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Chemical stability of positronic complexes with atoms and atomic ions

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A simple theory for establishing the stability or instability of positron-atomic systems against dissociation is presented. The theory consists of assuming that Morse-potential parameters for protonic diatoms are transferrable to the corresponding positronic molecules, and making appropriate reduced-mass modifications in the calculation of binding energies. The surprisingly good reliability of the method is established by appealing to the well-known positronium affinities of atomic hydrogen and fluorine. Positronium (Ps) binding is found for about half of the 42 atoms tested. In addition, instability is indicated for all nine positron-atom systems tested, and stability is indicated for seven of eight negatively charged systems tested; e.g., PsO^-.

I. INTRODUCTION

The low-energy interactions of positrons with atoms and molecules is a rapidly developing field, and in particular the chemistry of the positron and positronium is currently being investigated by many active workers around the world.[1] Further growth in this interesting area is hampered because we do not know whether most of the positron-atom complexes with which we deal experimentally are stable with respect to dissociation. Most of the very sparse evidence on this question has come from quantum-mechanical calculations; experimental work has contributed much less to our knowledge of bound states. Clearly the question of chemical stability is central, and must be dealt with if progress in this area is to continue.

Accurate quantum-mechanical calculations are expensive and thus limited in applicability to only the simpler systems, so there seems to be a need for reliable empirical methods for estimating binding energies. In this paper we present such a method and its results, and we compare our results to other evidence. All the systems we consider here are annihilatively unstable, of course, but annihilation lifetimes are ~1 nsec which is very long compared to atomic times (e.g., the time required for the electron in a Bohr hydrogen atom to complete an orbit).

II. THEORY

One of the first thoughts one has when considering positron or positronium (Ps) binding to an atom is, "Can we use existing information on the interaction of a proton or a hydrogen atom with the atom of interest?" Potential-energy curves for the H^+-A and H-A interactions are accurately known from molecular spectroscopy for many atoms A. The e^+-A potential-energy curve is exactly the same as that of H^+-A in the adiabatic approximation. The principal error in using the H^+-A potential for e^+-A comes from positron-nuclear distances close to but larger than the position of the potential minimum, where the positron is highly accelerated. For Ps-A and H-A there are additional differences because the adiabatic potentials are not the same. The static potential seen by a test charge is identically zero for Ps but not for H, and the dipole polarizability of Ps is eight times that of H. In the van der Waals region, the static potential of H is negligible, so the only significant difference is that dispersion forces for H-A are less than those of Ps-A. As the distances grow smaller, the electron and positron in Ps become increasingly differentiated by the growing exchange interaction. It seems to us that as the atoms Ps and H become more distorted to growing valence effects, and the electrons in Ps and in H become more involved in the electronic environment of the developing diatomic molecule, the difference between Ps-A and H-A will decline. Calculations[2] show that the probability density of the positron is significant in both regions. The point we want to make is: The (unknown) e^+-A potential is higher than the H^+-A potential near its minimum, and the (unknown) Ps-A potential is probably higher than the H-A potential near its minimum and certainly lower in the van der Waals region. Thus the e^+-A potential is overestimated, and errors in using the H-A potential for positronium calculations will tend to cancel. In the simple application of this idea carried out here, we deliberately overestimate the Ps-A potential in the van der Waals region, which tends to underestimate binding energies. Therefore, if our calculations indicate binding for e^+-A or Ps-A, it seems to be reasonable evidence that binding actually takes place. Clearly our argument is more compelling for e^+-A interactions than for Ps-A interactions.

For the e^+-A and H-A interactions, we adopt the Morse potential

$$V(r)=D(1-e^{-\beta(r-r_e)})^2 . \tag{1}$$

r is the proton-nuclear distance, D is the minimum energy of the potential curve compared to the energy of separated atoms at rest, r_e is the position of the minimum and β is related to the force constant. The energy levels for this potential were worked out many years ago in the case of no rotational excitation,[3] for which it was found that

$$E_{0,v}=\omega_e(v+\tfrac{1}{2})-\omega_e x_e(v+\tfrac{1}{2})^2 . \tag{2}$$

v is the vibrational quantum number which has nonnegative integral values up to a maximum of

$$v_{\max}=\frac{\omega_e}{2\omega_e x_e}-\tfrac{1}{2} \tag{3}$$

and

$$\omega_e=\beta\hbar\left[\frac{2D}{\mu}\right]^{1/2},$$

$$\omega_e x_e=\frac{\beta^2\hbar^2}{2\mu}, \tag{4}$$

μ being the reduced mass of the vibrating atoms. To the extent that the true H-A potential follows Eq. (1), D is the same as D_M given by

$$D_M=\frac{\omega_e^2}{4\omega_e x_e}, \tag{5}$$

which can be used as a consistency test of our method.

