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Dear Michael,

Thanks for your letter of Nov 10 — sorry it's been so long since I responded. I too enjoyed meeting you — and our conversation. I can assure you that any scientific disagreements we may have are no problem from my side. I actually enjoy them!

I've enclosed a preliminary version of my contribution to the NASA conference report. I hope you find it interesting — in spite of its length. Also, I've enclosed 2 recent C-cluster papers from the groups. To my mind, the $C_N M^+$ cluster model which has M^+ completely surrounded by the C_n cage is now proven.

Wrt the Homann work I may agree with you if what you mean as "soot particles" are single, growing graphitic sheets. In our picture these curl to form the "fullerenes" like C_{60}, or spiral + continue growth to form the macroscopic soot particles. I think this is consistent with Homann's statements + observations. What do you think?

Regards,

Rick S.

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November 10, 1987

Professor Rick E. Smalley
Department of Chemistry
Rice University
Houston, TX 77001

Dear Rick:

I am sorry I did not have a chance to say to you "good bye" last Friday -- Sherwood Chang wanted to talk to me about Penn State diamond project.

Enclosed is a copy of the last page of the Homann's paper, where I marked what I regard as Homann's conclusions on the formation mechanism of clusters observed in their flame study. I still interpret them as the clusters are secondary to soot particles, *i.e.*, the clusters are formed after (or even from) the soot particles.

I believe you and I will find ways to reconcile our results. For example, it is very possible that the growth of soot particles after they reach a certain size proceeds through shell structures, you and Kroto advocate. This actually may explain the "aging" of soot particles.

In any event, I hope that the differences in our scientific views will not prevent us from possible future interactions on this fascinating subject. I really enjoyed meeting you (I would not say it about Kroto) and am looking forward to other opportunities when our roads will cross.

With best regards,

Sincerely,

Michael

Michael Frenklach

Associate Professor of Fuel Science

P.S. I have also enclosed some of our soot modeling papers.

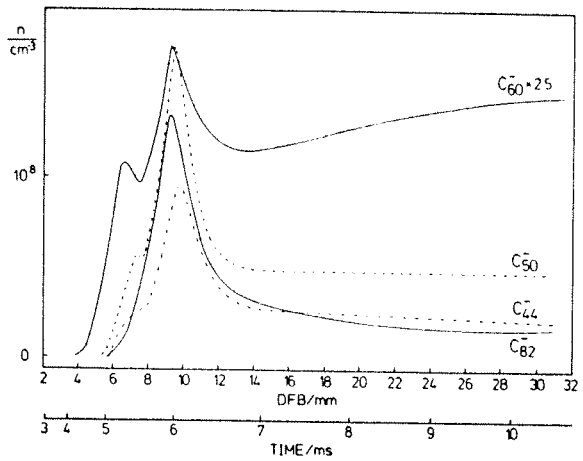

Fig. 2. Concentration profiles of negative polyhedral ions in a benzene flame; C/O = 0.76, v_u = 42 cm s^{-1}. The secondary maximum might be due to a disturbance of the concentration profile caused by a discontinuous plasma potential at this distance from the burner.

ilar soot production, polyhedral ions are more abundant (by a factor of about two) in benzene flames where the maximum temperature is about 100 K higher than in acetylene flames. The absolute number concentration was determined in separate experiments by measuring the total ion current through the quartz sampling probe. In an acetylene flame the total negative ion concentration is 1×10^9 cm^{-3} (C/O = 1.05), in a benzene flame (C/O = 0.8) it is at least twice as high.

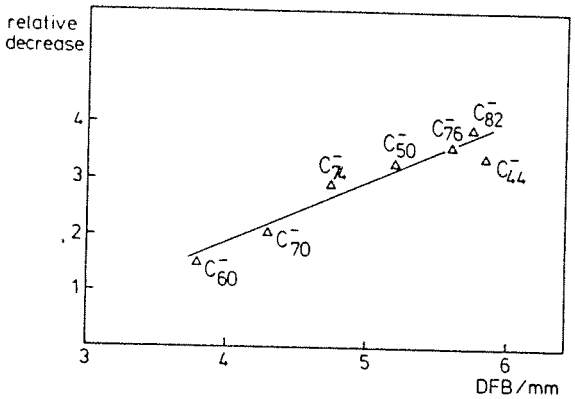

Fig. 3. Relative decrease in concentration (concentration at the maximum/concentration after the steep decline) of several ions versus the distance from the burner of their first appearance.

4. Discussion and conclusions

From the mass distribution of all ions and its dependence on reaction time we conclude that polyhedral carbon ions are not formed from the small polyyne ions but directly from polyaromatic particles of the same mass range or from single soot particle layers. The diameter of crystalline soot particles was determined by X-ray scattering experiments to be not more than 2 nm [13]. This is in good agreement with the mass distribution of negative polyhedral ions and indicates a connection between single soot particle layers and polyhedral particles.

After reaching a maximum the concentration of polyhedral ions declines probably due to reactions with small reactive particles, which could be free radicals (H, OH) or young soot particles as well as to recombination with oppositely charged ions. Considering the constant abundance of polyhedral ions at larger distances from the burner recombination processes seem to be of minor importance.

The comparatively early increase in concentration of certain ions that are more stable than others, e.g. C_{60}^-, is not fully understood at present. The results presented here are consistent with those from the graphite vaporization experiments, if one assumes that polyhedral particles are formed directly from single soot particle layers or single graphite particle layers, respectively.

Acknowledgement

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References

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[2] H.W. Wenz, Dissertation, Technische Hochschule Darmstadt (1983).
[3] D.B. Olson and H.F. Calcote, Eighteenth Symposium (International) on Combustion (The Combustion Institute, Pittsburgh, 1981) p. 453.
[4] P. Michaud, J.-L. Delfau and A. Barassin, Eighteenth Symposium (International) on Combustion (The Combustion Institute, Pittsburgh, 1981) p. 443.