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Transition energies and optical oscillator strengths for inner-shell excitations of a quark nitrogen molecule

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Received 12 May 1997; in final form 25 August 1997

Abstract

Experimental evidence for the model of quarks as the basic blocks of matter are only indirect. An alternative way to prove their existence is to look for changes in spectroscopic properties that could be influenced by fractionally charged nuclei, formed by the incorporation of an extra quark. In this Letter, we present results of ab initio calculations of the transition energies and optical oscillator strengths for a nitrogen molecule with fractionally charged nuclei. Our results show that both the transition energies and oscillator strengths for inner-shell excitation of the quark nitrogen molecule differ significantly from the normal molecule, being prone to experimental detection. © 1997 Elsevier Science B.V.

1. Introduction

Although the model of quarks as basic blocks of matter is a widely accepted one, there is no direct experimental evidence accounting for their existence. Evidence of quarks comes only from investigation of the properties of hadrons, quark-made particles, in high-energy particle accelerators [1–6]. Quantum chromodynamics (QCD) states that color particles cannot exist as free entities, being always confined to the interior of hadrons. However, there may be a tiny concentration of primordial quarks that have not found their partners in the expanding big-bang universe. These unpaired quarks could have been incorporated to ordinary nuclei. According to QCD, a fourth quark brought up to a baryon would be repelled by one quark and attracted by the two others. It has to be pointed out that what must be confined is color, not electric charge, so a fourth quark would generate a fractionally charged nucleus [7]. Several

experiments have been carried out to look for fractionally charged atoms or molecules [8]. In these experiments it is important to know what to expect from the interaction of $\pm 1/3$ or $\pm 2/3$ electric charge with ordinary atomic matter, what has been called *quark chemistry* [9]. A fractional quark charge in the nucleus of an atom will, of course, change its electronic energy levels, eventually changing transition energies and oscillator strengths in comparison to the atom or molecule in their usual constitution. An appropriate spectroscopic technique should be able to detect this change and assign transitions between energy levels perturbed by the presence of an extra quark in a given nucleus.

It has been already shown for the sodium atom that the wavelength of the $^2P \Leftarrow {}^2S$ transition is highly dependent on the nuclear charge of the quark–atom system [10]. The nitrogen molecule (N_2) is one of the most abundant molecules in space and in our planet. As the concentration of these quark

molecules should be very small, the chances of detection are increased if we search for spectroscopic alterations in abundant molecules. However, the spectroscopic property that should be most influenced by a fractionally charged nucleus is the transition energy associated to inner-shell electronic excitations. In this paper, we calculate the effects caused by quarks attached to a nitrogen nucleus, on some electronic excited states (transition energies and oscillator strengths) of the N_2 molecule. The system studied was proposed by Schaad et al. [9] and consists of a neutral nitrogen molecule in which there is one $+1/3e$ quark attached to one nucleus, and a $-1/3e$ quark attached to the other.

2. Computational details

In order to perform reliable calculations on these exotic nuclei, we optimized specific basis sets for each of the nuclei involved: $N(-1/3e)$ and $N(+1/3e)$. Based on the Huzinaga [11] basis sets for the first-row atoms of the periodic table (B, C, N, O, F, Ne), we constructed Padé type II approximants [12] to represent each of the Huzinaga's exponents as a function of the nuclear charge. From the Padé approximants, we obtained the optimum exponents for all fractionally charged nuclei considered here. The other exponents, two diffuse s and p, and a polarization function d, came from a previous work where these exponents were optimized for the N_2 molecule [13]. The final exponents are shown in Table 1.

