# Higher-order $C_n$ dispersion coefficients for hydrogen

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The complete set of second-, third-, and fourth-order van der Waals coefficients $C_n$ up to $n=32$ for the H($1s$)-H($1s$) dimer have been determined. They are computed by diagonalizing the nonrelativistic Hamiltonian for hydrogen to obtain a set of pseudostates that are used to evaluate the appropriate sum rules. A study of the convergence pattern for $n \leqslant 16$ indicates that all the $C_{n \leqslant 16}$ coefficients are accurate to 13 significant digits. The relative size of the fourth-order $C_n^{(4)}$ to the second-order $C_n^{(2)}$ coefficients is seen to increase as $n$ increases and at $n=32$ the fourth-order term is actually larger.

## I. INTRODUCTION

The long-range interaction between two spherically symmetric atoms can be written in the general form

$$V(R \rightarrow \infty) = -V_6(R) - V_8(R) - V_{10}(R) - V_{11}(R) - \cdots, \tag{1}$$

where the dispersion potential $V_n(R)$ of order $n$ is written as

$$V_n(R) = \frac{C_n}{R^n}. \tag{2}$$

The $C_n$ parameters are the van der Waals dispersion coefficients. The even ($n=6, 8, \ldots$) dispersion coefficients are calculated using sum rules derived from second-order perturbation theory and provide an attractive interaction. The odd ($n=11, 13, \ldots$) terms come from third-order perturbation theory and are repulsive [1,2]. Contributions from fourth-order perturbation theory start at $n=12$ [1,3].

The dispersion interaction for the simplest system—namely, the hydrogen dimer—is only known precisely to $n=11$. The latest calculations by Yan and Dalgarno (YD) [2] reported almost exact values for the second-order even dispersion parameters up to $n=16$. They also gave almost exact results for the third-order coefficients, up to $n=15$. However, it is known that contributions from fourth-order perturbation theory start at $n=12$ [1,3,4], so the dispersion potential computed from the YD $C_n$ is incomplete for $n>11$.

In this article, the complete set of dispersion parameters from $C_6$ to $C_{16}$ is computed by using a large pseudostate expansion to evaluate the appropriate sum rules. The contributions from fourth-order perturbation theory to $C_{12}$, $C_{14}$, and $C_{16}$ are explicitly included.

## II. CALCULATION OF THE DISPERSION PARAMETERS

All the dispersion coefficients computed in this paper were computed by first diagonalizing the nonrelativistic Hamiltonian in a large basis of orthogonal Laguerre-type orbitals (LTO's) [5] defined by

$$\chi_\alpha(r) = N_\alpha r^{\ell+1} \exp(-\lambda_\alpha r) L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r), \tag{3}$$

where the normalization constant is

$$N_\alpha = \sqrt{\frac{(2\lambda_\alpha)^{2\ell+3}(n_\alpha - \ell - 1)!}{(\ell + n_\alpha + 1)!}}. \tag{4}$$

The function $L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r)$ is an associated Laguerre polynomial that can be defined in terms of a confluent hypergeometric function [6] as

$$L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r) = \frac{(n_\alpha + \ell + 1)!}{(n_\alpha - \ell - 1)!(2\ell + 2)!}$$
$$\times M(-(n_\alpha - \ell - 1), 2\ell + 3, 2\lambda_\alpha r). \tag{5}$$

All the matrix elements can be written in analytic forms provided a common $\lambda_\alpha$ is adopted throughout the calculation. However, in the present work, the radial wave functions were placed on a numerical grid and all matrix elements computed by Gaussian quadratures. This was done for reasons of convenience as the diagonalization could be done with an existing program used in previous calculations of the dispersion parameters and the structures of positronic atoms [7,8]. This program can achieve close to machine precision in almost all radial matrix computations.

Once the Hamiltonian diagonalization is complete, sum rules involving radial matrix elements were used to determine the dispersion parameters. The specific sum rules used are those derived by Ovsiannikov, Guilyarovski, and Lopatko (OGL) [1]. Their expressions are a bit simpler than those developed by other authors [2,3]. There were some omissions in their published equations [9], and a more thorough description of the sum rules is presented here.

