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The study of the effect of changing the substituted on electron and orbital properties of the drug 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol on nano structure fullerene using Hartree- fock method

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Abstract

In this research work at The first compounds [C60- 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65-2X]$^{+}$ (X=F,Cl,Br) were optimized. Then the calculation of natural bond orbitals was performed with the NBO technique. All calculations using Hartree- fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results showed that the energy levels of molecular orbital (HOMO & LUMO) in the RF has the lowest value. C65-X has a length of the shortest bond and the bond has most power. Comparison of the dipole moments of compounds shows this trend: RF> R-Cl> R-Br. Both ratio Core / charge and the valence / charge for carbon atoms 31, 55, 65 and 63 in the RF has the highest value.

Keywords: Bond lenhgt , Dipole moment , fullerene , 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol

1. Introduction

Carbon in nature has five diatomite, graphite, nanotube, carbon-shaped and fullerene allotropes, all solid. Fullerenes consist of a large number of carbon molecules. In a general hollow form, they are circular, elliptical, or tubular in nano-metric dimensions. Fullerene, the first known carbon-spherical carbon molecule with arranged carbon, is in the form of a Korean ball. The base of fullerenes is the pages in the graphite, except that in the atomic structure of the fullerenes, instead of the regular hexagons in the graphite plates, there is a series of hexagonal and regular pentagons that are arranged together in one another. Taken and Fullerene Butter. Determine the fullerenes according to the number of atoms in their building. To name the fullerenes, a letter C is used that represents the carbon atom in their structure. The carbon atoms are hybridized in sp2. (Figure 1)

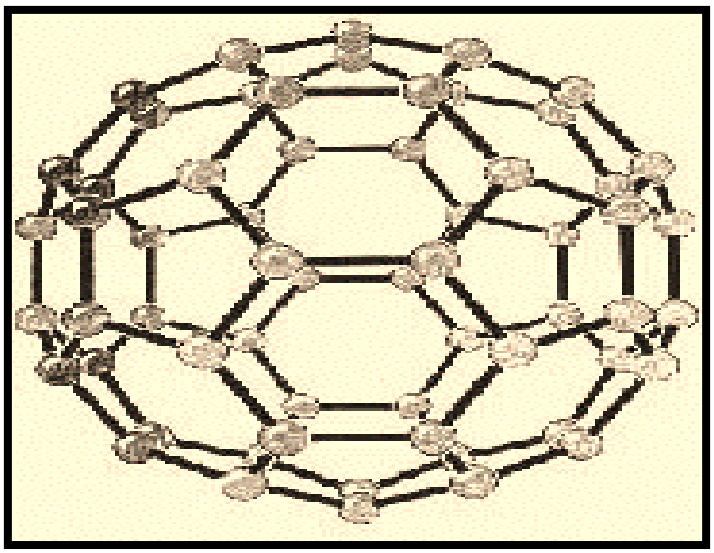

Fig 1. View of Fullerene C_{60}

2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol hydrochloride is a fast-acting nasal drops of 0.05% and an ophthalmic droplet of 5.1%. It can imitate the action of the body's catecholamines as a sympathomimetic drug. Directly affects the alpha-adrenergic receptors in the head or conjunctival and mucosal cerebellum and narrowing the vessels, decreases the blood flow locally and leads to loss of congestion of the nose and conjunctiva. In the eye of the radial muscle, the pupil opening in the iris, which is a smooth muscle and receptor, affects the activation of these receptors in the eye and causes eye irritation. (Figure 2) [1-5]

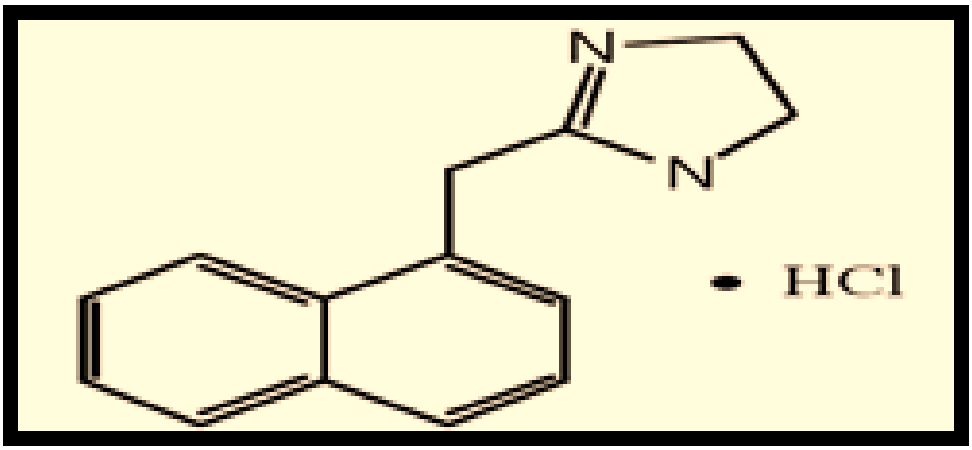

Fig 2. View of 2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol hydrochloride drug structure (C14H14N2H.Cl)

