Pressure-induced high temperature superconductivity in H$_3$X (X=As, Se, Br, Sb, Te and I)

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The discovery of high critical temperature $T_c$ superconductivity in highly compressed H$_3$S has opened up the question of searching for strong electron-phonon coupling in the hydrides outside the transition metal series. In this work, we performed Linearized Augmented Plane Wave (LAPW) calculations for many different volumes in the $Im\bar{3}m$ structure for H$_3$X (X=As, Se, Br, Sb, Te and I). We then applied the multiple scattering-based theory of Gaspari and Gyorffy to obtain the Hopfield parameters and the McMillan–Allen–Dynes theory to estimate $\lambda$ and $T_c$. Based on our analysis, all materials considered show an increase of the Hopfield parameters with increasing pressure for both the H and X-element components, which is a key ingredient for the strong electron-phonon coupling and the high $T_c$. Our calculations for H$_3$Se, in agreement with other studies, find a $T_c\sim$110K. For the other materials in our study we obtain $T_c$ well below 100 K. However, according to both of our rigid band model and virtual crystal analysis, we predict a $T_c\sim$ 180 K for H$_3$Br with a small amount of additional hydrogen.

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I. INTRODUCTION

Recently high temperature superconductivity at temperatures exceeding 200 K was predicted by Duan et al.¹ at extreme pressures above 200 GPa in H$_3$S in the $Im\bar{3}m$ crystal structure.² The prediction was immediately confirmed experimentally by Drozdov et al.³ This breakthrough has motivated numerous theoretical and experimental studies⁴–¹⁸ and the consensus developed that conventional BCS electron-phonon coupling is in play. Researchers in this field are exploring other elements to stabilize hydrogen at high pressures and already have been reports of near room temperature (RT) superconductivity in the compound H$_{10}$La [⁸, ¹⁶]. The idea of metallization of hydrogen that was proposed long ago by Wigner and Huntington has been pursued vigorously and Ashcroft’s prediction of RT superconductivity in metallic hydrogen under high pressures is getting close to reality [²⁰].

Using the Gaspari–Gyorffy (GG) theory [²¹], which is the basis of the present work, Papaconstantopoulos and Klein [²²] predicted the electron-phonon coupling $\lambda = 1.86$ and superconducting temperature $T_c = 234$ K at a pressure of 460 GPa for metallic hydrogen.

However, metallizing hydrogen requires extremely high pressure [²³]. Recent theoretical studies also suggest that it would require pressure at roughly 500 GPa [²⁴]. The hydrides are thus introduced as an alternative which offers a rather satisfactory trade-off since they could form metallic states at much lower pressure.

The hydrides are considered as unusual but conventional superconductors since their behavior can be explained with traditional electron-phonon interaction while a few details differ from the conventional ones [²⁵]. H$_3$S is a prominent example because of its optimal electronic states and the separation of the acoustic from the optical phonon modes. It is believed that sulfur lacks a specific role in terms of its contribution to enhancing superconductivity but it helps hydrogen forming metallic states. To carry this idea forward, there have been several attempts at targeting other hydrides, replacing sulfur with different elements within the same $Im\bar{3}m$ crystal structure [³, ⁶, ⁹, ¹⁰, ¹³, ²⁶], which includes iso electronic counterparts such as Se [⁶, ¹¹, ¹³].

Although it is commonly accepted that hydrogen is the main contributor to $T_c$ in H$_3$S, other hydride-forming elements may have a dramatic impact on the hydrogen contribution. The purpose of this work is to present a comprehensive study of the electronic structure of the hydrides H$_3$X (X=As, Se, Br, Sb, Te and I) in the $Im\bar{3}m$ crystal structure and using the GG theory to calculate the Hopfield parameter $\eta$. To explore the possible superconducting properties of these materials and compare with the well established H$_3$S, we make estimates of the phonon frequencies from Refs. [³, ⁹] and we conclude that a large value of the $\eta$ parameter is the strongest indication of high $T_c$ in these materials as in the case in H$_3$S.

II. COMPUTATIONAL DETAILS

The electronic structure calculations are performed with the all-electron Linearized Augmented Plane Wave (LAPW) method [²⁷] specifically the Wei-Krakauer-Singh code [²⁸] developed at the U.S. Naval Research Laboratory. In the present calculations the Hedin-Lundqvist form of the local density approximation was used.