### A. Second-order terms

The second-order dispersion coefficients for the H—H system have been determined to high accuracy [2,10,11], even for high $n$. The working expression adopted for computation is

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$$C_{2\lambda+6}^{(2)} = \sum_{\ell_1=1}^{\lambda+1} \frac{(2\lambda+4)!}{(2\ell_1+1)!(2\ell_1'+1)!}$$
$$\times \sum_{i_1,i_1'} \frac{\langle 0,0|r^{\ell_1}|i_1,\ell_1\rangle^2 \langle 0,0|r^{\ell_1'}|i_1',\ell_1'\rangle^2}{(E_{i_1}+E_{i_1'}-2E_0)}, \quad (6)$$

where $\ell_1'=\lambda+2-\ell_1$. The state vector $|i_1,\ell_1\rangle$ represents the radial part of the state $i_1$ with orbital angular momentum $\ell_1$ and energy $E_{i_1}$. The ground state energy is $E_0$. The sum rule

$$T^{(\ell)} = \sum_i \langle 0,0|r^\ell|i,\ell\rangle^2 = \frac{(2\ell+2)!}{2^{(2\ell+1)}} \quad (7)$$

is a useful diagnostic check of the accuracy of the underlying discretization of the H spectrum.

### B. Third-order terms $C_{11}$ and $C_{13}$

The dispersion coefficients $C_{11}$ and $C_{13}$ arise from third-order perturbation theory [1–4,12]. Close to exact dispersion parameters for the H—H system have been published [2]. The general expression for the third-order $C_{2\lambda+11}$ is [1]

$$C_{2\lambda+11} = -\sum_{\ell_1 k_1 \ell_2} \sum_{\ell_1' k_1' \ell_2'} \sum_{i_1 i_1' i_2 i_2'} \frac{G(\lambda,\ell_1,\ell_1',\ell_2,\ell_2',k_1,k_1')}{(E_{i_1 i_1'}-2E_0)(E_{i_2 i_2'}-2E_0)}$$
$$\times \langle 0,0|r^{\ell_1}|i_1,\ell_1\rangle\langle i_1,\ell_1|r^{k_1}|i_2,\ell_2\rangle\langle i_2,\ell_2|r^{\ell_2}|0,0\rangle$$
$$\times \langle 0,0|r^{\ell_1'}|i_1',\ell_1'\rangle\langle i_1',\ell_1'|r^{k_1'}|i_2',\ell_2'\rangle\langle i_2',\ell_2'|r^{\ell_2'}|0,0\rangle, \quad (8)$$

with the notation $E_{i_1 i_1'}=E_{i_1}+E_{i_1'}$ being used in the energy denominator. The parameter $\lambda$ is defined,

$$2\lambda+8 = \ell_1+k_1+\ell_2+\ell_1'+k_1'+\ell_2' \quad (9)$$

and all of the angular momentum indices are greater than zero. Defining $J=(\ell_1+k_1+\ell_2)/2$ and $J'=(\ell_1'+k_1'+\ell_2')/2$, the coefficient $G$ is defined as

$$G(\lambda,\ell_1,\ell_1',\ell_2,\ell_2',k_1,k_1') = (\lambda+4)!A(J,\ell_1,k_1,\ell_2)$$
$$\times A(J',\ell_1',k_1',\ell_2')B(\lambda,\ell_1,\ell_1')$$
$$\times B(\lambda,k_1,k_1')B(\lambda,\ell_2,\ell_2'), \quad (10)$$

where

$$B(\lambda,\ell_1,\ell_2) = \frac{[2(\lambda+4-\ell_1-\ell_2)]!}{(\lambda+4-\ell_1-\ell_2)!} \quad (11)$$

and

$$A(J,\ell_1,k_1,\ell_2) = \frac{J!}{(2J+1)!(J-\ell_1)!(J-k_1)!(J-\ell_2)!}. \quad (12)$$

### C. Fourth-order contributions to $C_{12}$ and $C_{14}$

As far as we know, there have only been two explicit calculations of the fourth-order contribution to $C_{12}$. Bukta and Meath [3] gave estimates of $C_{12}^{(2)}$ and $C_{12}^{(4)}$ for the hydrogen dimer. Ovsiannikov et al. [1] developed a general and

compact expression for the evaluation of $C_n^{(4)}$, and in addition they reported values of $C_{12}^{(4)}$ for all possible combinations of hydrogen and the alkali-metal atoms. Rectifying some omissions in their published equations [9], one writes

$$C_{2\lambda+12}^{(4)} = b_{2\lambda+12} - \sum_{\lambda_1=0}^{\lambda} C_{2\lambda_1+6}^{(2)} a_{2\lambda_2+6}, \quad (13)$$

where $\lambda=\lambda_1+\lambda_2$.

