rate constants [18].

The aim of the present letter is to explore and take the achievable precision further for H₃, a simple prototype for poly-electronic and polyatomic molecular systems, using explicitly correlated Gaussian functions.

2. Method
The Schrödinger equation (in Hartree atomic units) with \( N_{\text{nuc}} \) nuclei clamped at the \( R \) configuration and \( n_e \) electrons,

\[
H\psi(r; R) = E(R)\psi(r; R)
\]
\begin{equation}
H = \frac{1}{2} \sum_{i=1}^{N_e} p_i^2 - \sum_{i=1}^{N_e} \sum_{a=1}^{N_R} \frac{Z_a}{r_{ia}} + \sum_{i<j}^{N_e} \frac{1}{r_{ij}} + \sum_{a<b}^{N_R} \frac{Z_a Z_b}{R_{ab}}.
\end{equation}

is solved for the ground state of \( \text{H}_3 \) using a set of floating ECG basis functions,

\begin{equation}
\psi(r, R) = \mathcal{A} \sum_{n=1}^{N_s} c_n \phi_n(r, A_n, s_n) \chi_n(\theta)
\end{equation}

\begin{equation}
\phi_n(r; A_n, s_n) = \exp \left[ - (r - s_n)^T A_n (r - s_n) \right],
\end{equation}

where \( A_n = A_n \otimes I_1 \), \( A_n \in \mathbb{R}^{n_H \times n_H} \) is the exponent matrix and \( r, s \in \mathbb{R}^{3n_H} \) are the coordinate vectors of the electrons and the Gaussian centers, respectively. \( \mathcal{A} \) is the anti-symmetrization operator, and \( A \) is parameterized in the \( A = L^T L \) Cholesky-form, with an \( L \) lower-triangular matrix, to ensure positive definiteness of \( A \) and square integrability of the basis functions. The \( A_1 \) point group (in the \( C_{3v} \) point group) of the ground-state wave function is realized by constraining the Gaussian centers to the \( z \) axis.

The \( \chi_n(\theta) \) three-particle spin function corresponding to the doublet multiplicity of the ground-state is obtained as a linear combination of the two possible couplings of the elementary, one-electron spin functions \( \sigma_i(1) \frac{1}{2}, \frac{1}{2} \) to a doublet state \( [21] \),

\begin{equation}
\chi_n = d_{n_1} \left\{ \left( \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right)_{l=0} \sigma(3) \frac{1}{2} \right\} \frac{1}{2}, \frac{1}{2} + d_{n_2} \left\{ \left( \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right)_{l=0} \sigma(3) \frac{1}{2} \right\} \frac{1}{2}, \frac{1}{2},
\end{equation}

where the square brackets denote angular momentum coupling, using the Clebsch–Gordan coefficients \( \{ j_1, m_{j_1}, j_2, m_{j_2}, j_3, m_{j_3} \} \). For example, coupling two spin-1/2 particles to a singlet function is labelled as

\begin{equation}
\left[ \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right]_{l=0,0} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \left( \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right)_{\frac{1}{2}, \frac{1}{2}},
\end{equation}

\begin{equation}
\left[ \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right]_{l=0,1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \left( \sigma(1) \frac{1}{2}, \sigma(2) \frac{1}{2} \right)_{\frac{1}{2}, \frac{1}{2}} = \frac{1}{\sqrt{2}} \left( \left| \uparrow \downarrow \right> - \left| \downarrow \uparrow \right> \right).
\end{equation}

Considering the normalization condition as well, the doublet three-electron spin functions can be parameterized by a single \( \theta_n \) parameter as

\begin{equation}
d_{n_1} = \sin \theta_n \quad \text{and} \quad d_{n_2} = \cos \theta_n,
\end{equation}

and \( \theta_n \) is optimized together with the nonlinear parameters of the basis set.

