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THE SYNTHESIS, DEGRADATION, AND STRUCTURE OF POLYPHOSPHAZENES. (U)
NOV 78 H R ALLCOCK DAHC04-75-6-0143

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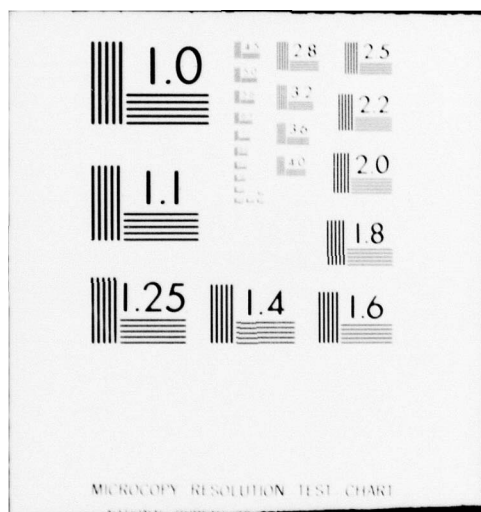
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19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Phosphazene high polymers, synthesis, X-ray structure, transition metal complexes, conformational energy calculations.		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Poly(organophosphazenes) and their cyclic oligomeric analogs have been used as ligands for transition metal complexes. X-Ray structural work has shown that platinum binds to the skeleton of specific organophosphazenes. X-Ray structural work and conformational energy calculations have been used to deduce the relationships between structure and properties in polyphosphazenes.		

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THE SYNTHESIS, DEGRADATION, AND STRUCTURE OF POLYPHOSPHAZENES

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Final Report

The Synthesis, Degradation, and Structure of Polyphosphazenes

May 1, 1975 - August 31, 1978

A. Summary of Research Progress

The objectives of this work were to synthesize new phosphazene high polymers that may be of practical value, to study their chemical properties, and to investigate the relationship between the structure and properties of these materials in order to predict the properties of polymers not yet prepared.

The synthesis work has yielded examples of the first polyphosphazene-transition metal adducts, in the form of platinum-polymer coordination compounds. Such species are active as antitumor agents and, at the same time, have demonstrated the potential for future synthetic work with metallo-polyphosphazenes.

X-Ray structural work has been completed on the platinum-phosphazene adducts. The binding of the transition metal is through the skeletal nitrogen atoms of the phosphazenes. Extensive X-ray and other morphological research has now been completed on poly(dichlorophosphazene). The physical behavior of this compound is now fairly well understood in terms of the molecular structure.

Finally, non-bonding conformational energy calculations have been carried out on a wide range of poly(organophosphazenes). The results have shown that the physical properties (particularly flexibility and T_g) of the polymers can be correlated with the size and conformational mobility of the side groups.

B. List of Publications

Mechanism of the Reactions between Ortho Dinucleophiles and Cyclophosphazenes, H. R. Allcock, R. L. Kugel, and G. Y. Moore, Inorganic Chemistry, **14**, 2831 (1975).

Conformational Analysis of Poly(dihalophosphazenes), H. R. Allcock, R. W. Allen, and J. J. Meister, Macromolecules, **9**, 950 (1976).

Conformational Analysis of Poly(alkoxy- and aryloxyphosphazenes), R. W. Allen and H. R. Allcock, Macromolecules, **9**, 956 (1976).

Synthesis of Platinum Derivatives of Polymeric and Cyclic Phosphazenes, H. R. Allcock, R. W. Allen, and J. P. O'Brien, J. Am. Chem. Soc., **99**, 3984 (1977).

Crystal and Molecular Structure of a Platinum-Cyclophosphazene Complex: cis-Dichloro[octa(methylamino)cyclotetraphosphazene-N,N'']platinum(II), R. W. Allen, J. P. O'Brien, and H. R. Allcock, J. Am. Chem. Soc., **99**, 3987 (1977).

Antitumor Agents Synthesized from K_2PtCl_4 and Polymeric or Cyclic Phosphazenes,
H. R. Allcock, R. W. Allen, and J. P. O'Brien, J. Chem. Soc., Chem. Commun.,
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Phosphazenes as Coordinative Ligands for Platinum: Crystal and Molecular
Structure of Cis-Dichloro[octamethylcyclotetraphosphazene-N,N']Platinum
(II)-Acetonitrile, H. R. Allcock and J. P. O'Brien, Inorganic Chemistry
(submitted for publication).

Crystal and Molecular Structure of a Platinum-Cyclophosphazene Salt: [N,N'-
Dihydro(octamethylcyclotetraphosphazanium)Tetrachloroplatinate, $[H_2N_4P_4-$
 $(CH_3)_8^{2+}PtCl_4^{2-}$, J. P. O'Brien, R. W. Allen, and H. R. Allcock,
Inorganic Chemistry, (submitted for publication).

The Morphological Properties of Poly(dichlorophosphazene), H. R. Allcock and
R. A. Arcus (to be submitted to Macromolecules).

The Crystal and Molecular Structure of Poly(dichlorophosphazene), H. R. Allcock,
R. A. Arcus, and E. G. Stroh (to be submitted to Macromolecules).

Polyphosphazenes: New Polymers with Inorganic Backbone Atoms,
H. R. Allcock, Science, 193, 1214 (1976).

Poly(organophosphazenes) - Unusual New High Polymers,
H. R. Allcock, Angew. Chemie, 16, 147 (1977).

C. List of Reports Submitted (period covered)

October 1, 1974 - March 31, 1975
April 1, 1975 - September 30, 1975
July, 1975 - July, 1976
January 1, 1977 - June 30, 1977
July 1, 1977 - December 31, 1977
January 1, 1978 - June 30, 1978

D. List of Personnel

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John P. O'Brien	"
Robert A. Arcus	"
Timothy J. Fuller	"
Karen M. Smeltz	"
James L. Schmutz	"