The factor $a_{2\lambda_2+6}$ is

$$a_{2\lambda_2+6} = \sum_{\ell_1=1}^{\lambda_2+1} \frac{(2\lambda_2+4)!}{(2\ell_1+1)!(2\ell_1'+1)!}$$
$$\times \sum_{i_1,i_1'} \frac{\langle 0,0|r^{\ell_1}|i_1,\ell_1\rangle^2 \langle 0,0|r^{\ell_1'}|i_1',\ell_1'\rangle^2}{(E_{i_1}+E_{i_1'}-2E_0)^2}, \quad (14)$$

where $\ell_1+\ell_1'=\lambda+2$. The expression for $a_{2\lambda+6}$ is practically the same as Eq. (6) for $C_{2\lambda+6}^{(2)}$, the only difference being an extra factor in the energy denominator [compare with Eq. (10) of [1]].

The factor $b_{2\lambda+12}$ is more complicated and defined as

$$b_{2\lambda+12} = \sum_{\ell_1,\ell_2,\ell_3} \sum_{\ell_1',\ell_2',\ell_3'} \sum_{k_1,k_2,k_1',k_2'} \sum_K \sum_{i_1 i_1' i_2 i_2' i_3 i_3'}$$
$$\times \left[ \frac{\hat{L}_1!\hat{K}_1!\hat{K}_2!\hat{L}_3!}{2\ell_1!2\ell_1'!2k_1!2k_1'!2k_2!2k_2'!2\ell_3!2\ell_3'!} \right]^{1/2}$$
$$\times \langle \ell_1 0 k_1 0|\ell_2 0\rangle\langle \ell_1' 0 k_1' 0|\ell_2' 0\rangle$$
$$\times \langle k_2 0 \ell_3 0|\ell_2 0\rangle\langle k_2' 0 \ell_3' 0|\ell_2' 0\rangle$$
$$\times \langle L_1 0 K_1 0|K0\rangle\langle K_2 0 L_3 0|K0\rangle$$
$$\times \begin{Bmatrix} \ell_1 & \ell_1' & L_1 \\ k_1 & k_1' & K_1 \\ \ell_2 & \ell_2' & K \end{Bmatrix} \begin{Bmatrix} k_2 & k_2' & K_2 \\ \ell_3 & \ell_3' & L_3 \\ \ell_2 & \ell_2' & K \end{Bmatrix}$$
$$\times \frac{1}{(E_{i_1 i_1'}-2E_0)(E_{i_2 i_2'}-2E_0)(E_{i_3 i_3'}-2E_0)}$$
$$\times \langle 0,0|r^{\ell_1}|i_1,\ell_1\rangle\langle i_1,\ell_1|r^{k_1}|i_2,\ell_2\rangle$$
$$\times \langle i_2,\ell_2|r^{k_2}|i_3,\ell_3\rangle\langle i_3,\ell_3|r^{\ell_3}|0,0\rangle$$
$$\times \langle 0,0|r^{\ell_1'}|i_1',\ell_1'\rangle\langle i_1',\ell_1'|r^{k_1'}|i_2',\ell_2'\rangle$$
$$\times \langle i_2',\ell_2'|r^{k_2'}|i_3',\ell_3'\rangle\langle i_3',\ell_3'|r^{\ell_3'}|0,0\rangle, \quad (15)$$

where $L_1=\ell_1+\ell_1'$, $L_3=\ell_3+\ell_3'$, $K_1=k_1+k_1'$, and $K_2=k_2+k_2'$. We use $\hat{L}=(2L+1)$. The sums are constrained by the condition

$$L_1+K_1+K_2+L_3 = 2\lambda+8. \quad (16)$$

While $\ell_1$, $\ell_1'$, $\ell_3$, and $\ell_3'$ must be greater than 0, it is possible for $\ell_2$ and $\ell_2'$ to be equal to 0. None of $k_1$, $k_1'$, $k_2$, or $k_2'$ can be zero. Since $\ell_2$ and $\ell_2'$ can both be equal to zero, the possibility of $i_2, i_2'$ both occupying the ground state must be explicitly excluded from the summation.