The parameters D_0^0, ω_e, and $\omega_e x_e$ are tabulated with sufficient precision for 37 diatomic hydrides by Huber and Herzberg[4] to be useable for our purpose, and recent molecular beam results on H noble-gas interactions[5] enable us to extend our investigations to a total of 42 cases. D is calculated from D_0^0 by adding to it the zero-point energy $E_{0,0}$. If the e^+-A or H-A potential is exactly Morselike, then, neglecting the enhanced van der Waals interaction of Ps compared to H and the greater spread of electronic charge of Ps compared to H and making the adiabatic approximation, we can compute the e^+-A or Ps-A interaction by solving the same Schrödinger equation solved by Morse but with an appropriate modification of the numerical value of the reduced mass. This amounts to (using tildes to denote quantities which pertain to e^+-A or PsA) s-type positronium energy levels given by

$$\tilde{E}_{0,v}=\tilde{\omega}_e(v+\tfrac{1}{2})-\tilde{\omega}_e\tilde{x}_e(v+\tfrac{1}{2})^2, \tag{6}$$

where

$$\tilde{\omega}_e=\omega_e\sqrt{\mu/\tilde{\mu}}$$

$$\tilde{\omega}_e\tilde{x}_e=\omega_e x_e\frac{\mu}{\tilde{\mu}}. \tag{7}$$

Positron or positronium affinities are then given by

$$\tilde{D}_0^0=D-\tilde{E}_{0,0}. \tag{8}$$

In order for the system e^+A or PsA to be chemically stable, the affinity must be positive, as must

$$\tilde{v}_{\max}=\frac{\omega_e}{2\omega_e x_e}\sqrt{\tilde{\mu}/\mu}-\tfrac{1}{2}. \tag{9}$$

III. RESULTS FOR NEUTRAL SPECIES

Our results are summarized in Table I. There, under the symbol of each element, are three data entries. The middle of these refers to the stability of PsA. If a bound state exists, the dissociation product of lowest energy is invariably Ps + A. In order for another arrangement to be more stable, either the electron affinity of A would have to be greater than the ionization potential of positronium (6.8 eV), or the ionization potential of A would have to be less than the electron affinity of Ps (0.327 eV).[13–15] Since no atoms satisfy either condition, the middle entry under each atomic symbol in Table I has to do with the positronium affinity of A. The entry is either: the positronium affinity in eV [calculated from Eq. (8) with the reduced mass $\tilde{\mu}$ being that of Ps and A], the word "no" which means binding is indicated by our calculations *not* to take place, or a dash indicating that sufficient data to do a calculation is not available. In each case where binding is indicated by our calculations, $\tilde{v}_{\max}$ is less than unity, which means that excited bound s states do not exist. We have not applied our method to non-s states.

For hydrogen we obtain a positronium affinity of 0.63 eV, which is less than the very accurate value 1.021 eV.[16] This confirms our expectation, stated above, that our calculations are conservative. For fluorine we obtain a positronium affinity of 0.98 eV. A calculation of PsF in the restricted Hartree-Fock approximation[2] and estimates of the error due to the neglect of the correlated motion of leptons in PsF yield likely lower and upper bounds on this quantity of 1.83 eV (Ref. 2) and 1.91 eV,[17] and Schrader's calculated value is 1.86 eV.[18] Again, the present calculations are seen to be conservative. For the other halogens, upper bounds for the positronium affinities are not available due to the absence of certain necessary theoretical data,[17] but likely lower bounds of 1.11, 0.55, and −0.19 eV, for Cl, Br, and I, respectively, have been reported.[2] The present result for these atoms, 0.54, 0.25, and 0.00 eV, again show our method to be conservative, with iodine as a possible exception. Experimentally, positronium halides have been observed in aqueous environments[19,20] and as graphite intercalated compounds.[21,22] The order of binding energies found here and in other calculations[2,18] is confirmed for the graphite intercalated compounds, and for aqueous systems[23] when the hydration energies of the halide ions are considered.[24,25]