To ensure sufficient accuracy for convergence, the to-
The key step to estimate $T_c$ is the determination of the electron-phonon coupling $\lambda$, which, as pointed out by McMillan [30] and Hopfield [31], can be written as

$$\lambda_j = \frac{\eta_j}{M_j \langle \omega_j^2 \rangle} = \frac{N(E_F) \langle I^2 \rangle}{M_j \langle \omega_j^2 \rangle}$$  \hspace{1cm} (1)

where $N(E_F)$ is the total DOS per spin at the Fermi level $E_F$, $\langle I^2 \rangle$ is the electron–ion matrix element, $\langle \omega_j^2 \rangle$ is the average phonon frequency and the index $j$ corresponds to $X$ element and hydrogen. The Hopfield parameter $\eta_j$, which only describes electronic properties, is calculated using the GG formula based on the scattering theory. This formula allows us to express the electronic contributions to the $\lambda_j$ in local terms in the following form

$$\eta_j = \frac{1}{N(E_F)} \sum_{l=0}^{2} 2(l + 1) \sin^2(\delta_j^l - \delta_j^{l+1}) v_j^l v_j^{l+1}$$  \hspace{1cm} (2)

where both $\delta_j^l$ and $v_j^l = N_j^l (\epsilon_F)/N_j^{l(1)}$ are orbital $l$ and site $j$ dependent. The phase shifts $\delta_j^l$ are defined through the following equation:

$$\tan \delta(R_s, E) = \frac{j_l^l - j_l^l(kR_s)L_l(R_s, E)}{n_l^l - n_l^l(kR_s)L_l(R_s, E)}.$$  \hspace{1cm} (3)

where $L_l = u_l'/u_l$ is the logarithmic derivative and $j_l$ and $n_l$ are spherical Bessel and Neumann functions. The free scatterer DOS $N_j^{l(1)}$ is defined as follows:

$$N_j^{l(1)} = (2l + 1) \int_0^{R_s} \left[ u_l^l(r, E_F) \right]^2 r^2 dr$$  \hspace{1cm} (4)

where $u_l$ is the radial wave function and the upper limit of the integral is the muffin-tin radius $R_s$.

Finally, $T_c$ is evaluated using the Allen–Dynes equation [32] as follows:

$$T_c = f_1 f_2 \omega_{\log} \frac{\omega_{\log}}{1.2} \exp \left[ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right]$$  \hspace{1cm} (5)

In Eq. (5) we have set the Coulomb pseudopotential $\mu^* = 0.1$ and $f_2 = 1$. $f_1$ is the strong coupling factor given by the following

$$f_1 = \left[ 1 + \frac{\lambda}{2.46 + 9.35\mu^*} \right]^{1/3}.$$

A further approximation for the phonon frequencies is made based on previous work [33] considering that the large mass difference between the hydrogen and element X results in a separation of H optical modes from the acoustic modes of the element X.

### III. RESULTS AND ANALYSIS

#### Electronic structure

Fig. 1 shows the energy bands of H$_2$Se under pressure (a) P=2.45 Mbar (b) P=1.69 Mbar and (c) P=0.

Our observation of the separated band at $P = 0$ is stated for completeness and not as an explanation of the occurrence of superconductivity at higher pressure. The overall bandwidth increases significantly with increasing pressure as expected. However, for the high pressure cases near the Fermi level $E_F$, the ordering and shape of the bands are
not seriously affected. We note that these bands look very similar to those of the prototype material H$_3$S. We have also calculated the energy bands of the other materials under investigation here i.e. for X=As, Br, Sb, Te and I. The difference is basically in the position of $E_F$, and therefore we will not present additional band structure figures but we will come back later to this point on the applicability of a rigid band behavior in these materials.

Similar information can also be found in Fig 2 which shows the total DOS (a)-(c), Se-site angular-momentum-decomposed DOS (d)-(f) and H-site DOS (g)-(i) of H$_2$Se where each column corresponds to $P=2.45$ Mbar, $P=1.69$ Mbar and $P=0$ respectively. Consistent with Fig 1 at high pressures the shape of the DOS is preserved around $E_F$, including the position of $E_F$ on a sharp peak (van Hove singularity). In the equilibrium case ($P=0$), the DOS at the Fermi level is composed of 50% of p-like Se and 20% of s-like H states suggesting a strong sp orbital hybridization. The d-like Se contribution to the DOS in Figs. 2(d)-(f), becomes larger as pressure increases. The percentage of d-like states is doubled from the DOS at the Fermi level is composed of 50% of p-like Se and 20% of s-like H states suggesting a strong sp orbital hybridization. The d-like Se contribution to the DOS in Figs. 2(d)-(f), becomes larger as pressure increases. The percentage of d-like states is doubled from the equilibrium condition ($P=0$), increases monotonically with the fastest rate in all cases. The important finding here is that the $p_H$ becomes significant at the high pressures where superconductivity occurs. We note that we present these results at low pressures to show the trends of the projected DOS within the $Im3m$ structure. However for these materials this structure is not stable at low pressures, as discussed in Ref. [34] the stable crystal structure is in the rhombohedral R3m space group [2].