TABLE I. The dispersion coefficients for the H–H dimer. All the results in the "Best previous" column come from [2] except that for $C_{12}^{(4)}$ which is taken from [3]. All values are in atomic units.

| Coefficient | 10 LTO's | 15 LTO's | 20 LTO's | Best previous |
|---|---|---|---|---|
| $C_6$ | 6.499 026 705 3305 | 6.499 026 705 4057 | 6.499 026 705 4059 | 6.499 026 705 4058 |
| $C_8$ | 124.399 083 58236 | 124.399 083 58362 | 124.399 083 58362 | 124.399 083 58362 |
| $C_{10}$ | 3285.828 414 9425 | 3285.828 414 9674 | 3285.828 414 9674 | 3285.828 414 9674 |
| $C_{12}^{(2)}$ | $1.214\,860\,208\,9619 \times 10^5$ | $1.214\,860\,208\,9686 \times 10^5$ | $1.214\,860\,208\,9686 \times 10^5$ | $1.214\,860\,208\,9686 \times 10^5$ |
| $C_{14}^{(2)}$ | $6.060\,772\,689\,1671 \times 10^6$ | $6.060\,772\,689\,1917 \times 10^6$ | $6.060\,772\,689\,1917 \times 10^6$ | $6.060\,772\,689\,1921 \times 10^6$ |
| $C_{16}^{(2)}$ | $3.937\,506\,393\,9865 \times 10^8$ | $3.937\,506\,393\,9985 \times 10^8$ | $3.937\,506\,393\,9985 \times 10^8$ | $3.937\,506\,393\,9992 \times 10^8$ |
| $C_{11}$ | −3474.898 037 8919 | −3474.898 037 8822 | −3474.898 037 8822 | −3474.898 037 8822 |
| $C_{13}$ | $-3.269\,869\,240\,4549 \times 10^5$ | $-3.269\,869\,24\,04407 \times 10^5$ | $-3.269\,869\,24\,04407 \times 10^5$ | $-3.269\,869\,24\,04407 \times 10^5$ |
| $C_{15}$ | $-2.839\,558\,063\,3179 \times 10^7$ | $-2.839\,558\,063\,2998 \times 10^7$ | $-2.839\,558\,063\,2997 \times 10^7$ | $-2.839\,558\,063\,2998 \times 10^7$ |
| $C_{12}^{(4)}$ | 1241.587 803 8317 | 1241.587 803 8462 | 1241.587 803 8462 | 1241.588 |
| $C_{14}^{(4)}$ | $3.009\,633\,558\,9570 \times 10^5$ | $3.009\,633\,559\,0035 \times 10^5$ | $3.096\,633\,559\,0035 \times 10^5$ | |
| $C_{16}^{(4)}$ | $4.745\,455\,287\,4168 \times 10^7$ | $4.745\,455\,287\,4083 \times 10^7$ | $4.745\,455\,287\,4079 \times 10^7$ | |
| $C_{12}$ | $1.227\,276\,087\,0002 \times 10^5$ | $1.227\,276\,087\,0071 \times 10^5$ | $1.227\,276\,087\,0071 \times 10^5$ | $1.227\,27609 \times 10^{5\text{a}}$ |
| $C_{14}$ | $6.361\,736\,045\,0628 \times 10^6$ | $6.361\,736\,045\,0920 \times 10^6$ | $6.361\,736\,045\,0921 \times 10^6$ | |
| $C_{16}$ | $4.412\,051\,922\,7282 \times 10^8$ | $4.412\,051\,922\,7393 \times 10^8$ | $4.412\,051\,922\,7393 \times 10^8$ | |

[a]This entry adds the BM $C_{12}^{(4)}$ to the YD $C_{12}^{(2)}$.

## III. RESULTS OF THE CALCULATION

The results of the calculations for the complete set of dispersion coefficients up to $C_{16}$ are given in Table I. The parameters are given for basis sets with 10, 15, and 20 basis functions per angular momentum, respectively. The exponent in the LTO was chosen to be $\lambda=1.0$ for all angular momenta. This choice resulted in much faster convergence of the dispersion parameters than that observed by Yan and Dalgarno in their calculations of the third-order dispersion coefficients. Table I also gives results reported by YD and a single calculation of $C_{12}^{(4)}$ by Bukta and Meath (BM) [3].