### 2.1. Optimized fragment initialization

The initial basis function parameters are usually generated in a pseudo-random manner, retaining those functions from a trial set that provide the lowest energy expectation value. This generation procedure is followed by extensive refinement of the parameterization based on the variational principle \([21]\). By increasing the number of electrons, the dimensionality of the parameter space, and hence, the optimization cost increases. To keep the computational cost low, it is useful to consider that the interaction between the electrons of the hydrogen molecule and the electron of the hydrogen atom is weak in the van-der-Waals well or if the two ‘fragments’ are not too close, in general. If the interaction is not too strong, then a \( \psi_0 \) initial approximation for the wave function can be written as the product of the wave functions optimized for the ‘fragments’ (atom and molecule for the present example):

\begin{equation}
\psi_0^H(r_1, r_2, r_3) = \psi_0^H (r_1, r_2) \psi_0^H (r_3),
\end{equation}

which corresponds to an initial parameterization of the three-electron basis set with

\begin{equation}
A^H_{kl} = \begin{pmatrix} A^H_{kl} & 0 \\ 0 & A^H_{kl} \end{pmatrix},
\end{equation}

and the 3-electron \( s \) vectors include the \( s \) vectors shifted according to the configuration of the ‘fragments’ in \( \text{H}_3 \):

\begin{equation}
s_{kl} = \begin{pmatrix} s_{kl}^H + R_{CM}^H s_{kl}^H \\ s_{kl}^H + R_{CM}^H s_{kl}^H \end{pmatrix},
\end{equation}

where \( R_{CM}^H \) is the center of mass of the protons in \( \text{H}_2 \).

This procedure is reminiscent of the monomer contraction method that was first introduced in Ref. \([22]\) for the helium dimer, although there are a few differences. First, we use the fragment (or monomer) basis set only to initialize the many(three)-electron basis, and we run repeated refinement cycles \([23, 24]\) using the Powell method \([25]\) for this initial basis. Second, retaining the full direct-product basis optimized for \( \text{H}_2 \) and separately for \( \text{H}_2 \) would be computationally very demanding, so instead, we truncate the direct-product basis according to the following strategy.

The ground-state wave function of the \( \text{H}_2 \) molecule was expanded over 1200 ECG functions, yielding \(-1.174 475 714 \) \( E_h \) for the ground state energy, which—compared to the
most accurate value obtained by Pachucki
−1.174 475 714 220 4434(5) Eh [26]—is con-
verged to a fraction of a nEh. The wave function
of the hydrogen atom was represented with
10 optimized Gaussian functions, resulting in
−0.499 999 332 Eh (in comparison with the exact
value, −0.5 Eh) ground-state energy. Inclusion of
all possible combinations of the \( H_2 \) and \( H \)
basis functions would result in a gigantic, 12 000-term
expansion. Such a long expansion would be
prohibitively expensive to extensively optimize
(refine), and it is unnecessary to have so many
functions for the reaching a \( 1 : 10^9 \) (ppb) precision.
To reduce the direct-product basis, it would be
possible to perform competitive selection over the
large basis space or to order (and then truncate)
the basis functions based on their importance in
lowering the energy [21]. In the present work, we
used a very simple construct that does not require
any computation: we have generated a set of 1200
functions by appending each \( H_2 \) basis function
from the 1200 set with a single \( H \) function. Out of
the 10 \( H \) functions, we have picked one based on
the basis index, \( i.e., \)
\[
\{ \phi_{10i} : \phi_{10i}^n \text{ where } n = 0, 1, \ldots, 119, i = 1, 2, \ldots, 10 \}
\]
\[
= \{ \phi_1^H, \phi_1^H \phi_2^H, \ldots, \phi_{10}^H \phi_{10}^H, \phi_1^H \phi_2^H, \phi_1^H \phi_3^H, \ldots, \phi_{10}^H \phi_{10}^H, \phi_1^H \phi_2^H, \phi_1^H \phi_3^H, \ldots, \phi_{10}^H \phi_{10}^H \}.
\]
(11)
The spin basis functions defined in Eq. (5), were
initialized by coupling the two electrons initially
localized on the \( H_2 \) fragment to a singlet state, \( i.e., \)
d\( n_1 = 0 \) and d\( n_2 = 1 \) corresponding to \( \vartheta_n = 0 \)
\( (n = 1, 2, \ldots, 1200) \) in Eqs. (5)–(7). All non-linear
parameters, including \( \vartheta_n \), of the initial basis set
were excessively optimized in repeated refinement
cycles (Fig. 1). The optimized fragment-based ini-
tialization of the basis set, described in this section,
allowed saving several weeks (months) of computer
time in comparison with Ref. [27] (see also Sec. 3).

