

Electrostatic traps for polar molecules

S. K. Sekatskiĭ¹⁾

Spectroscopy Institute, Russian Academy of Sciences, 142092 Troitsk, Moscow Region, Russia

(Submitted 10 November 1995)

Pis'ma Zh. Éksp. Teor. Fiz. **62**, No. 12, 900–904 (25 December 1995)

New types of traps are proposed for small polar molecules. The traps are based on the possibility that molecules, which possess a permanent dipole moment, can execute stable orbital motion around a thin, charged wire. The experimental conditions for realization of such traps are analyzed. © 1995 American Institute of Physics.

In the last few years considerable progress has been made in the development and investigation of electromagnetic traps not only for ions,^{1,2} but also for laser-cooled neutral atoms which is a more complicated task (Refs. 2–4). The building of such traps has made it possible to perform many interesting pioneering experimental studies of a number of fundamental physics problems and also to use cold atoms and ions for solving practical problems in metrology.^{1–4} On the other hand, virtually none of the electromagnetic traps which have previously been proposed and implemented can be used to trap molecules. This is attributable to the fact that molecular spectra are extremely complicated, that effective schemes for laser excitation of molecules cannot be found, and to other factors. There is no doubt, however, that developing different methods for handling molecules, for example, for investigating chemical reactions is important.

In the present letter I wish to call attention to the fact that electrostatic “wire” traps, which resemble the wire traps and wire guides recently proposed and used by Schmiedmayer^{5,6} for atoms possessing a magnetic moment $\vec{\mu}$, can be realized for molecules possessing a permanent dipole moment \mathbf{d} .

In Refs. 5 and 6 it was shown that an atom which possesses a magnetic moment $\vec{\mu}$ can execute stable orbital motion around a thin wire carrying a constant current I , since in such a system there exists an attractive potential which decays with distance as $1/r$. When the frequency of this motion is much lower than the Larmor precession frequency of the vector $\vec{\mu}$ around the magnetic field vector \mathbf{B} of the current-carrying wire, the adiabatic approximation is applicable and the motion of the atom in a plane perpendicular to the wire is classical Kepler revolution on closed elliptical orbits. A similar situation occurs for a polar molecule which possesses a dipole moment \mathbf{d} and which is located at a distance r from a charged wire with radius r_1 and linear charge density q (see Fig. 1): A radial electric field which decreases with distance as $1/r$,

$$E = 2q/r, \tag{1}$$

surrounds the wire and for a cylindrical capacitor (Fig. 1)

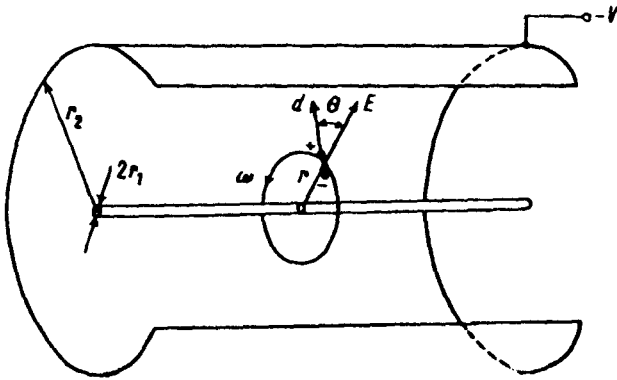


FIG. 1. Diagram illustrating the interaction of a dipole molecule with the electric field inside a cylindrical capacitor with electrode diameters r_1 and r_2 .

$$q = \frac{V}{2 \ln(r_2/r_1)}, \quad (2)$$

which corresponds formally to a potential energy of a dipole which decreases as $1/r$:

$$U = -\mathbf{dE}. \quad (3)$$

It is well known, however, that the average dipole moment d of any free molecule in a purely rotational state is equal to zero in the laboratory coordinate system. (The condition that the average dipole moment of any nondegenerate quantum system is equal to zero follows from the requirements of symmetry under time reversal. A detailed discussion of this question — can a molecule have a permanent dipole moment? — is given in, for example, Ref. 7.) Therefore, it is not obvious *a priori* that such a trap can be realized. Moreover, in contrast to atoms, the states of free molecules cannot be classified according to the values of the projection of the vector \mathbf{d} onto the direction of the field \mathbf{E} , so that the results of Refs. 5 and 6 cannot be used directly to analyze a trap.

