

REACTIONS OF HIGHER FULLERENES WITH CN⁻ MONITORED BY ESMS.

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Higher fullerenes undergo nucleophilic addition reactions similar to those of C₆₀ and C₇₀.¹

The successful reactions of [60]-fullerene (C₆₀) and [70]-fullerene (C₇₀) with NaCN,² monitored by ESMS, encouraged us to try similar reactions with a higher fullerene mixture composed mainly of [84]-fullerene (C₈₄).

We have found that these fullerenes react with CN⁻ readily, like their smaller homologs (C₆₀ and C₇₀); both singly (C₈₄(CN)⁻, C₉₀(CN)⁻,...) and doubly (C₈₄(CN)₂²⁻,...) charged anions are observed with the doubly charged produced at a much greater rate.

It was also found that the number of singly charged adducts (i.e., C_x(CN)_n⁻, x > 76 and n is odd) is less for the higher fullerenes than that in the case of C₆₀ and C₇₀. It is proposed that subsequently all the higher fullerenes react with CN⁻ and are transformed to a doubly charged, or neutral species. However there is a possibility that the sensitivity of the mass spectrometer can vary which prevents the observation of peaks with low abundances.

The initial semi-empirical quantum mechanical molecular orbital calculations obtained using the AM1 approximation with the MOPAC³ program can provide us with information on the preferred positions of the adducts and as to why the doubly charged anions in this case can be of such ease to form.

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