2.2. Gaussian-center scaling

Independent variational optimization of the basis
set at may points along the PEC (or over the PES)
would make the computations very computationally
intensive. Kolos and Wolniewicz [28] noted already
in 1964 that for a sufficiently large basis set, the
\( A_i \) exponents are insensitive to small displacements
of the nuclear coordinates. In 1997, Cencek and
Kutzelnigg proposed a scaling technique to gen-
erate a good initial ECG (re)parameterization for
the electronic basis set of diatomics upon small nu-
clear displacements [29]. They noted that their
approach can be generalized beyond diatomics. Pa-
vanello and Adamowicz implemented rescaling the
ECG centers (to have a good starting basis set) of
\( H_2 \) upon small nuclear displacements to gen-
erate a series of points to represent the 3D PES
[27, 30, 31, 32]. Upon a small \( \Delta R_a \) displacement of
the coordinates of the \( a \)th nucleus,
\[
R'_a = R_a + \Delta R_a ,
\]
(12)
the \( s_i \) in \( R^3 \) ECG centers corresponding to the \( i \)th
electron were transformed as
\[
s'_i = s_i + \Delta s_i ,
\]
(13)
where \( \Delta s_i \) is expressed as a function of the \( \Delta R_a \) nu-
clear displacement,
\[
\Delta s_i = \frac{1}{W_i} \sum_{a=1}^{N_{lec}} w_{ia} \Delta R_a
\]
(14)
with \( W_i = \sum_{a=1}^{N_{lec}} w_{ia} \). The \( w_{ia} \) ‘weight’ is a function
constructed based on simple arguments. It is chosen
to be the distance of the \( s_i \) center and the \( a \)th
nucleus, \( |s_i - R_a| \) and it is expected to have good
limiting properties. First, it must vanish if the \( s_i \)
center is very (infinitely) far from the displaced
nucleus, \( \lim_{|s_i - R_a| \to \infty} w_{ia} = 0 \). Second, the closer the \( s_i \)
center to the \( R_a \) nucleus position, the \( \Delta R_a \) dis-
placement has a larger contribution, \( i.e., \) larger \( w_{ia} \)
weight, to the \( \Delta s_i \) change.

These conditions allow several possible choices
for the weight function. For example, Coulomb-
like weights were used in Ref. [27]

\[ w^C_{ia} = \frac{1}{|s_i - R_a|}. \]  

(15)

After some experimentation with different possible functions, and inspired by the picture that the weight function can be intuitively defined as if there was some attraction between the centers and the nuclear positions by a central field, a Yukawa-like weight function appears to be a good choice

\[ w^Y_{ia} = e^{-\mu|s_i - R_a|}, \]  

(16)

where the parameter \( \mu \in \mathbb{R}^+ \) was set to unity in this work. For small nuclear displacements, a parameterization rescaled with Yukawa weights (with \( \mu = 1 \)) provided an energy lower than rescaling with Coulomb weights, Eq. (15).

The rescaling technique with the Yukawa weight function was used to generate the PEC corresponding to the \( \text{H}_2 \) molecule with a proton-proton distance fixed at \( R_{\text{H}_2} = 1.4 \) bohr. The \( R_{\text{H}_2} - \text{H} \) distance of the hydrogen atom was measured from the center of mass of the \( \text{H}_2 \) fragment. The starting value was \( R_{\text{H}_2} - \text{H} = 6.442 \) bohr, for which an initial basis set was generated using the optimized fragment initialization (Sec. 2.1) and the representation was improved through several Powell refinement cycles [25] of the non-linear parameters (Fig. 1). Then, initial basis sets were generated by making small \( \Delta R_{\text{H}_2} - \text{H} = \pm 0.1 \) bohr displacements, rescaling the centers according to Eq. (14) with Yukawa weights, Eq. (16), followed by 5 entire basis refinement cycles (that took 4 hours) before the next step was taken along the series of the nuclear configurations (the positive and the negative displacement series were run in parallel). All computations have been carried out using the QUANTEN computer program [24, 33, 34, 35].

The energies (Fig. 2) and optimized basis set parameters are deposited in the Supplementary Material.

3. Results and discussion

We have carried out extensive single-point computations for the near-equilibrium geometry in the van-der-Waals well with \( R_{\text{H}_2}^{(0)} = 1.4 \) bohr and \( R_{\text{H}_2}^{(0)} - \text{H} = 6.442 \) bohr first reported in Ref. [19]. This structure is close to the equilibrium geometry obtained with carefully conducted orbital-based computations [17] (Table 2). The energy of Ref. [19] computed with a small ECG basis is inaccurate, but later, large-scale computations were reported in Ref. [20].