### A. Second-order terms

The calculations of $C_n^{(2)}$ do not give new information, and Yan and Dalgarno [2] have given values which are converged to better than 15 significant figures. The present calculations with the $N=20$ basis are identical to 13 significant figures. The small differences in the last digit for some of coefficients arise from minor inaccuracies with the radial matrix elements. Hence we conclude that the present calculations are numerically reliable and that the pseudostate representation of the H spectrum is close to converged.

Besides the dispersion coefficients, the sum rule, Eq. (7) was evaluated and seen to be correct to 12 significant digits for all polarities relevant to the evaluation of $C_6-C_{16}^{(2)}$.

### B. Third-order terms

Since the third-order terms $C_n^{(3)}$ have already been given by YD, these calculations merely serve as a test of our numerical procedures. Once again, calculations with the 20 LTO basis agree with the YD results to 14 significant figures. It is worth noting that the present results required fewer terms than YD to achieve convergence. YD made the choice $\lambda_\alpha = 1/(\ell+1)$ in Eq. (3) and did not achieve convergence to the 14th digit place until the dimension of the LTO expansion was 50. The present basis with $\lambda_\alpha = 1.0$ achieves the same level of convergence with 20 LTO's.

### C. Fourth-order terms

The only previous explicit calculation of a fourth-order term was that made by BM [3], and the only parameter given was $C_{12}^{(4)}$. The OGL [1] estimate of $C_{12}^{(4)}$, $1.220 \times 10^5$ a.u., was made using an approximation to the Green's function and so perfect agreement is not expected. However, the present calculation agrees with the BM calculation of $C_{12}^{(4)}$ to all digits quoted: namely, seven.

The number of terms in the sum, Eq. (15), increases rapidly as $n$ increases. There are 4 terms for $C_{12}^{(4)}$, there are 64 terms for $C_{14}^{(4)}$, and finally there are 460 terms for $C_{16}^{(4)}$.

The dominant contribution to $C_n^{(4)}$ comes from $b_{2\lambda+12}$ with 96% of $C_{12}^{(4)}$ coming from $b_{12}$. The tendency for $b_{2\lambda+12}$ to be the dominant term in $C_n^{(4)}$ becomes more pronounced as $n$ increases, and for $n=16$ one has $|b_{16}-C_{16}^{(4)}|/|C_{16}^{(4)}|$ equal to $1.2 \times 10^{-3}$.

One feature of Table I concerns the relative size of $C_n^{(4)}$ to $C_n^{(2)}$. For $n=12$, the $C_n^{(4)}:C_n^{(2)}$ ratio is 1.02%. However, as $n$ gets larger, the ratio also gets larger. For $n=14$ the ratio is 4.97%, while for $n=16$ the ratio is 12.1%.

### D. Dispersion coefficients for $n \geq 17$

Higher-order contributions than fourth-order begin at $n=17$. There is a fifth-order contribution to $C_{17}$ and a sixth-order contribution to $C_{18}$ [1]. Estimates of $C_n^{(2)}$ for $n \geq 17$ have been made by a variety of authors [1,11,13–15]. How-

TABLE II. The $n \geqslant 16$ dispersion coefficients for the H—H dimer. All values are in atomic units.

| $n$ | $C_n^{(2)}$ | $C_n^{(4)}$ | $C_n^{(2)} + C_n^{(4)}$ | $-C_n^{(3)}$ |
|---|---|---|---|---|
| 17 | | | | $2.726\,099\,889 \times 10^9$ |
| 18 | $3.234\,218\,716 \times 10^{10}$ | $7.009\,061\,179 \times 10^9$ | $3.935\,124\,834 \times 10^{10}$ | |
| 19 | | | | $3.020\,900\,833 \times 10^{11}$ |
| 20 | $3.278\,573\,440 \times 10^{12}$ | $1.083\,922\,188 \times 10^{12}$ | $4.362\,495\,628 \times 10^{12}$ | |
| 21 | | | | $3.900\,227\,980 \times 10^{13}$ |
| 22 | $4.021\,082\,848 \times 10^{14}$ | $1.832\,218\,347 \times 10^{14}$ | $5.853\,301\,195 \times 10^{14}$ | |
| 23 | | | | $5.856\,636\,712 \times 10^{15}$ |
| 24 | $5.868\,996\,335 \times 10^{16}$ | $3.444\,924\,821 \times 10^{16}$ | $9.313\,921\,156 \times 10^{16}$ | |
| 25 | | | | $1.017\,059\,252 \times 10^{18}$ |
| 26 | $1.005\,294\,993 \times 10^{19}$ | $7.249\,737\,286 \times 10^{18}$ | $1.730\,268\,722 \times 10^{19}$ | |
| 27 | | | | $2.028\,440\,001 \times 10^{20}$ |
| 28 | $1.996\,944\,941 \times 10^{21}$ | $1.709\,243\,726 \times 10^{21}$ | $3.706\,188\,667 \times 10^{21}$ | |
| 29 | | | | $4.613\,037\,362 \times 10^{22}$ |
| 30 | $4.553\,288\,866 \times 10^{23}$ | $4.507\,006\,859 \times 10^{23}$ | $9.060\,295\,725 \times 10^{23}$ | |
| 31 | | | | $1.188\,007\,684 \times 10^{25}$ |
| 32 | $1.181\,107\,088 \times 10^{26}$ | $1.325\,398\,446 \times 10^{26}$ | $2.506\,505\,534 \times 10^{26}$ | |