This exhausts possibilities for calibrating our method, since no other reliable information on positronium binding energies exists. That is to say, existing calculations on Ps-A systems are either inconclusive,[26–32] too approximate to be useful,[33–35] or incorrect;[36–42] and experimental results to date do not contribute to our knowledge of binding in other positron-atomic systems. We believe that, in the case of hydrogen and the halogens, confirming evidence from experiment and from other calculations discussed above establishes the present method as a reasonably reliable indicator of positronium binding.

From Table I we see that for the first-row atoms, positronium binding is indicated for $_3$Li, $_5$B, $_6$C, $_8$O, and $_9$F. Negative results were found for $_4$Be and $_7$N. For neon and the other noble gases, we have extracted the needed spectroscopic constants for PsA from the experimental work of Toennies, Welz, and Wolf on AH.[5] The results are uniformly negative: None of these atoms are indicated by our calculations to bind positronium.

All the alkali-metal atoms for which the required spectral data is available show positronium binding as do all the group-IB metals $_{29}$Cu, $_{47}$Ag, and $_{79}$Au. In contrast,

TABLE I. Calculated binding energies for positronic complexes with atoms and atomic ions.[a]

H g .63 b ℓ																	He no f no fn –
Li no fh .62 c ℓ	Be g no e .4 cm											B g .60 b .77 cm	C g .14 c .9 cm	N no fh no e no em	O no f .08 c .35 bm	F no f .98 b –	Ne no fj no fn –
Na no fi ~.3 c ℓ	Mg g no e .4 cm											Al no f .85 c ℓ	Si g <.39 c .91 cm	P g ~.02 c ℓ	S g ~.4 b .35 cm	Cl g .54 c –	Ar no ek no fn –
K – .5 c ℓ	Ca – no e –	Sc – – –	Ti g – –	V – – ℓ	Cr – – ℓ	Mn g ~.5 b –	Fe g – –	Co g – –	Ni g ~.7 c –	Cu g .3 c –	Zn g no f –	Ga – <.75 c ℓ	Ge g ~1 c –	As g – –	Se g – –	Br g .25 c –	Kr – no fn –
Rb = – ℓ	Sr – no e –	Y – – –	Zr g – –	Nb g – –	Mo g – –	Tc g – –	Ru g – –	Rh g – –	Pd g – –	Ag g .06 c –	Cd g – –	In – .53 b ℓ	Sn g – –	Sb g – –	Te g – –	I g .00 c –	Xe g no fn –
Cs – .56 b ℓ	Ba – <.25 d –	La – – ℓ	Hf g – –	Ta g – –	W g – ℓ	Re g – –	Os g – –	Ir g – –	Pt g ≲.6 b –	Au g .3 c –	Hg g – –	Tl – .09 c ℓ	Pb g no e –	Bi g <.83 c –	Po g – –	At g – –	Rn g – –
Fr – – ℓ	Ra – – –	Ac g – –															

Ce – – –	Pr – – –	Nd – – –	Pm – – –	Sm – – –	Eu – – –	Gd – – –	Tb – – –	Dy – – –	Ho – – –	Er – – –	Tm – – –	Yb – ≲.3 c –	Lu – ~1 b –
Th – – –	Pa – – –	U – – –	Np – – –	Pu – – –	Am – – –	Cm – – –	Bk – – –	Cf – – –	Es – – –	Fm – – –	Md – – –	No – – –	Lr – – –

[a] The three data under the chemical symbol for each atom A are binding energies for: e^+A (top value), PsA (middle value), and PsA^- (bottom value). Dashes signify that no information is available. Binding energies are given in eV. All data is from Ref. 4 unless otherwise indicated.

[b] D and D_M [Eq. (5)] for HA differ by less than 3%, indicating that the true H-A potential is accurately given by Eq. (1). This implies a high degree of consistency in our use of Eqs. (7) for the system PsA.