In this project, some of the properties in the composition were investigated by changing the halogen component in carbon position 65 (Fig. 3)

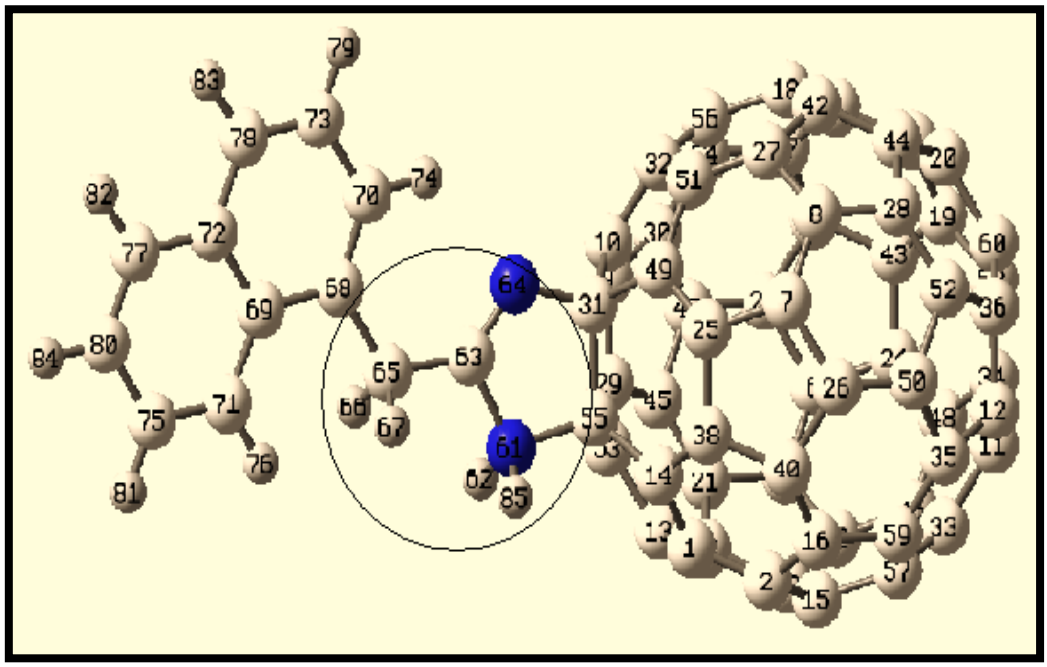

Fig.3. Optimized Compound Structure] + 2X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at HF / 6-31 G *

2. Calculations and results

In this research, the compounds were optimized [+ 2X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br)]. Subsequently, calculations of natural molecular orbitals were performed using the NBO technique. All computations were performed using the Hartree-Fake method in the 6-31G * series, using GaussView software, Vogocin software (Gaussian version 03W). Then, using the results of calculations of HOMO and LUMO electron microscopy properties and changes in the length of the C65-X bond and bipolar moments, and the Core / charge and valence / charge ratios for carbon atoms 31, 55, 65, and 63 in the ion-ion-ion-ion-phonon-fullerene 2X] + - [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-

imidazol-C65 (X = F, Cl, Br) at the level of HF / 6-31 G * was evaluated by the addition of halogen groups. The forms (4-8) [6- 10]