The core hole states, generated by the inner-shell excitations ($1\sigma \rightarrow 2\pi$ and $2\sigma \rightarrow 2\pi$) were first optimized at the Hartree–Fock (HF) level of calculation, in order to account for relaxation effects. The procedure used to converge these localized states has been described in a previous work [13]. Following the self-consistent (SCF) calculations, a set of configuration interaction (CI) calculations have been performed using the orbitals generated at the SCF level plus virtual orbitals, obtained at the IVO [14] level, one set for each one of the states involved. The CI calculations have been performed allowing up to double excitations from all the occupied orbitals to the virtual space formed by 11 IVO orbitals, to generate the correlated wave functions. This level of

Table 1
The exponents of the basis set for the quark atoms

	$N(-1/3e)$	$N(+1/3e)$
s	5324.47	6520.09
	799.172	979.733
	184.106	226.493
	53.7005	66.3715
	17.9445	22.1735
	6.47717	7.94144
	2.44101	2.93388
	0.62726	0.77637
	0.19322	0.23636
	0.11460	0.14018
p	23.9231	29.5966
	5.30573	6.60040
	1.51807	1.90031
	0.46572	0.59089
	0.13687	0.16764
	0.04656	0.05702
d	0.736	0.832

calculation has proven to yield accurate values for transition energies as well as oscillator strengths for the neutral molecule [13,15] and hopefully will do the same for the quark molecule. At this level of calculation, the optimized internuclear distance for the quark molecule is 1.120 Å.

From the CI calculations the transition energies were determined. For the oscillator strength calculations, each state was represented by its own wave function and the matrix elements involving non-orthogonal orbitals were calculated using a bi-orthogonalization procedure already described in previous papers [15,16].

3. Results and discussion

The results of our calculations for the vertical transitions are shown in Table 2. For the sake of comparison, the results obtained for the ordinary N_2 molecule are also presented [15,17,18]. There is an enormous difference in the transition energy (≈ 40 eV) for both core excitations ($1\sigma_{g,u} \rightarrow 1\pi_g$) relative to the nitrogen molecule. As expected, the optical oscillator strength is somewhat smaller for the quark nitrogen molecule. This can be understood in terms of localized excitations. For the nitrogen molecule, the two nuclei are equivalent and contribute equally

Table 2
Transition energies and optical oscillator strengths for electronic excitations of the ordinary nitrogen molecule and the one with fractionally charged nuclei

Excitation	ΔE (eV)	OOS
N——N		
$1\sigma_u \to 1\pi_g$	402.55	0.20
$1\sigma_g \to 1\pi_g$	402.62	
$2\sigma_u \to 1\pi_g$	44.40	0.41
N(+1/3)——N(−1/3)		
$1\sigma\{N(+1/3)\} \to 2\pi$	445.00	0.11
$2\sigma\{N(−1/3)\} \to 2\pi$	363.25	0.15
$4\sigma \to 2\pi$	16.51	0.68

to the total oscillator strength. On the other hand, in the quark molecule, the two nuclei are different and the value of the oscillator strength, as a measure of the intensity of the transition, should reflect this asymmetry. If the hole states were completely localized, one should expect the oscillator strength for the transition originated at the positively charged nucleus to be less than half the value of the normal molecule, and the one at the negatively charged nucleus to be more than half of that value. The results in Table 2 are in agreement with this picture but also reflect the fact that the hole states are not completely localized [19].

The next optically allowed transition of the N_2 molecule that should be more affected by the nuclear charge corresponds to the $2\sigma_u \to 1\pi_g$ ($b^1\Pi_u$) excitation. The equivalent transition in the quark molecule is the $4\sigma \to 2\pi$. In this case a much smaller difference (2.11 eV) was observed between the two transition energies. For other transitions, involving the outer orbitals, an even smaller difference was observed (≈ 1 eV). Besides, those transitions occur in a somehow congested region of the N_2 spectra (12–14 eV) what makes them less useful for the purpose of identifying the quark N_2 molecule.

4. Conclusions

It was shown that the incorporation of quarks to a nitrogen molecule brings remarkable alterations in the spectroscopic region associated to inner-shell excitations. The results suggest that these differences should be detectable provided enough time of exposition and a powerful source of light (for instance, *sincrotron* radiation), are employed.

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