At this geometry, the best energy obtained from the present work with 1200 ECGs (constructed by the initial fragment initialization, Sec. 2.1, followed by \( n_{\text{Powell}} = 3000 \) Powell refinement cycles of the entire basis set) is \(-1.674\; 561\; 687\; \text{E}_\text{h}\) (upper part of Table 1). Table 1 also shows the computed energy values for smaller basis sets that allow assessment of the convergence and extrapolation to the complete basis set (CBS) limit [36].

Direct comparison with Ref. [20] requires further computation, because the extensively optimized energy reported in Ref. [20] appears to belong to a 6.442 bohr distance of the hydrogen atom not from the center of nuclear mass of the \( \text{H}_2 \) unit, but from the closer proton of \( \text{H}_2 \). We think that this nuclear structure was used in Ref. [20], because we obtain good agreement for the energies when we perform the computation at this geometry, shown in the lower part of Table 1, corresponding to \( R_{\text{H}_2}^{(0)} = 1.40 \) bohr and \( R_{\text{H}_2} - \text{H}' = R_{\text{H}_2} - \text{H}^{(0)} + R_{\text{H}_2}^{(0)}/2 = 6.442 \) bohr + 0.700 bohr = 7.142 bohr.

We also note that the best energy value of Ref. [20] computed in 6 months (using 12 CPU cores) was reproduced in this work (corresponding to the structure given in footnote b of Table 1) using the optimized fragment initialization technique (Sec. 2.1) followed by a few Powell refinement cycles in in 4 days. The computational benefit of the optimized fragment technique is significant in comparison with a computation [20] constructed from ‘scratch’ immediately for the three-particle problem.

Then, we continued the extensive refinement of the basis parameterization based on the variational
Table 1: Convergence of the non-relativistic, ground-state energy of H₂ near the van-der-Waals equilibrium structure at \(R_{\text{H}_2} = 1.4\) bohr and \(R_{\text{H}_2\cdot\text{H}} = 6.442\) bohr taken from Ref. [19].

| \(N_b\) | Ansatz | \(n_{\text{Powell}}\) | \(E [E_b]\) |
|--------|--------|----------------|------------|
| 600    | \(\langle \psi_{\text{H}_2}^{(0)} \rangle \cdot \langle \psi_{\text{H}_2}^{(1)} \rangle\) | 2000       | -1.674 560 470 |
| 800    | \(\langle \psi_{\text{H}_2}^{(0)} \rangle \cdot \langle \psi_{\text{H}_2}^{(1)} \rangle\) | 2000       | -1.674 561 379 |
| 1000   | \(\langle \psi_{\text{H}_2}^{(0)} \rangle \cdot \langle \psi_{\text{H}_2}^{(1)} \rangle\) | 2000       | -1.674 561 583 |
| 1200   | \(\langle \psi_{\text{H}_2}^{(0)} \rangle \cdot \langle \psi_{\text{H}_2}^{(1)} \rangle\) | 3000       | -1.674 561 687 |

\[\text{[Extrapolation to } N_b \rightarrow \infty: \text{ } -1.674 561 75(3)]\]

\(R_{\text{H}_2} = 1.40\) bohr, \(R_{\text{H}_2\cdot\text{H}} = 7.142\) bohr. \(^a\)

\(R_{\text{H}_2} = 1.40\) bohr, \(R_{\text{H}_2\cdot\text{H}} = 6.442\) bohr, measured from the nuclear center of mass (NCM) of the \(\text{H}_2\) unit. \(^b\)

Geometry \(^c\) is claimed in Ref. [20], but it appears to be \(^b\). The difference amounts to whether the distance of the hydrogen atom is measured from the NCM or the nearer proton.