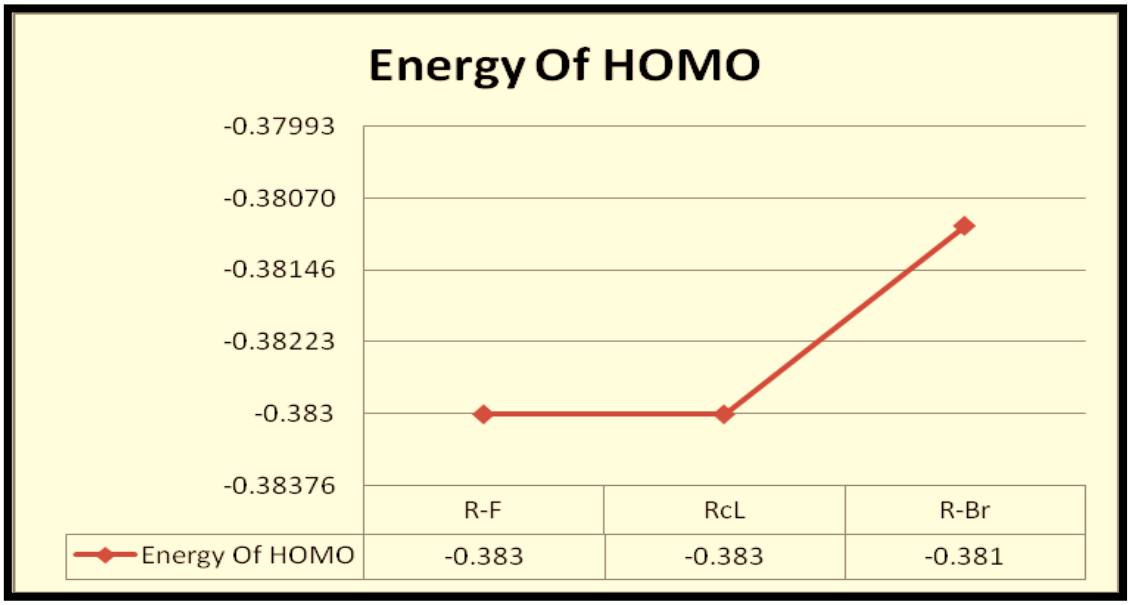

Fig 4: HOMO molecular orbital energy value (in terms of (ev in the composition)

X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at the HF / 6-31

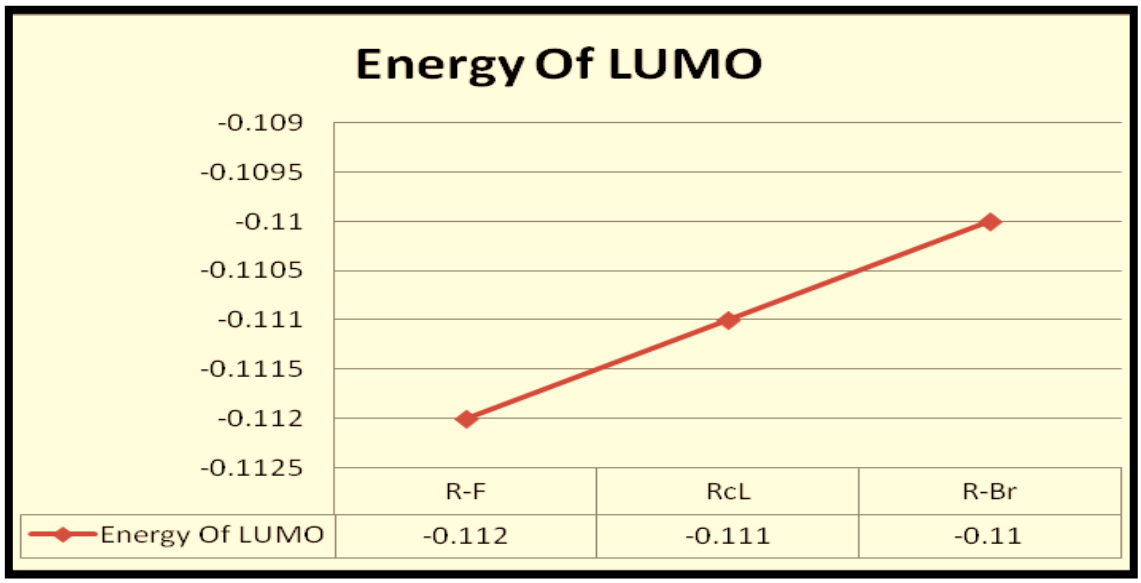

Fig5. LUMO molecular orbital energy value (in terms of ev in combination

[C60-2X] -2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at the HF / 6-31 G level *