**Hopfield parameter $\eta$**

We have calculated the Hopfield parameter $\eta_j$ using Eq. 2 in Section II. In this formulation the index $j$ indicates that we obtain separate $\eta_j$ for hydrogen and the element X. This also results in having two separate electron-phonon coupling constants $\lambda$. This approach is differs from the approach of other authors, who directly compute the total $\lambda$. Our approach has the advantage of studying the electronic contribution to $\lambda$ from each element separately and being able to pin down which aspects of the band structure affect superconductivity as is described below. The summation Eq. 2 in a cubic approximation, has three terms which we identify as the sp (for $l=0$), pd (for $l=1$) and df (for $l=2$) channels. For the hydrogen component $\eta_H$ the dominant term comes from the sp channel. For the X component, $\eta_X$ of the H$_3$X compounds the dominant term comes from the pd channel. It should also be noted that each term of the sum consists of the product $\sin^2(\delta_l^j - \delta_{l+1}^j)\nu_l^j\nu_{l+1}^j$. The $\nu_l^j\nu_{l+1}^j$ term of the product is usually larger but the $\sin^2(\delta_l^j - \delta_{l+1}^j)$ is not negligible. In Fig. 4 $\eta_j$ is plotted versus pressure for the six materials we have studied.
The values of $\eta_H$ have been multiplied by three because of the three crystallographic sites of hydrogen. From the six compounds, it is found that H$_3$Se has the largest values of $\eta$ and is also comparable to those of the prototype material H$_3$S as shown in Fig. 4 (b). The others have lower values of $\eta$ especially those of the second row. We now proceed to analyze the relative importance of the two terms of the product shown in Fig. 5 and 6.

The term $v_1^2 v_{(j+1)}^2$ in Eq. 2 plotted against pressure is shown in Fig. 5. One can see it retains the general trends and certain features such as few jumps and flatness at various pressure by comparing Fig. 5 to Fig. 3. Although the difference between X=Se and Te is more pronounced than others which can be attributed to the relative location of Fermi level to the peak in DOS, the rest are roughly in the same magnitude.

The second factor, $\sin^2(\delta_j^X - \delta_j^{X+1})$, on the other hand, which describes the effect of phase shift as shown in Fig. 6 amplifies the difference and its influence can be summarized by the following trends. For H-site, while the $\sin^2(\delta_j^H - \delta_j^{H+1})$ term in the upper row is generally larger than that in the bottom row, $\sin^2(\delta_j^H - \delta_j^{H+1})$ within the same row are nearly identical. For X elements the most significant contribution to $\sin^2(\delta_j^X - \delta_j^{X+1})$ term corresponds to the pd channel (with square symbols) in Fig. 6 going from H$_3$As to H$_3$Br we note a substantial increase with pressure, while being vanishingly small in all three materials in the bottom row. The phase shifts de-
pend on the logarithmic derivatives $L_i$ in Eq. 8 which in turn depend on the crystal potential that strongly varies from one material to another. Finally, from Eq. 1 we see that the Hopfield parameter is defined as the product of the total DOS at $E_F$, $N(E_F)$, and the electron-ion matrix elements $\langle I_j^2 \rangle$ for each of the two components X and H.

As an example we plot the quantities $N(E_F)$, $\eta_X$ and $\eta_H$ for X=Br and Se in Fig. 7. we note that although $\eta$’s generally increase with increasing pressure, the underlying reasons are a bit different. In the case of H$_3$Se, $N(E_F)$ is slowly varying with pressure while $\eta$ and $\langle I_j^2 \rangle$ have a rapid increase with pressure. In the case of H$_3$Br, on the other hand, the $N(E_F)$ decreases rapidly and competes with increasing $\langle I_j^2 \rangle$. However, the important message is that the increase of $\langle I_j^2 \rangle$ dominates over the $N(E_F)$ with the resulting $\eta$ to always increase with pressure.