The possibility of orienting polar molecules in an electric field has been studied extensively, both theoretically and experimentally (see, for example, Refs. 8–11 and the references cited there). It was shown that the typical small polar molecules with dipole moment d of the order of 0.1–10 D and a rotational constant C of the order of 0.1–1 cm^{-1} in initial states with low total angular momentum $J \leq 2-4$ can be oriented rather well in fields with intensity E such that the coupling parameter

$$p \equiv dE/C \geq 1. \quad (4)$$

[From the standpoint of quantum theory, orientation means that the molecules are not in pure rotational states, and that their states are characterized by a superposition of quantum states with different values of the quantum numbers J and K (the projection of the vector \mathbf{J} onto the symmetry axis) and others.] For the typical polar molecules mentioned above (KCl, ICl, CH_3I , etc.), this corresponds to fields of 10–100 kV/cm. Such fields are realized in the trap which we are considering. It is easy to see that for the case $r_1 = 0.1$ mm, $r_2 = 1$ cm, and $V = 10$ kV (see Fig. 1) the electric field E at a distance $r = 0.7$ mm

from the inner electrode is equal to 30 kV/cm. The technique of ultrasonic molecular jets is successfully employed in experiments to produce a beam of molecules with small values of J , which is necessary for orienting dipole molecules; this technique makes it possible to cool molecules to rotational temperatures of the order of several Kelvins. For large values of the angular momentum J the rotation of the molecules predominates over their orientation, and alignment of the vector \mathbf{d} along the field \mathbf{E} does not occur.

The results of Refs. 9 and 10 can be used to analyze the problem further. It is shown there that, for example, an ICl molecule ($d=1.24$ D, $C=0.1142$ cm⁻¹) in an initial state $J=0$, which enters a uniform static electric field of 20 kV/cm is oriented, as a result of adiabatic evolution, along the vector \mathbf{E} , so that the average $\langle \cos \vartheta \rangle = 0.631$. For the same molecule in the initial state $J=1$ the quantity $\langle \cos \vartheta \rangle$, averaged over all possible initial values of the quantum number $M=0$ and 1 of the projection of \mathbf{J} onto \mathbf{E} (evidently, this formulation of the problem pertains to our case), is equal to 0.1849. The quantity $\langle \cos \vartheta \rangle$ increases with the field E and decreases rapidly as the angular momentum J increases. For KCl ($d=10.27$ D, $C=0.1286$ cm⁻¹) and CH₃I molecules $\langle \cos \vartheta \rangle$ behaves similarly. For example, for KCl molecules with $J=0$ and $E=30$ kV/cm $\langle \cos \vartheta \rangle$ is close to 1, for $J=1$ and $E=30$ kV/cm $\langle \cos \vartheta \rangle \sim 0.8$, and so on.

The potential energy of molecules in the trap being considered can thus be written in the form

$$U = -\mathbf{dE} = -dE \cos \vartheta = -\frac{2dq}{r} \cos \vartheta. \quad (5)$$

Therefore, if the angle ϑ between the vectors \mathbf{d} and \mathbf{E} remains unchanged, i.e., the orientation of the dipole moment \mathbf{d} follows adiabatically the field \mathbf{E} during the motion of the molecule, we have the same $1/r$ interaction potential in the system, and all well-known results of the analysis of the classical Keplerian orbital motion of particles can be applied to it.^{5,6,12} (The fact that the quantity $\langle \cos \vartheta \rangle$ in turn depends on the electric field intensity E , of course, introduces some differences in the interaction potential of a dipole molecule, but it does not change the qualitative nature of the motion. Here the most important circumstance is that the orbital motion of the particles is stable for potentials which decay more slowly than $1/r^2$ (Ref. 12). A detailed analysis of the motion of dipole molecules will be published later.) In the simplest case of a circular orbit of radius r a molecule revolves steadily around the wire with velocity

$$v = \sqrt{2dE(r) \cos(\vartheta) / M} \quad (6)$$

and angular velocity

$$\omega = v/r, \quad (7)$$

where M is the mass of the molecule. The motion of the molecule along the wire in this case is free (the case of a wire particle guide). The adiabaticity criterion here is the fact that the frequency ω_{ext} of the external orbital revolution of the molecules around the wire must be much smaller than the frequency ω_{int} of the internal (i.e., intrinsic) rotation of the molecules; it is obvious that in this case there is easily "enough time" for the vector

