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Contributions to the Theoretical Treatment of Ammonium. I.

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In this paper we determine the electron distribution, the binding energy, and the ionic radius of the positive ammonium molecule ion. The general idea of our method is that the molecule is divided by a spherical surface which contains the protons and it is supposed, in our first approximation, that the charge of protons is distributed uniformly on this surface. Now, we we have inside our sphere a nitrogen nucleus, the charge of which is over compensated by ten electrons and so a N^{3-} ion is formed. The whole formation can be regarded from the outside of the sphere as similar to the Na^+ ion, because the charge of the four protons has been added to the charge of the N nucleus. In a second approximation we pay attention to the fact that the protons are not exactly uniformly distributed on the spherical surface but on the points of a tetrahedron. We have taken into consideration the inhomogeneous field of protons by using the perturbation calculation. The ionic radius of our molecule ion is determined as usual in the statistical theory of atoms. Finally, we check our result with a cycle process. We do not use semi-empirical parameters.

IT is interesting that there exist radicals composed of non-metallic atoms which have the same properties as metals. The most common example is ammonium, which forms salts similar to those of alkali metals. It is obvious that the four protons of the radical penetrate the electron cloud of the nitrogen and it may be presumed that the molecule has, in addition to the closed shell of the positive ammonium radical, one *s*-electron, just as the alkali metals have.

The theoretical treatment of ammonium is an especially interesting problem, because pure ammonium is experimentally unknown. Consequently, its constants have not been established. We cannot ignore the exceedingly remarkable fact that, on the one hand, ammonium (just as alkali metals do) forms an amalgam, which, though sufficiently liable to decay, can be prepared under high pressure and has the same properties as the amalgams of alkali metals; on the other hand, up till now pure ammonium metal has not been produced.

In the first part of our paper we shall determine the electron distribution, binding energy, nitrogen-proton distance, and ionic radius of the positive ammonium ion; in the second part the wave function of the valence electron, ionization energy of ammonium, and the eigenfrequencies of NH_4^+ will be determined.

I.

In the case of the positive ammonium ion, nitrogen is linked with four hydrogens, while one electron is given to the anion. The four protons are on the surface of a sphere, which has a radius R, and the molecule ion has tetrahedral symmetry.

The theoretical treatment of molecules of such type would be possible generally on grounds of

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