**Electron-phonon coupling $\lambda$ and $T_c$**

According to Eq. 11 which gives the electron-phonon coupling $\lambda$, we need the force constants $M_i \langle \omega_X^2 \rangle$ in the denominator of Eq. 11 as well as the Hopfield parameter $\eta$. At this point we want to emphasize that we want to retain the two component approach separating the acoustic from the optic modes in these materials as justified by the small mass of hydrogen and also verified by the lattice dynamics calculations of other groups. Since we have not performed full phonon spectrum calculations, we extract the phonon frequencies $\langle \omega^2 \rangle$ by the following approximate procedure. From the work of Flores-Livas 6 on H$_3$Se we obtain the values of $\langle \omega_{log} \rangle$ for three different pressures shown in Table I. Then the individual acoustic mode $\langle \omega_X \rangle$ and optical mode $\langle \omega_H \rangle$ are estimated by equating the ratios $\langle \omega_X \rangle / \langle \omega_{log} \rangle = \omega_X^2 / \omega_{log} = 0.39$ and $\langle \omega_H \rangle / \langle \omega_{log} \rangle = 1.18$. The separation to acoustic and optical modes is well justified due to the very small mass of hydrogen 53 so the total $\lambda$ entering the Allen-Dynes equation is given by $\lambda = \lambda_X + 3\lambda_H$

For a given mass, an increase of the phonon frequency gives a larger $\omega_{log}$ but a smaller $\lambda$. This means that in the $T_c$ equation $\omega_{log}$ and $\lambda$ have an opposite effect and since $\lambda$ is within the exponential term, it has the strongest effect. For the neighboring elements in the same row, the mass difference induces a frequency change that is often negligible. Even for the X that belongs to a different row, within the same crystal structure, we could still expect $\omega_H$ to stay within a reasonable range.

By applying the estimated phonon frequencies listed in Table I to the Eq. 5 for H$_3$Se we obtained $T_c = 118$ K, 120 K and 122 K at $P = 1.0$, 1.5 and 2.0 Mbar respectively, which are in excellent agreement with previous works 6 11. This confirms the validity of our approximation on phonon frequencies.

Fig. 8 shows $T_c$, $\lambda$ and the decomposed $\lambda$ contrition for Se and H. The $\lambda_H$ almost assembles the total $\lambda_{H,Se}$ which indicates that the contribution is predominately coming from the H-sites.

The values of $\lambda$ for other materials are also listed in Tab II. Although in the cases such as H$_3$As and H$_3$Br, where the values of $\eta_H$ and $\eta_X$ are rather comparable, the $\lambda_H$ in most cases is 10 times larger than $\lambda_X$ in all the materials considered. This is due to the fact that the mass of the X element, which appears in the denominator of Eq. 11 is nearly two orders of magnitude larger than that of hydrogen. This result further confirms the role of hydrogen as the main contributor to high $T_c$. By the same token, one could expect the difference will become more extreme in the the second row materials.

The dependence of $T_c$ under pressure can be understood as the interplay between $\lambda_j$ and $\omega_{log}$ where $\lambda_j$ also depends on $\eta$ and $\omega_j$. All the frequencies generally go up with increasing pressure but with different rates, they have the opposite effects on the $T_c$ as described above. The value of $\eta$ in most cases increases with pressure as shown in Fig. 2. From a numerical standpoint, a high $T_c$ is the optimal result of the interplay of $\lambda_j$ and $\omega_{log}$. $\eta$, which depends solely on the electronic structure is the only factor can be optimized independently, therefore serves as an indicator of possible high $T_c$ compounds. H$_3$Br in Fig. 4(c), as an example, has values of $\eta$ which are comparable to those in H$_3$Se at $P=2$ Mbar indeed shows the second largest $T_c$.

The three materials in the second row, due to their larger masses, are expected to have larger force constants and therefore smaller $\lambda_X$. In addition, the Hopfield pa-

| Pressure (Mbar) | $\langle \omega_{log} \rangle$ (eV/Å$^2$) | $\langle \omega_X \rangle$ (eV/Å$^2$) | $\langle \omega_H \rangle$ (K) |
|----------------|----------------------------------|----------------------------------|------------------|
| 1.0 Mbar       | 0.8176                           | 0.5254                           | 0.0254           |
| 1.5 Mbar       | 3.8962                           | 1.6777                           | 0.0914           |
| 2.0 Mbar       | 5.5643                           | 2.1087                           | 0.0973           |