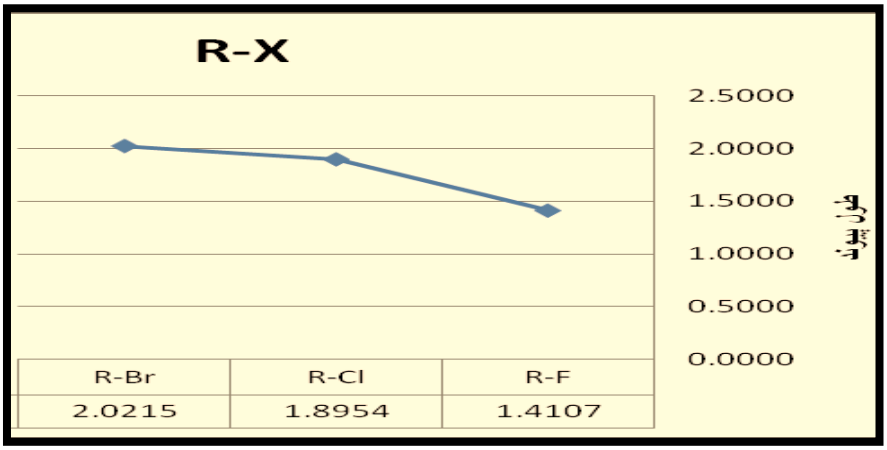

Fig 6: Comparison of the length of the C65-x bond (expressed in terms of angstrom) in the combinations of [+ 2X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at HF / 6-31 G *

Studies on bipolar momentum variations were performed by changing the displacements in the composition, and the process of bipolar momentum changes was evaluated and it was observed that the bipolar momentum strength depends on the type of added groups in the carbon position 65, and with increasing electronegativity Heterogeneous halogenation increases. Figure (7)[11].

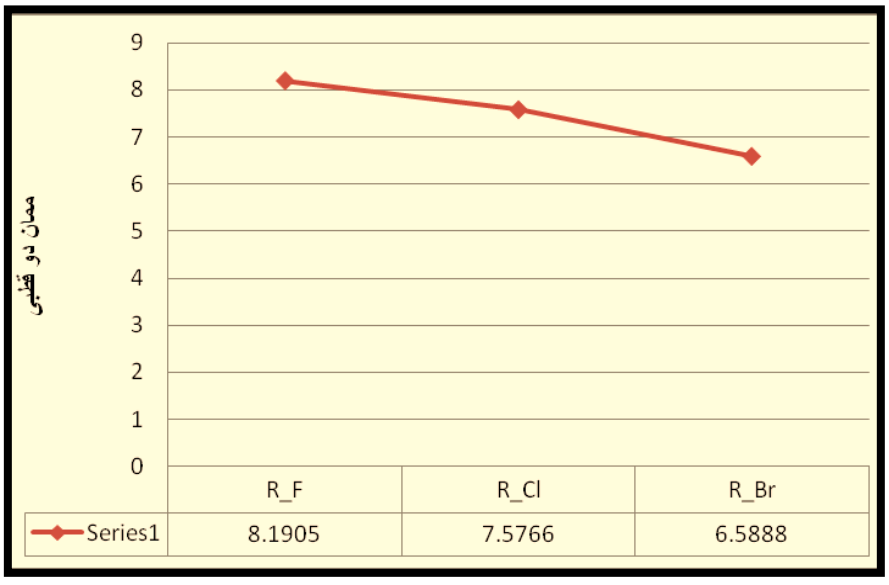

Fig. 7 The bipolar moments of variation in the composition [+ 2X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at the HF / 6-31 G level *