Table 2: Comparison of energies of various \(ab\) \(initio\) computations. The equilibrium geometry, determined at the MRCI/aug-cc-pV6Z level is \(R_{\text{H}_2} = 1.4015\) bohr and \(R_{\text{H}_2\cdot\text{H}} = 6.51205\) bohr [17].

| Source | \(E [E_b]\) |
|--------|------------|
| aug-cc-pVDZ \(^a\) | -1.664 339 |
| aug-cc-pVTZ \(^a\) | -1.672 540 |
| aug-cc-pVQZ \(^a\) | -1.673 902 |
| aug-cc-pV5Z \(^a\) | -1.674 332 |
| aug-cc-pV6Z \(^a\) | -1.674 445 |
| aug-mcc-pVTZ \(^a\) | -1.672 553 |
| aug-mcc-pVQZ \(^a\) | -1.673 917 |
| aug-mcc-pV5Z \(^a\) | -1.674 298 |
| aug-mcc-pV6Z \(^a\) | -1.674 430 |
| aug-mcc-pV7Z \(^a\) | -1.674 488 |
| MBE\(^{\text{cc}}\text{(3,4 CBS)}\) \(^b\) | -1.674 566 |
| MBE\(^{\text{mcc}}\text{(6,7 CBS)}\) \(^c\) | -1.674 562 |
| Present work \((N_b = 1200)^d\) | -1.674 562 264 |

\(^a\) Ref. [17]: MRCI energy.
\(^b\), \(^c\) Ref. [17]: extrapolated CBS energy corresponding to the aug-cc-pVXZ \((X = 3, 4)\) and aug-mcc-pVXZ \((X = 6, 7)\) basis sets, respectively.
\(^d\) Rescaled from the basis set optimized for the \((R_{\text{H}_2}^{(0)}, R_{\text{H}_2\cdot\text{H}}^{(0)})\) structure in Table 1 followed by 1000 Powell refinement cycles.

4. Summary, conclusion, and outlook

In summary, we have computed a benchmark-quality one-dimensional segment of the Born–Oppenheimer potential energy surface of the \(\text{H}_3\) system for a series of collinear nuclear configurations. The electronic energies are estimated to be converged on the sub-parts-per-million level.

The depth of the van-der-Waals well was predicted to be \(86(1)\) \(\mu E_b\) at the \(R_{\text{H}_2} = 1.4015\) bohr and \(R_{\text{H}_2\cdot\text{H}} = 6.51205\) bohr geometry in MRCI computations underlying the currently most precise potential energy surface of \(\text{H}_2\) [17]. The variational computations reported in this work and using a (relatively small) explicitly correlated Gaussian basis set confirm this value and improve upon its precision by two orders of magnitude, \(86.54(3) \mu E_b\). In order to achieve a similar precision for non-collinear nuclear structures, which have a lower order or no point-group symmetry, it will be necessary to use a larger basis set, which is certainly feasible.
Regarding the broader context of this work, (non-)adiabatic perturbation theory [37, 38, 39, 40, 41] combined with leading-order relativistic and quantum electrodynamics (QED) corrections [42, 43] are expected to provide a state-of-the-art theoretical description for this system. This framework has already been extensively used and tested for the lightest diatomic molecules [44, 35]. For the ground-electronic state of the H2 molecule, the effect of the non-adiabatic-relativistic coupling has also been evaluated and was found to be non-negligible [45]. In this direction, the computation of a precise representation of the electronic wave function is a necessary first step that was demonstrated in this work to be feasible. The adiabatic, non-adiabatic and (regularized) relativistic and QED corrections can be evaluated at a couple of points using currently existing procedures [41, 46, 35, 47]. At the same time, for a complete description of a polyatomic system like H2, these corrections must be computed over hundreds or thousands of nuclear configurations. This requires a fully automated evaluation and error control of all corrections, which may be especially challenging for the singular terms in the relativistic and QED expressions, and this requires further methodological and algorithmic developments that is left for future work.

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Table 3: Potential energy curve of collinear H$_2$ with collinear hydrogen atoms and the H$_3$ structure fixed at $R_{H-}$ = 1.4 bohr.