| TABLE I: Averaged phonon frequencies $\langle \omega_{log} \rangle$, $\langle \omega_X \rangle$ and $\langle \omega_H \rangle$ at pressure 1.0, 1.5 and 2.0 Mbar. |

| Pressure (Mbar) | $\eta_A$ (eV/Å$^2$) | $\eta_H$ (eV/Å$^2$) | $\lambda_A$ | $\lambda_H$ | $\lambda$ (K) |
|----------------|---------------------|---------------------|-------------|-------------|---------------|
| 1.0 Mbar       | 0.8176              | 0.5254              | 0.0254      | 0.0254      | 0.1792        |
| 1.5 Mbar       | 3.8962              | 1.6777              | 0.0914      | 0.0914      | 1.1332        |
| 2.0 Mbar       | 5.5643              | 2.1087              | 0.0973      | 0.0973      | 1.4366        |

| TABLE II: Site-projected $\lambda$, total $\lambda$ and $T_c$ for H$_3$X |

| Pressure (Mbar) | $\langle \omega_{log} \rangle$ (eV/Å$^2$) | $\langle \omega_X \rangle$ (eV/Å$^2$) | $\langle \omega_H \rangle$ (K) |
|----------------|----------------------------------|----------------------------------|------------------|
| 1.0 Mbar       | 0.8176                           | 0.5254                           | 0.0254           |
| 1.5 Mbar       | 3.8962                           | 1.6777                           | 0.0914           |
| 2.0 Mbar       | 5.5643                           | 2.1087                           | 0.0973           |

| TABLE I: Averaged phonon frequencies $\langle \omega_{log} \rangle$, $\langle \omega_X \rangle$ and $\langle \omega_H \rangle$ at pressure 1.0, 1.5 and 2.0 Mbar. |
rameters are in general smaller than those in the first row. Assuming that the phonon frequencies on the H sites are the same as in the first row, the $\lambda_H$ is smaller than in the first row given the small values of $\eta_H$ (see Table I).

### Rigid-band model

Fig. 9 shows the total DOS and partial DOS for all three materials in the first row (X=As, Se and Br) at Pressure around 2 Mbar. By comparing the three panels, one can see that the shape of DOS around $E_F$ is well preserved. The relevant electronic properties can thus be explained with a rigid-band model where the change in electronic states corresponds directly to Fermi level shift due to a small amount of alloying and indirectly affect $T_c$ through $\eta$'s.

To better understand how the electronic properties could potentially affect $\lambda$ and $T_c$, we also consider $T_c$ versus electron number within a rigid band model. This is shown in Fig. 10. Each materials has its Fermi level near a peak in the density of states, even without alloying. By shifting the Fermi level toward the peak, the $\lambda$ and $T_c$ can be enhanced dramatically. However for $H_3Se$ the enhancement is limited since $E_F$ is very close to the van Hove singularity.

This gives an interpretation on the role of the element X from a different perspective and provides certain guidelines for optimizing hydrides to achieving high $T_c$. Of special interest is the case of $H_3Br$, where a small amount of additional electrons can enhance the $T_c$ to nearly 180 K. This may be accomplished by increasing the hydrogen content in $H_3Br$. We confirmed this rigid band prediction by performing a virtual crystal calculation by increasing the hydrogen amount by 0.15 electrons.

### Stability and elastic constants

Thorough examinations of the structural stability of $H_3X$ have been done in previous work [6] [11]. In this section we briefly test the mechanical stability of the first row materials (X=As, Se and Br) by calculating the elastic constants $C_{11} - C_{12}$ and $C_{44}$. Both elastic constants in the cubic high-pressure $Im3m$ structure are determined using standard finite-strain methods [35]. Fig. 11 shows the energy versus the square of the distortion for $C_{11} - C_{12}$ and $C_{44}$ for the lattice constant $a=6.2$ which corresponds to pressure around 1.0 Mbar. Both $H_3As$ and $H_3Se$ have positive $C_{11} - C_{12}$ and $C_{44}$ elastic constants suggesting its stability against long-wavelength distortions. However the result for $H_3Br$ indicates a very small negative slope for $C_{44}$ suggesting that the structure is unstable. Nevertheless, $H_3Br$ needs to be investigated.
further given our prediction in the previous section that higher $T_c$ may be reached by increasing the H content.