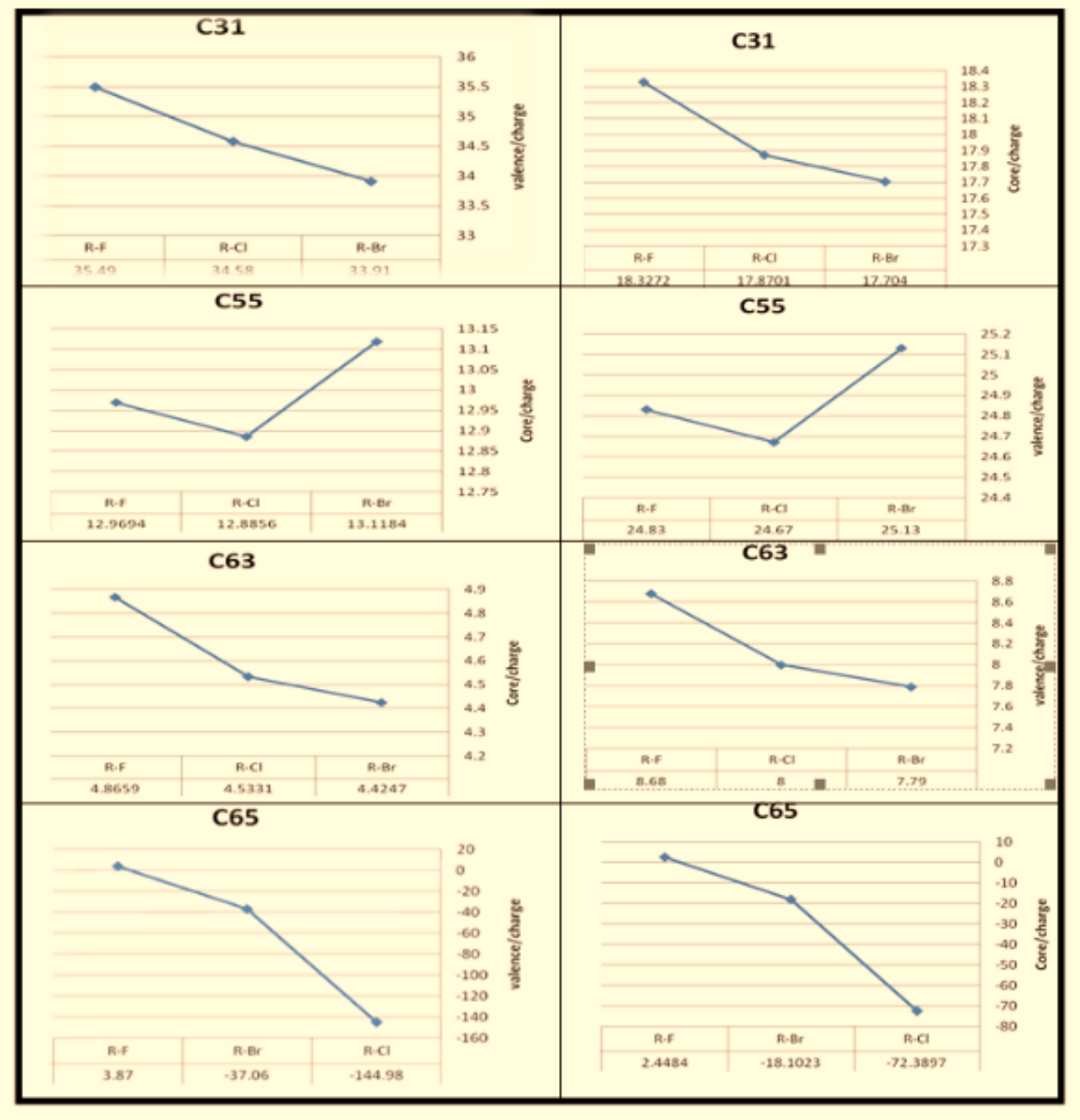

Figure 8 shows the ratio of Core / charge and valence / charge for carbon atoms of 31, 55, 65 and 63, ion-ion combination of pheozolin-fullerene [+2X- [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at HF / 6-31 G level *

3. Conclusion

The presence of halogens causes variations in the length of the bonds and as a result of the strength of the bonds. The modifications of these changes depend on the type of halogen and its location. By changing the substitutions on the composition, it was observed that by increasing the electronegativity of the halogen atom and increasing the inclination The ratio of the atom to the attraction of the pair of adjacent electrons of the neighboring atoms in a molecule and the increase in the relative relative tendency of that atom to reduce the electrons of a covalent bond toward its core decreases the length of the bond. Fluorine is the electronegative atom in the halogens group, which has the shortest bond length and the highest binding strength. Fig. 6 is the dipole moment of a polarization in a molecule. A polar molecule is a molecule with a positive and negative head, that is, one side is positive and the other is negative. For each polar bond, one can consider a polarized vector whose direction towards the atom is electronegative and its length is different The electronegativity of the two atoms depends. The greater the electronegativity difference between the two atoms, the more polar the polar is, and the polar bond. The comparison of the bipolar moments in the compounds shows this trend: R-F> R-Cl> R-Br Fig. 7. Both Core / charge and valence / charge ratios for carbon atoms of 31, 55, 65, and 63 were investigated in the ionized Phenazolin-Fuller ion [+ CX] [C60-2-(naftalin-1-ilmetil)-4,5-dihidro-1H-imidazol-C65 (X = F, Cl, Br) at HF / 6-31 G * level both The ratio in RF is highest. Figure (8)

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