| $R_{H-}$ [bohr] | $E$ [E$_h$] | $R_{H-}$ [bohr] | $E$ [E$_h$] | $R_{H-}$ [bohr] | $E$ [E$_h$] |
|----------------|-------------|----------------|-------------|----------------|-------------|
| 3.942          | -1.671 027 070 | 7.742          | -1.674 527 262 | 11.542         | -1.674 480 330 |
| 4.042          | -1.671 542 481 | 7.842          | -1.674 524 133 | 11.642         | -1.674 480 079 |
| 4.142          | -1.671 995 736 | 7.942          | -1.674 521 142 | 11.742         | -1.674 479 843 |
| 4.242          | -1.672 392 125 | 8.042          | -1.674 518 294 | 11.842         | -1.674 479 622 |
| 4.342          | -1.672 736 967 | 8.142          | -1.674 515 593 | 11.942         | -1.674 479 415 |
| 4.442          | -1.673 035 388 | 8.242          | -1.674 513 039 | 12.042         | -1.674 479 220 |
| 4.542          | -1.673 292 312 | 8.342          | -1.674 510 633 | 12.142         | -1.674 479 036 |
| 4.642          | -1.673 512 388 | 8.442          | -1.674 508 369 | 12.242         | -1.674 478 864 |
| 4.742          | -1.673 699 926 | 8.542          | -1.674 506 245 | 12.342         | -1.674 478 702 |
| 4.842          | -1.673 858 896 | 8.642          | -1.674 504 254 | 12.442         | -1.674 478 549 |
| 4.942          | -1.673 992 934 | 8.742          | -1.674 502 391 | 12.542         | -1.674 478 405 |
| 5.042          | -1.674 105 325 | 8.842          | -1.674 500 651 | 12.642         | -1.674 478 269 |
| 5.142          | -1.674 198 999 | 8.942          | -1.674 499 026 | 12.742         | -1.674 478 141 |
| 5.242          | -1.674 276 566 | 9.042          | -1.674 497 510 | 12.842         | -1.674 478 020 |
| 5.342          | -1.674 340 341 | 9.142          | -1.674 496 096 | 12.942         | -1.674 477 906 |
| 5.442          | -1.674 392 365 | 9.242          | -1.674 494 779 | 13.042         | -1.674 477 799 |
| 5.542          | -1.674 434 419 | 9.342          | -1.674 493 552 | 13.142         | -1.674 477 697 |
| 5.642          | -1.674 468 056 | 9.442          | -1.674 492 409 | 13.242         | -1.674 477 601 |
| 5.742          | -1.674 494 619 | 9.542          | -1.674 491 345 | 13.342         | -1.674 477 510 |
| 5.842          | -1.674 515 270 | 9.642          | -1.674 490 355 | 13.442         | -1.674 477 424 |
| 5.942          | -1.674 531 005 | 9.742          | -1.674 489 433 | 13.542         | -1.674 477 343 |
| 6.042          | -1.674 542 675 | 9.842          | -1.674 488 574 | 13.642         | -1.674 477 266 |
| 6.142          | -1.674 551 007 | 9.942          | -1.674 487 775 | 13.742         | -1.674 477 193 |
| 6.242          | -1.674 556 616 | 10.042         | -1.674 487 030 | 13.842         | -1.674 477 124 |
| 6.342          | -1.674 560 021 | 10.142         | -1.674 486 337 | 13.942         | -1.674 477 058 |
| 6.442          | -1.674 561 676 | 10.242         | -1.674 485 691 | 14.042         | -1.674 476 996 |
| 6.542          | -1.674 561 899 | 10.342         | -1.674 485 088 | 14.142         | -1.674 476 937 |
| 6.642          | -1.674 561 042 | 10.442         | -1.674 484 527 | 14.242         | -1.674 476 880 |
| 6.742          | -1.674 559 343 | 10.542         | -1.674 484 003 | 14.342         | -1.674 476 827 |
| 6.842          | -1.674 557 010 | 10.642         | -1.674 483 515 | 14.442         | -1.674 476 777 |
| 6.942          | -1.674 554 214 | 10.742         | -1.674 483 058 | 14.542         | -1.674 476 728 |
| 7.042          | -1.674 551 095 | 10.842         | -1.674 482 632 | 14.642         | -1.674 476 683 |
| 7.142          | -1.674 547 764 | 10.942         | -1.674 482 234 | 14.742         | -1.674 476 639 |
| 7.242          | -1.674 544 313 | 11.042         | -1.674 481 862 | 14.842         | -1.674 476 598 |
| 7.342          | -1.674 540 812 | 11.142         | -1.674 481 514 | 14.942         | -1.674 476 559 |
| 7.442          | -1.674 537 318 | 11.242         | -1.674 481 188 | 15.042         | -1.674 476 521 |
| 7.542          | -1.674 533 875 | 11.342         | -1.674 480 883 | 15.142         | -1.674 476 485 |
| 7.642          | -1.674 530 514 | 11.442         | -1.674 480 598 | 15.242         | -1.674 476 451 |