**IV. CONCLUSIONS**

We have calculated the parameters determining superconductivity in the group of hydrides $H_3 X$ (X=As, Se, Sb, Te and I). Our approach is based on LAPW electronic-structure calculations in the $Im\overline{3}m$ crystal structure and the Gaspari–Gyorffy and McMillan-Allen-Dynes theories. We conclude that the elements X play the role of stabilizer of these compounds to keep H metalized under pressure. The highest superconducting transition temperature 112 K is found for $H_3Se$, which is iso-electronic to the well-established $H_3S$. From a rigid band model extrapolation and a VCA calculation we suggest that, assuming the $Im\overline{3}m$ structure is maintained, higher $T_c$ may be achieved by electron doping in the $H_3Br$. Finally, we find that the road to high $T_c$ depends mainly on high values of the Hopfield parameters on the hydrogen sites. Our analysis shows that the variation of the parameters $\eta_F$ or of the matrix element $\langle I^2 \rangle$ is more important than the variation of the phonon frequency. Therefore, concentrating on the variation of $\eta$ justifies bypassing the computationally very demanding phonon spectra calculations. Finally, in Refs. [5, 7] the possibility of achieving higher $T_c$ in $H_3S$ by adding small amount of phosphorus is explored with conflicting results. Also, Heil and Boeri [13] suggest raising $T_c$ in $H_3S$ by replacing sulfur with oxygen. In our present study we did not find ways to raise $\langle I^2 \rangle$ or $\eta$ resulting in a higher $T_c$ in the group of compounds $H_3X$ that we used. Ref. [10] reports a very large $\eta_F = 17.5$ eV/Å$^2$ for $H_3F$, but the stability of this material is in question. In a preliminary calculation for $H_3O$ we have found a very large value of $\eta_0 = 18.4$ eV/Å without exploring the stability of the $Im\overline{3}m$ structure.

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**Appendix A**

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TABLE III: Total and projected DOS, Hopfield parameter $\eta$ and the two terms of the products in Eq. 2

| $\Delta V (\text{eV})$ | Projected DOS (States/Ry/f.u.) | $\Delta V (\text{eV})$ | Projected DOS (States/Ry/f.u.) |
|---------------------|-------------------------------|---------------------|-------------------------------|
| 0.8798              | 2.6325                        | 0.8687              | 2.1525                        |
| 0.8530              | 2.6399                        | 0.8413              | 2.1237                        |
| 0.8201              | 2.5524                        | 0.8000              | 2.0000                        |
| 0.7957              | 2.4235                        | 0.7790              | 1.8444                        |
| 0.7714              | 2.3595                        | 0.7551              | 1.8085                        |
| 0.7512              | 2.3025                        | 0.7290              | 1.7444                        |
| 0.7322              | 2.2544                        | 0.7040              | 1.6994                        |
| 0.7166              | 2.2125                        | 0.6790              | 1.6551                        |
| 0.7021              | 2.1705                        | 0.6440              | 1.6158                        |
| 0.6897              | 2.1325                        | 0.6140              | 1.5904                        |
| 0.6793              | 2.1105                        | 0.5840              | 1.5551                        |
| 0.6689              | 2.0885                        | 0.5540              | 1.5144                        |
| 0.6586              | 2.0665                        | 0.5240              | 1.4735                        |
| 0.6483              | 2.0445                        | 0.4940              | 1.4324                        |
| 0.6381              | 2.0225                        | 0.4640              | 1.3924                        |
| 0.6280              | 2.0005                        | 0.4340              | 1.3533                        |
| 0.6180              | 1.9785                        | 0.4040              | 1.3144                        |
| 0.6080              | 1.9565                        | 0.3740              | 1.2755                        |
| 0.5980              | 1.9345                        | 0.3440              | 1.2364                        |
| 0.5880              | 1.9125                        | 0.3140              | 1.1976                        |
| 0.5780              | 1.8905                        | 0.2840              | 1.1587                        |
| 0.5680              | 1.8685                        | 0.2540              | 1.1198                        |
| 0.5580              | 1.8465                        | 0.2240              | 1.0809                        |
| 0.5480              | 1.8245                        | 0.1940              | 1.0419                        |
| 0.5380              | 1.8025                        | 0.1640              | 1.0029                        |
| 0.5280              | 1.7805                        | 0.1340              | 0.9639                        |
| 0.5180              | 1.7585                        | 0.1040              | 0.9249                        |
| 0.5080              | 1.7365                        | 0.0740              | 0.8859                        |
| 0.4980              | 1.7145                        | 0.0440              | 0.8469                        |
| 0.4880              | 1.6925                        | 0.0140              | 0.8079                        |
| 0.4780              | 1.6705                        | 0.0000              | 0.7689                        |

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