[c] D and D_M differ by more than 3% and less than 30%. See note b.

[d] D and D_M differ by more than 30% and less than 70%. See note b.

[e] $\tilde{D}_0^0$, Eq. (8), is negative.

[f] $\tilde{v}_{\max}$, Eq. (9), is negative.

[g] Our method does not apply to the stability of e^+A because the ionization potential of A is between 6.8 and 13.6 eV.

[h] ω_e and $\omega_e x_e$ from Ref. 6; dissociation energy from Ref. 7.

[i] ω_e and $\omega_e x_e$ from Ref. 6; dissociation energy from Ref. 8.

[j] ω_e and dissociation energy from Ref. 9 and $\omega_e x_e$ from Ref. 10.

[k] Spectral constants from Ref. 11.

[l] Our method does not apply to the stability of PsA^- because the electron affinity of A is between 0.327 and 0.754 eV.

[m] Spectral parameters for AH^- are given in Ref. 12.

[n] Spectral parameters are calculated by the present authors from the van der Waals potentials deduced from molecular beam results.[5]

none of the alkaline-earth atoms (except possibly $_{56}$Ba) show binding nor does the group-IIB metal $_{30}$Zn. The group-IIIB metals are indicated to be consistent binders of positronium. Several other transition metals and two lanthanides also show binding. The second-row nonmetals $_{14}$Si, $_{15}$P, $_{16}$S, and $_{17}$Cl all show positronium binding in our method, although the calculated binding energy for P is small and uncertain. Altogether, our method indicates positronium binding to be fairly general and very widespread in the periodic chart. Of the 42 atoms for which the necessary spectral constants for the diatomic hydrides are available,[4,5] at least 16 and possibly as many as 30 pass our tests for being capable of binding positronium. Twelve give unambiguously negative results, and of these, four are alkaline earths and five are noble gases.

IV. RESULTS FOR POSITIVE SPECIES

In order for our method to be applicable to the stability of the species e^+A, the lowest-energy dissociation product of AH^+ and e^+A must correspond. However, if the ionization of the atom A is between 6.8 (that of Ps) and 13.6 eV (that of H), then the dissociation products do not correspond

$$
\begin{aligned}
&AH^+ \rightarrow A^+ + \mathrm{H} \\
&e^+A \rightarrow A + e^+ .
\end{aligned}
\tag{10}
$$

In this case our method does not apply, and we can learn nothing from it about the stability of e^+A. Forty-nine atoms are known to be in this category. We consider the hydrogen atom itself to be a member of this category because its ionization potential makes it an ambiguous case. Nevertheless some other authors[43] recently used a method similar to our own on the system e^+H.

Of the remaining atoms, sufficient data exists for only nine to do calculations with our method. Two of these are the lighter alkali metals and Al for which e^+A dissociates into $A^+ + \text{Ps}$. $\tilde{\mu}$ in Eqs. (6)–(9) is therefore taken to be that of Ps and A^+, and our calculations have to do with the positronium affinity of A^+. The remaining six atoms are all light nonmetals or noble gases and have as the lowest energy of the separated atoms $A + e^+$. In these cases $\tilde{\mu}$ is that of A and e^+, and the calculations have to do with the positron affinity of A. In all cases, binding is unambiguously indicated not to take place.

${}_3\text{Li}^+$ and ${}_{11}\text{Na}^+$ are indicated by our calculations to be unable to bind Ps because both have negative values of $\tilde{v}_{\text{max}}$. Good quantum-mechanical calculations ${}_{19}\text{KH}^+$ exist[44] but they are not quite good enough for our purposes. We need an accurate value of $\omega_e x_e$, which is proportional to the curvature of the potential curve at its minimum. The value of this sensitive parameter is easily extractable from results given by Olson *et al.*,[44] but when we do this for their results for NaH$^+$, we find serious disagreement with the more accurate results.[6] For this reason, we do not consider that sufficiently accurate parameters for KH$^+$ are available.