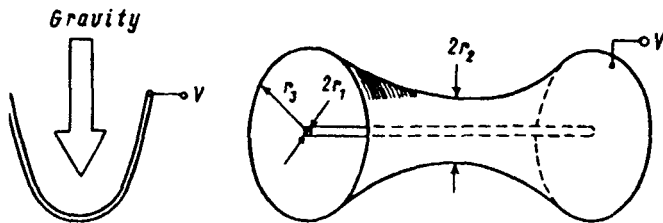


FIG. 2. Three-dimensional traps for polar molecules: a — The charged wire is located in a gravitational field; b — a capacitor in which the diameter of the outer plate varies along the length of the capacitor and has a minimum at the center (i.e., it is shaped like a hyperboloid). This idea can also be implemented for the case in which the diameter of the inner electrode varies along the length of the capacitor.

d to be oriented along the vector **E** during the orbital motion of the molecules (compare the discussion of the adiabaticity criterion in Ref. 9). Expressing ω_{int} in terms of the rotational constant C

$$\omega_{\text{int}} = 2C(J+1)/\hbar \quad (8)$$

and taking into account expressions (6) and (7), we obtain the adiabaticity criterion

$$p \cos \vartheta = dE \cos \vartheta / C \ll 2C(J+1)^2 M r^2 / \hbar^2, \quad (9)$$

where \hbar is Planck's constant. It is easy to see that the condition (9) holds for all reasonable values of the parameters which appear in it.

In summary, I have shown that two-dimensional trapping of molecules around charged wires is possible. Note that the velocity v of the orbital motion of the molecules is very high: For example, for KCl molecules with $J=0$ and $E=30$ kV/cm we obtain $v=3.4 \times 10^3$ cm/s. Therefore, KCl molecules from a supersonic beam of cooled molecules which moves with average velocity $v \sim 6 \times 10^4$ cm/s can be trapped in the indicated trap even for a beam with a divergence ~ 0.05 (of course, the beam is directed into the trap parallel to the charged wire).

The possibility of building three-dimensional (3D) traps on the basis of the principle indicated above is very interesting. This question will be examined in greater detail in a future paper. Here I wish to indicate only the following two possibilities (Fig. 2). In the first case, similarly to the wire traps for atoms,⁵ the trap is closed as a result of the presence of gravity. In the second case the potential attracting the dipole molecules decays not only in the radial direction, but also in the direction of the wire from the center to the edges as a result of the inhomogeneous linear charge density in such a geometry. Of course, such 3D traps can be realized only for sufficiently cold atoms: The depth of the confining potential in Fig. 2b is $\sim 5 - 10$ K. To cool molecules to such a temperature and to load the traps, it is possible to use, for example, a recently proposed technique for cooling molecules in a cold buffer gas (helium).¹³

I thank J. Schmiedmayer for discussions which stimulated the completion of this work.

- ¹ H. Demelt, *Rev. Mod. Phys.* **62**, 521 (1990).
- ² E. Arimondo, W. D. Phillips, and F. Strumia [Eds.], *Laser Manipulation of Atoms and Ions*, North-Holland, Amsterdam, 1992.
- ³ A. Migdall, J. Prodan, W. Phillips *et al.*, *Phys. Rev. Lett.* **54**, 2596 (1985).
- ⁴ W. Paul, *Rev. Mod. Phys.* **62**, 531 (1990).
- ⁵ J. Schmiedmayer, *Phys. Rev. A* **52**, R13 (1995).
- ⁶ J. Schmiedmayer, *Appl. Phys. B* **60**, 169 (1995).
- ⁷ W. Klemperer, K. K. Lehmann, J. K. G. Watson, and S. C. Wofsy, *J. Chem. Phys.* **97**, 2413 (1993).
- ⁸ B. Friedrich, D. P. Pullman, and D. R. Herschbach, *J. Phys. Chem.* **95**, 8118 (1991).
- ⁹ H. J. Loesch and A. Remscheid, *J. Chem. Phys.* **93**, 4779 (1990).
- ¹⁰ H. J. Loesch and J. Moller, *J. Phys. Chem.* **97**, 2158 (1993).
- ¹¹ B. Friedrich and D. Herschbach, *Phys. Rev. Lett.* **74**, 4623 (1995).
- ¹² L. D. Landau and E. M. Lifshitz, *Mechanics*, Pergamon Press, N. Y. [Russian original, Nauka, Moscow, 1988].
- ¹³ J. M. Doyle, *Bull. Am. Phys. Soc.* **39**, 1166 (1994).

Translated by M. E. Alferieff