ever, the only estimate of the third- and fourth-order terms with $n \geqslant 17$ are those of OGL [1]. By explicit calculation they obtained $C_{17}^{(3)} = -2.739 \times 10^9$ a.u., which agrees with the present more extensive calculation to within 1%. Making an approximation to the greens function they estimated $C_{18}^{(4)} = 3.3 \times 10^9$ a.u., which is about half the size of the present value.

The dispersion parameters up to $C_{32}$ from the present calculation are tabulated in Table II. The reason for taking the calculations so far rests in the relative size of the $C_n^{(4)}$ and $C_n^{(2)}$ terms. It was noticed that the $C_n^{(4)} : C_n^{(2)}$ ratio got larger as $n$ increased. So the calculations were extended to $C_{32}$ in order to demonstrate explicitly that the $C_n^{(4)} : C_n^{(2)}$ ratio can actually become larger than 1.0.

The precision of the entries in Table II is not as high as those in Table I. The calculations of $C_n^{(4)}$ did become more time consuming as $n$ increased. There were 922 064 different $(\ell_1, k_1, \ell_2, \ldots)$ combinations by the time $n=32$ was reached. Also the number of radial integrals in Eq. (15) increases as $N^6$ where $N$ is the number of LTO's for any given $\ell$. So the $N=20$ calculation is 64 times more intensive than the $N=10$ calculation.

The $C_n^{(2)}$ and $C_n^{(3)}$ entries in Table II were taken from the calculation with 15 LTO's. The $C_n^{(4)}$ entries were taken from a $N=15$ calculation up to $n=20$; thereafter, the $N=10$ basis was used. The values of $C_n^{(2)}$ agree with those of Thakkar [11] for all ten digits given in Table II. Comparisons between $N=10$ and $N=15$ calculations for $C_n^{(3)}$ suggest that the convergence is slower as $n$ increases and that $C_{31}^{(3)}$ is reliable to about six digits. A similar level of accuracy can be expected for $C_n^{(4)}$ and a comparison between the $N=10$ and $N=15$ values for $C_{20}^{(4)}$ gives agreement for the first nine digits.

## IV. CONCLUSIONS

The higher-$n$ dispersion parameters from $C_{11}$ to $C_{16}$ have been computed to an accuracy of 13 significant figures for the H–H dimer. Since the fourth-order contributions were included for $C_{12}$, $C_{14}$, and $C_{16}$, the adiabatic dispersion interaction can now be regarded as complete up to terms of order $R^{-16}$.

While the tabulations of dispersion coefficients report many digits, only the first five or so digits can be expected to correspond to the actual coefficients of two real hydrogen atoms. The present data have all been computed in the non-relativistic limit and therefore relativistic corrections to the energies and transition moments will alter the dispersion coefficients in the later digits.

The time taken to evaluate the dispersion coefficients was not excessive. For example, a calculation using 20 LTO's took about 17 min to determine all terms up $C_{16}$ on a 850 MHz CPU. Hence the pseudostate method adopted here, and in other similar works (e.g., [2,3]), could be used to make explicit calculations of the fifth-order correction to $C_{17}$ and even the sixth-order correction to $C_{18}$ [1]. Therefore, it is certainly possible with existing technology to determine the complete dispersion interaction for the H–H interaction for all terms up to and including $C_{22}$.

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