The nonmetals ${}_7\text{N}$, ${}_8\text{O}$, and ${}_9\text{F}$ fail to bind e^+ for the same reason: $\tilde{v}_{\text{max}}$ is negative. This is also true of ${}_2\text{He}$ and ${}_{10}\text{Ne}$. ${}_{18}\text{Ar}$ fails to bind e^+ in our approximation because D_0^0 is negative. Our results for ${}_7\text{N}$, ${}_2\text{He}$, and ${}_{10}\text{Ne}$ agree with those of Golden and Epstein,[45] who showed that these three atoms fail to satisfy a necessary condition for binding positrons.

V. RESULTS FOR NEGATIVE SPECIES

The species $A\text{H}^-$ and $\text{Ps}A^-$ will have comparable lowest-energy dissociation products only if the electron affinity of A does not lie between that of Ps and H, namely 0.327 (Refs. 13–15) and 0.754 eV.[46] If the electron affinity of A is below that range, then we are dealing with the affinity of A for Ps$^-$; if above, then, the positronium affinity of A^-. Using the electron affinities compiled by Smirnov,[46] we find that 16 atoms have electron affinities within this range, and hence our method does not apply. The 16 include all the alkali metals and all the group-III*A* elements except boron.

Adequate spectral parameters exist for $A\text{H}^-$ for eight other atoms A. Most of these are from the high quality quantum-mechanical calculations of Rosmus and Meyer.[12] Experimental values listed by Rosmus and Meyer are used in preference to the calculated values, except for ω_e for ${}_{16}\text{SH}^-$ for which the listed experimental value is uncertain. Otherwise, results of the coupled electron pair approximation are used. Using the appropriate reduced mass in our calculations, we find stability of $\text{Ps}A^-$ in all cases except PsN$^-$. The lowest-energy dissociation products are $A + \text{Ps}^-$ for $A = {}_4\text{Be}$, ${}_5\text{B}$, ${}_7\text{N}$, and ${}_{12}\text{Mg}$; and $A^- + \text{Ps}$ for $A = {}_6\text{C}$, ${}_8\text{O}$, ${}_{14}\text{Si}$, and ${}_{16}\text{S}$.

VI. CONCLUSIONS, CRITIQUE, AND SUGGESTIONS FOR FUTURE WORK

Over half of the 42 atoms tested by our method show positronium binding. These include the alkali metals, the "coinage" metals, the group-III*A* metals, and most of the nonmetals. The principal counterexamples are the noble gases, ${}_7\text{N}$, the four lightest alkaline earths, and ${}_{30}\text{Zn}$. Positronium is uniformly unsuccessful in forming stable van der Waals complexes. Our calculations indicate that the three lightest noble gases fail to bind e^+ as do all the other five atoms tested, which are the lighter alkali metals and the most electronegative first row nonmetals. The stability of the negatively charged species $\text{Ps}A^-$ is indicated for all the eight atoms tested except N.

In view of the crudity of our method and the very large mass corrections required, it must be said that our conclusions are quite tentative. This work is intended to provide rough predictions and a guide to trends and relationships in the periodic chart regarding e^+-, Ps-, and Ps$^-$-atom interactions, rather than accurate predictions for any individual atom. In particular, our negative results for the existence of bound states of positronium with the noble gases should not be viewed as definite proof that they do not exist. As noted in Sec. II, our method depends upon a cancellation of errors in the valence and van der Waals regions. For H—noble-gas complexes, there is no valence region comparable to those in other hydrogen-containing diatomic molecules, so we are very likely underestimating the strength of the Ps—noble-gas interaction over the whole of its attractive region. Bound states of PsKr and PsXe have been conjectured to account for anomolous positronium yields for positrons slowing down in gaseous Kr and Xe.[47]

Implicit in the approach described here is our choice of the CMN (center of mass of the nuclei) coordinate system.[48] This choice introduces into the vibronic problem for Ps-A systems angular momentum terms which couple different states except (in our case) for Σ electronic states. We are ignoring these in the present work and they may be significant.

A more realistic diatomic potential function than the simple Morse potential (1) might be used in the future. The Morse potential is incorrect at short range because it does not correctly give the internuclear Coulomb repulsion, and also at long range because it does not correctly reflect the dispersion forces.

The nonadiabatic corrections for the positronic species can be estimated from electronic wave functions for the corresponding protonic species.[49] This represents a very much larger calculation than we report in the present work. Much larger still would be a calculation in which the electronic wave functions themselves are modified to account for nonadiabatic effects.

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